A NOVEL AND RATIONAL APPROACH TOWARDS DESIGNING ALUMINIUM CHELATORS

SHAQIL HAIDER CHAUDARY

Doctor of Philosophy

THE UNIVERSITY OF ASTON IN BIRMINGHAM

December 1999

DEDICATION

To my late father, an inspiration in my life

'To seek knowledge is a religious duty for every Muslim, male ar
female'

A saying of the prophet (pbuh)

A prayer from the Quran (20:114)

'... and say my Lord! Increase me in knowledge.'

ASTON UNIVERSITY

A NOVEL AND RATIONAL APPROACH TOWARDS DESIGNING ALUMINIUM CHELATORS

SHAQIL HAIDER CHAUDARY

Doctor of Philosophy

1999

SUMMARY

Aluminium (Al) is known to be neurotoxic and has been associated with the aetiology of Alzheimer's Disease. To date, only desferrioxamine (DFO), a trihydroxamic acid siderophore has been used in the clinical environment for the removal of Al from the body. However, this drug is expensive, orally inactive and is associated with many side effects. These studies employed a theoretical approach, with the use of quantum mechanics (QM) via semi-empirical molecular orbital (MO) calculations, and a practical approach using U87-MG glioblastoma cells as a model for evaluating the influence of potential chelators on the passage of aluminium into cells.

Preliminary studies involving the Cambridge Structural Database (CSD) identified that Al prefers binding to bidentate ligands in a 3:1 manner, whereby oxygen was the exclusive donating atom. Statistically significant differences in M-O bond lengths when compared to other trivalent metal ions such as Fe^{3+} were established and used as an acceptance criterion for subsequent MO calculations. Of the semi-empirical methods parameterised for Al, the PM3 Hamiltonian was found to give the most reliable final optimised geometries of simple 3:1 Al complexes. Consequently the PM3 Hamiltonian was used for evaluating the ΔH_f of 3:1 complexes with more complicated ligands. No correlation exists between published stability constants and individual parameters calculated via PM3 optimisations, although investigation of the dicarboxylates reveals a correlation of 0.961 showing promise for affinity prediction of closely related ligands.

A simple and inexpensive morin spectrofluorescence assay has been developed and optimised producing results comparable to atomic absorption spectroscopy methods for the quantitative analysis of Al. This assay was used in subsequent *in vitro* models, initially on *E. coli*, which indicated that Al inhibits the antimicrobial action of ciprofloxacin, a potent quinolone antibiotic. Ensuing studies using the second model, U87-MG cells, investigated the influence of chelators on the transmembrane transport of Al, identifying 1,2-diethylhydroxypyridin-4-one as a ligand showing greatest potential for chelating Al in the clinical situation.

In conclusion, these studies have explored semi-empirical MO Hamiltonians and an *in-vitro* U87-MG cell line, both as possible methods for predicting effective chelators of Al.

KEYWORDS: *E. coli*, semi-empirical, U87-MG, X-ray crystallography

ACKNOWLEDGMENTS

I gratefully acknowledge my supervisors, Carl Schwalbe and Peter Lambert for their support and guidance throughout my time at Aston. I would also like to thank Professor Hider, Kings College for his generous donation of hydroxypyridinones which I used in the latter stages of the studies. The work in this thesis was funded by a studentship from the Biotechnology and Biological Sciences Research Council (BBSRC).

I would like to thank my family for their support throughout my Ph.D., and in particular my wife, Shazia for her patience and tolerance.

Finally I would like to thank Pakeeza for support during the final stages of these studies and two friends in particular, Alim and Taeeba, for their moral support and good humour throughout my university education.

LIST OF CONTENTS

LIST OF FIGURES

LIST OF TABLES

LIST OF ABBREVIATIONS

ACh	Acetylcholine
AMP	Adenosine monophosphate
ATP	Adenosine triphosphate
Al	Aluminium, Aluminium ion (+3)
AD	Alzheimer's Disease
APP	Amyloid Precursor Protein
Å	Angstrom, 10^{-10}m
AAS	Atomic Absorption Spectroscopy
AM1	Austin Method 1 Hamiltonian
ASP	Automated Similarity Package
BPB	Background-peak-background
BBB	Blood Brain Barrier
CSSD	Cambridge
CCDC	Cambridge Crystallographic Data Centre
CSD	Cambridge Structural Database
cm, mm, μm, nm	Centimetre, millimetre, micrometre, nanometre
CFA	Central Field Approximation
cip	Ciprofloxacin
CNDO	Complete Neglect of Differential Overlap
CADD	Computer Assisted Drug Design
CAMD	Computer Assisted Molecular Design
CI	Configuration Interaction
Cu	Copper
CC	Coupled Cluster Theory
cssr	Crystal Structure Search Retrieval format file
°	Degree
°C	Degrees Celsius
°K	Degrees Kelvin
DFT	Density Functional Theory
DNA	Deoxyribonucleic acid
DFO	Desferrioxamine

DSC	Differential Scanning Calorimetry
DMSO	Dimethylsulphoxide
R	Discrepancy factor
d/d water	Double Distilled water
DMEM	Dulbecco's Modified Eagle Medium
E. coli	*Escherichia coli* W3110
EDTA	Ethylenediaminetetraacetic acid (tetrasodium salt)
ECACC	European Collection of Animal and Cell Cultures
FLDMM	Fluorescence Data Manager Manual
FCS	Foetal Calf Serum
Ga	Gallium
GTO	Gaussian Type Orbitals
GVB	Generalised Valence Bond
GAMESS	General Atomic Molecular Electronic Structure System
G	Gibbs free energy
GABA	γ-aminobutyric acid
GMP	Glucose-6-monophosphate
GOF	Goodness of Fit
g, mg, μg, ng	Grams, Milligrams, Micrograms, Nanograms
HF	Hartree Fock
HPs	Hydroxypyridinones
IR	Infra-red
ICSD	Inorganic Crystal Structural Database
INDO	Intermediate Neglect of Differential Overlap
Fe	Iron, Ferric ion
LCAO	Linear Combination of Atomic Orbitals
R^2	Linear regression correlation coefficient
pKa	Log association constant
MS	Mass spectroscopy
m.pt.	Melting point
ML	Metal ion + Ligand

M-D	Metal-Donor (oxygen or nitrogen)
MIC	Minimum Inhibitory Concentration
MNDO	Modified Neglect of Differential Overlap
M, mM, μM, nM	Molar, Millimolar, Micromolar, Nanomolar
MEPmap	Molecular Electrostatic Potential map
MM	Molecular Mechanics
MO	Molecular Orbital
MOPAC	Molecular Orbitals Package
MP	Möller Plesset perturbation theory
Mo	Molybdenum
MCSCF	Multi-Configurations Self Consistent Field
NFS	Networked File Storage
NFT	Neurofibrillary tangles
Nth	North format file
NMR	Nuclear Magnetic Resonance
NA	Nutrient Agar
NB	Nutrient Broth
OD, OD_{470nm},	Optical Density, Optical Density at 470nm,
OD_{510nm}	Optical Density at 510nm.
MEOXAL	Oxalic acid dihydrate
PM3	Parameterisation Model 3 Hamiltonian
K_{part}	Partition coefficient
MTT	is 3-[4,5-dimethylthiazol-2-yl]-2,5-diphenyl tetrazolium bromide
ppb	Parts per billion
PBS	Phosphate Buffered Saline
PDB	Protein Databank
QSAR	Quantitative Structure Activity Relationship
QM	Quantum Mechanics
QMC	Quantum Monte Carlo method
rpm	Revolutions per minute
RNA	Ribonucleic acid
SCF	Self Consistent Field
SP	Senile Plaques

STO	Slater Type Orbitals
K_{stab}	Stability constant
SD	Standard deviation
TADS	Thermal Analysis Data Station
3-D	Three dimensional
Tsar	Tools for Structure Activity Relationships
2-D	Two dimensional
Mgm^{-3}	Units of density, Megagrams per metre cubed, (works out to be gcm^{-3})
v/v, w/v	Volume in volume, weight in volume
λ	Wavelength

CHAPTER ONE

INTRODUCTION

1.1 ALUMINIUM (AL) IN THE ENVIRONMENT AND THE HUMAN BODY

Aluminium (Al), the third most abundant element on the surface of the earth and the most abundant of its metallic constituents, is not known to participate in any natural metabolic process and as such is not thought to be an essential component of the diet (Perl, 1988).

Most investigated foodstuffs contain <5 $\mu g\ g^{-1}$ of Al the highest concentrations were determined in cocoa products (33 $\mu g\ g^{-1}$), spices (145 $\mu g\ g^{-1}$) and black tea leaves (899 $\mu g\ g^{-1}$). In general, Al content of frequently consumed food, increased in the following order: beverages, food of animal origin, food of plant origin (Muller, 1998). The total adult body burden has been estimated at 30-50mg, of which about 50% is assigned to the skeleton, 25% to the lungs and the remaining 25% is attributed to soft tissue (Martin, 1986).

Al is normally insoluble, but it dissolves in the acid environment and becomes toxic to both plants and animals (Delhaize, 1995). The accelerated pollution acidification in industrialised countries since the 1950s has led to one of the greatest ecological changes in historical times.

Al has been associated with osteomalacia, osteoporosis and Alzheimer's disease (AD). Although its precise role is not known in AD, it is widely recognised as a neurotoxin and consequently much effort has been put into research on Al specific chelating agents over the past two decades (Yokel, 1994). It has been suggested that the rate of accumulation of Al in the brain would result in toxic levels after 100 to 150 years (Ganrot, 1986). This may occur sooner in people with impaired renal function, those

receiving large oral Al exposure via Al containing antacids-phosphate binders or those receiving parenteral Al exposure. The accumulation and toxicity of Al can be avoided when Al sources are identified and exposure prevented.

To date, no suitable alternative to Desferal (desferrioxamine, DFO) as an Al chelating agent has been found. DFO has been shown to slow the progression of AD in some patients, hence the suspected link between Al and AD. Research on AD is continually increasing and is discussed later.

1.2 ALZHEIMER'S DISEASE (AD)

AD, a form of dementia, was first described in 1906 by Alois Alzheimer (Alzheimer, 1907), a German scientist describing the symptoms of a 51 year old woman showing signs of memory loss, aphasia, hallucination, delusions and behavioural disturbance. Currently AD is the fourth most common cause of death in the elderly (Ohm, 1997).

1.2.1 Aetiology

The cause of AD is at present unknown, although there is a definite aetiological genetic connection. Both age and Down's syndrome are also thought to be causal factors.

The amyloid precursor protein (APP) found on the long arm of chromosome 21 was also found to be associated with AD, although this only accounted for approximately 25% of AD sufferers (Clarke, 1993). The remaining 75% of AD cases were found to correlate with chromosome 14 by a gene designated as presenilin 1.

A hypothesis that a metal-induced immune disorder may be involved in the pathogenesis of some forms of AD has been proposed (Armstrong, 1995). The classical complement pathway is activated in AD and T cells and reactive microglia appear in the brain. Studies of metal induced autoimmunity and the use of compounds containing Al as vaccine adjuvants suggest that metals activate complement and are

taken up by antigen presenting cells. The consequent immune response may contribute to neuronal damage, P-amyloid deposition and cell death.

1.2.2 Epidemiology

At present AD is the most common type of dementia that occurs in the elderly, with an estimated 5-10% of all the population over the age of 65 showing signs of AD. Approximately 10% of all AD occur as early as 50 years of age (Sobow, 1994). With the growing elderly population, the impact of AD is expected to become more pronounced, having major social and financial implications. The number of elderly people in both the developed and developing world is rapidly increasing with an estimated average population growth of 20% in developed countries and 73% in developing countries from 1975 to 2000. Consequently, the total number of 'elderly' people is hugely increased resulting in an elevated abundance of AD patients. Table 1.1 shows the prevalence rates of AD relative to age.

Thus, there is increasing pressure on the scientific community to understand the cause of the disease and develop drugs to treat AD and or at least arrest its progression. AD is notably different from other forms of dementia in than its onset can occur in patients below the age of 65 (presenile dementia), although its prevalence is very low when compared to the over 65 year age group.

TABLE 1.1 Age specific prevalence rates (per 100 population) for AD

Ages (years)	Prevalence (Europe) (Rocca, 1991)
35-59	0.2
60-69	0.3
70-79	3.2
80-89	10.8

It has been suggested that Al plays a role in the aetiology of AD (Yokel, 1991). Although its precise function is controversial, at least 60 neurochemical reactions are disrupted by Al. (Crapper, 1989).

1.2.3 Neuropathology

The original pathological description of AD was the presence of neurofibrillary tangles (NFT) and senile plaques (SP) in the brain (Gilman, 1997). Since then other features have been recognised, such as granulovacuolar degeneration, Hirano bodies (found in the hippocampus) and Lewy bodies.

1.2.4 Neurochemistry

AD is associated with deficits in the cholinergic system, although deficiencies in other neurotransmitters have also been reported (Burns, 1997). Deficits in acetylcholine (Ach) are probably due to a deficit of the enzyme, choline acetyltransferase, responsible for catalysing Ach synthesis (from acetylcoenzyme A and choline). Low levels of Ach are particularly found in the hippocampus and temporal cortex.

In addition to abnormalities in the cholinergic system deficits in noradrenaline and seratonin have been found. Noradrenaline reduction is indicated by reduced activity of dopamine hydroxylase and reduced noradrenaline uptake into nerve terminals *in vitro*. Reduced seratonin levels have been found within the cortex, which probably relate to histopathological changes resulting in deficits also in the basal nuclei.

1.2.5 Clinical presentation and diagnosis

Clinically, AD is an insidious fatal dementia. The first clinical symptom is usually a loss of short term memory which progressively increases, deterioration of mental ability, disturbances in language and spatial orientation. Patients often develop symptoms that lead to gross behavioural disturbances, including suspiciousness to the point of paranoia, hallucination, both visual and auditory, agitation and depression. Towards the end stage of the disease patients are unable to look after themselves and tend to become bedridden.

The definite diagnosis of AD can be confirmed by a neuropathological examination of the brain post mortem or brain biopsies (Gearing, 1995). However, as brain biopsies of AD patients are rarely justified, diagnosis is generally made clinically. Three main sets of diagnostic criteria have widely accepted; the DSM-IV (American Psychiatry Association), ICD-10 (the World Health Organisation 10th International Classification of Diseases, and the NINCDS/ADRDA (Stroke/Alzheimer's Disease and Associated Disorders Association). All are generally based on the gradual decline in the four areas outlined below.

1. Behaviour; may become anti-social with a loss of interest and reduced initiative. The person becomes increasingly anxious and irritable.
2. Thinking; thoughts become slower and reduced in content.
3. Mood; can alter suddenly from swings of depression to elation.
4. Cognitive function; gradual memory loss (recent memory loss being affected first).

The accuracy of clinical diagnosis based on these criteria varies; some studies show a diagnostic accuracy as high as 88% in research centres where clinical diagnosis of probable AD was made before post mortem examination. (Gilman, 1997; Berg, 1994).

1.2.6 Cost of AD

A report submitted for the NHS executive estimated an annual cost of almost £8,000 per AD patient in the city of London, and extrapolating this cost to the UK, with an estimated 16,737 AD patients resulted in an estimated annual resource cost of between £110-156 million (Harvey, 1998). Thus, a need for cheaper alternative therapies that could ultimately cure or prevent the disease is firmly established.

1.2.7 Association of Al with AD

There is some circumstantial evidence that Al may be involved in the aetiology of AD, although the so-called Al hypothesis is controversial (Crapper McLachlan, 1989; Doll, 1993; Nieboer, 1995). AD has, although not undisputed (Wood, 1988; Wettstein, 1991; Landsberg 1992), been associated, on the one hand, with Al accumulation in the nuclear chromatin (Crapper McLachlan, 1980; Good, 1992), in the NFT (Perl, 1980; Good, 1992) and focally in specific regions of the brain (Xu, 1992) and, on the other hand, with Al in drinking water (Flaten, 1986; Vogt, 1986; Martyn, 1989; Crapper McLachlan 1996)

Al dissolves in an acid environment and can be resorbed in the intestine, especially after complexing with organic acids such as tartaric and citric acids, both of which are common in foods (Slanina, 1986). The Al absorption varies greatly between individuals, increases with age and is raised with patients suffering from AD (Taylor, 1992). Most resorbed Al leaks slowly into the cells and may interfere with the transcription of DNA (Lukiw, 1992), increase the production of β-amyloid from the amyloid precursor protein (Clauberg, 1993; Zatta 1993), induce aggregation of the β-amyloid (Mantyh 1993; Kawahara, 1993; Exley 1995) and contribute to the formations of NFT (Shin, 1995; Zatta, 1995).

Four independent lines of evidence implicate Al's role in AD:

1. Toxicological studies and laboratory observations of the learning and memory performance of animals.
2. A large number of documented biochemical changes at concentrations of Al similar to those found in various subcellular compartments in AD affected brains.
3. Epidemiological evidence of the increased incidence of AD in relation to exposure to Al in drinking water (Still, 1980; Flaten, 1990)
4. The slowing of the clinical progression of AD by drugs such as DFO, that removes Al from the body. A two year prospective, single-blind clinical trial was conducted using DFO showing a decline in progression of AD (Crapper McLachlan, 1991).

AD starts in the entorrhinal cortex, progresses to the hippocampus and then ultimately spreads to the cerebral hemispheres as depicted by figure 1.1.

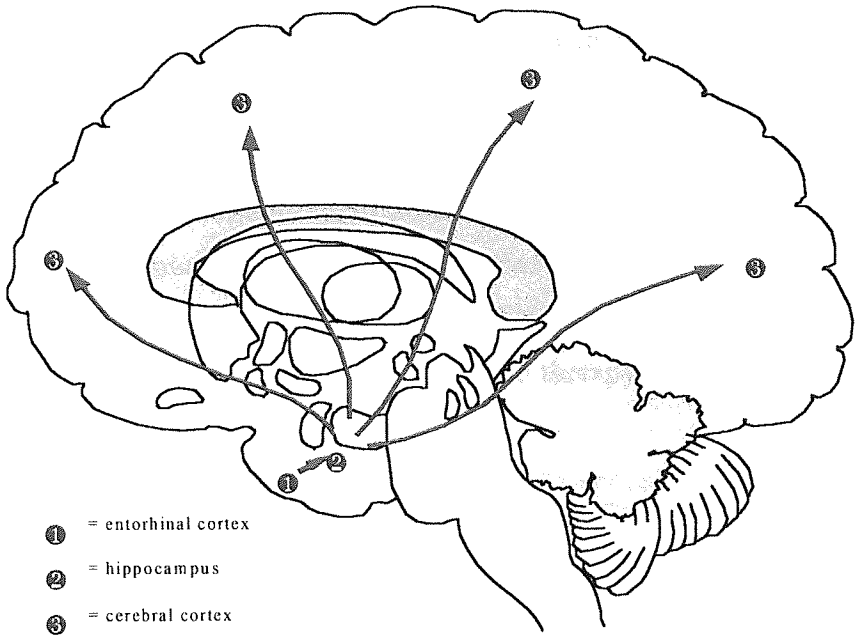


FIGURE 1.1 Human brain illustrating the areas of the brain affected by AD

McDermott *et al* (1977) have shown that Al levels in the brain increase with age and the density of NFT in AD brains is 6-40 times greater than brains of mentally normal age matched controls. Studies have shown remarkably high concentrations of Al levels in NFT (300μg/g dry weight)(Crapper McLachlan, 1998). Studies of AD brains with age matched controls have shown significant increases in Al levels, present as aluminosilicates (Krishnan, 1988; Yoshida, 1996) and have been estimated to be approximately 1.4 times the level overall (Trapp, 1977).

Unfortunately, Al exposure, accumulation and toxicity continue to occur due to its ubiquitous distribution in our environment, water and food, as well as in dialysate solutions and pharmaceuticals.

Desferrioxamine (DFO), a trihydroxamic acid iron siderophore, has been used to treat Al accumulation and toxicity with some success but not in all cases. A patient with

progressive motor neurone disease who had used a facial cream containing 30% Al oxide for twenty years showed a positive DFO test response and clinical improvement over the first and second year of prolonged DFO treatment (0.01mmol/kg intramuscularly every twelve hours) (Kruck, 1989). Crapper McLachlan *et al* (1991) compared 25 probable AD patients, who received 125mg (0.19mmol) DFO in twice daily doses for two years, to a matched group that did not receive DFO. The DFO treated group had lower mortality and rate of deterioration of their activities of daily living scores. Melograna (1983) conducted further studies on rabbits to objectively assess Al chelation activity. An Al loaded (20 subcutaneous injections of Al lactate of 0.6mmol/kg) rabbit model was used, whereby DFO therapy significantly raised serum Al concentrations and urinary Al output.

However, DFO is not orally effective, rather expensive and produces side effects including auditory neurotoxicity (Freedman, 1988) and hypotension. Given the limitations of DFO, an orally effective, less expensive and less toxic Al chelator would be beneficial, particularly for long term prevention or treatment of Al accumulation.

1.2.8 Current research in AD and treatments

To date, only two drugs, namely tacrine (trade name Cognex) and donepezil (trade name Aricept) are currently used in the United States for the treatment of AD, these are both anticholinesterases aimed at increasing the levels of Ach in the brain, a neurotransmitter involved in cognitive function. Only donepezil is currently marketed in the UK. However, neither of these drugs are curative, they merely slow the progression of the disease (Rogers, 1996; Geldmacher, 1997).

Another line of research is the slowing down of brain cell death. The development of AD is thought to be associated with the death of cholinergic cells. The grafting of genetically modified cells rich in nerve growth factor into brains of monkeys which naturally suffer with a disease similar to AD, resulted in reduction from 60% to 20% in the number of cholinergic brain cells that died (Mestel, 1994).

Ultimately, if Al is an aetiological factor of AD, then its removal in those patients known to have excessive quantities of Al, would possibly prevent or even cure AD. With this hypothesis in mind, the studies in this thesis are aimed at moving one step in the right direction in the hope of identifying a therapeutically viable Al chelator.

1.3 ACTIONS OF AL AT A CELLULAR LEVEL

While abundant in the environment, Al is only present in trace amounts within biological systems, and has no known biologically useful role. Al affects many biochemical and neurochemical processes of the brain, which may be causal factors for its associated neurotoxicity. The effects can be categorised into five groups.

1. Nuclear effects

- binds to DNA phosphate and bases (Karlik, 1980)
- decreases RNA in neuroblastoma cells (Miller, 1974)
- blocks RNA initiation sites for RNA polymerase (Sarkander, 1983) and RNA polymerase activity *in vitro* (Crapper McLachlan, 1983)
- decreases cell division and alters DNA synthesis (Sampson, 1965)

2. Cytoplasmic effects

- induces conformational changes in calmodulin (Farnell, 1985)
- reduces sugar phosphorylation (Rorison, 1965)
- decreases respiration (Foy, 1978)
- inhibits ATP (Trapp, 1980)
- elevates cyclic AMP and GMP levels (Johnson, 1987)
- induces an alteration in Tau that is recognised by antibodies to Alz 50 (Guy, 1991)

3. Cytoskeletal effects

- induces neurofibrillary degeneration composed of 10nm fibres identical in chemical composition to normal neurofilaments (Munoz-Garcia, 1986)
- alters phophorylation of cytoskeletal proteins (Johnson, 1987)

4. Effects on membranes and membrane bound enzymes

- alters physical properties of membrane lipids (Viestra, 1978)
- binds to positive and negative charged sites in membranes *in vitro* (Deleers, 1985)
- alters membrane structure (Idem, 1986)
- enhances brain specific lipid peroxidation (Gutteridge, 1985)
- increases permeability of BBB to neuropeptides (Banks, 1988)

5. Synaptic and neurotransmitter effects

- blocks high affinity uptake of γ-aminobutyric acid (GABA) (Sturman, 1983)
- inhibits acetylcholinesterase (Marquis, 1982)

1.4 OVERVIEW OF CHELATING CLASSES OF CLINICAL INTEREST

If chelators are to be used in the clinical situation, there are many restrictions on the chemical design of the molecule, in addition to that of selectivity. In general, both the free ligand and the complex should be water-soluble and yet, if the role of the ligand is to scavenge a metal, it must be able to penetrate cell membranes. Thus, the ligand should possess no charged functional groups at neutral pH values and the resulting complex should be neutral if it is to enter living host cells. These properties, coupled with water solubility, impose considerable constraints on the molecular design. Neutral ligands are likely to be orally active, but if their molecular weight is less than 400, they may penetrate the BBB and thereby trigger considerable side effects. Consequently, the net charge and the molecular weight of the ligand have considerable influence on its distribution *in vivo*. As a general rule, oligodentate ligands are more kinetically inert than their bidentate analogues and therefore scavenge metals more efficiently, without causing redistribution (Hider and Hall, 1991).

The group III metals, Al, Fe, gallium and the lanthanides all interact with anions of high charge density, and in particular, oxyanions. Consequently, they have relatively low affinities for dinitrogen, disulphur, and mixed nitrogen-sulphur ligands in aqueous media (Hider and Hall, 1991). *In vivo*, Al exists only as a trivalent cation. Reactions with Al are characterised by polymerisation, slow kinetics, and extensive hydrolysis. As a hard Lewis acid, Al is highly electropositive and not easily polarised. It generally forms ionic or electrostatic bonds. Al prefers to co-ordinate with hard Lewis bases (ligands), such as OH^-, F^-, PO_4^{3-}, SO_4^{3-}, CH_3COO^-, ROH, RO^-, and RNH_2, that donate electrons to the acid's vacant electron orbitals (Pearson, 1973; Jones, 1984).

In general Al has lower log K_1 values than either gallium(III) (Ga) or iron(III) (Fe), supporting the theory put forward by Hider *et al* (1991) regarding the 'oxygen octahedral field' theory. Hider and co-workers (1991) have shown that a perfect package of six oxygen atoms (van der Waals radius of 1.4Å) in an octahedral manner would result in a central cavity radius being produced of 0.58Å. However, if these oxygens were part of a ligand, the octahedral arrangement would be distorted as depicted in figure 1.2, resulting in a cavity of 0.7Å, a perfect size for a ferric ion.

While this cavity would still allow the smaller Al ion, the fit would not be as tight, resulting in a lower affinity of a dioxygen ligand for Al relative to Fe.

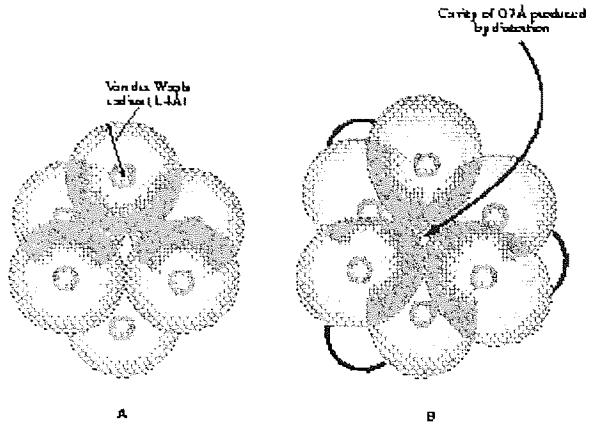


FIGURE 1.2 Influence of chelation on six oxygen atoms arranged in an octahedral manner to the cavity produced

Most bidentate ligands have at least three possible complexes with Group III metals; namely ML, ML_2, ML_3, where M is the metal ion and L is the ligand. The relative proportions of these complexes depend on the pH of the solution. As protons and the cation compete with each other for the ligand, alkaline pH values favour ML_3 whereas acid pH values favour ML; the precise position of the equilibrium depending on the log association constant (pKa) and the stepwise formation constant ($\beta 3$) values. The ratio of metal to ligand can also influence the relative population of the three species; thus a high L:M ratio will shift the equilibria to the right hand side and favour the formation of ML_3 species. Hider *et al* (1991) have shown a clear relationship between the pKa values of the ligands and the K_1 value for iron(III), indicating the dominant influence of electrostatic interaction between the metal and the ligating atoms. Thus, dioxygen-containing ligands with relatively high pKa values would be ideal for this type of cation. Examples of such cations are depicted in figure 1.3; lactate (6) would be classed as a poor chelating agent (log K_{stab} for Al, 5.8) (Martell and Smith, 1974-1977, 1982)

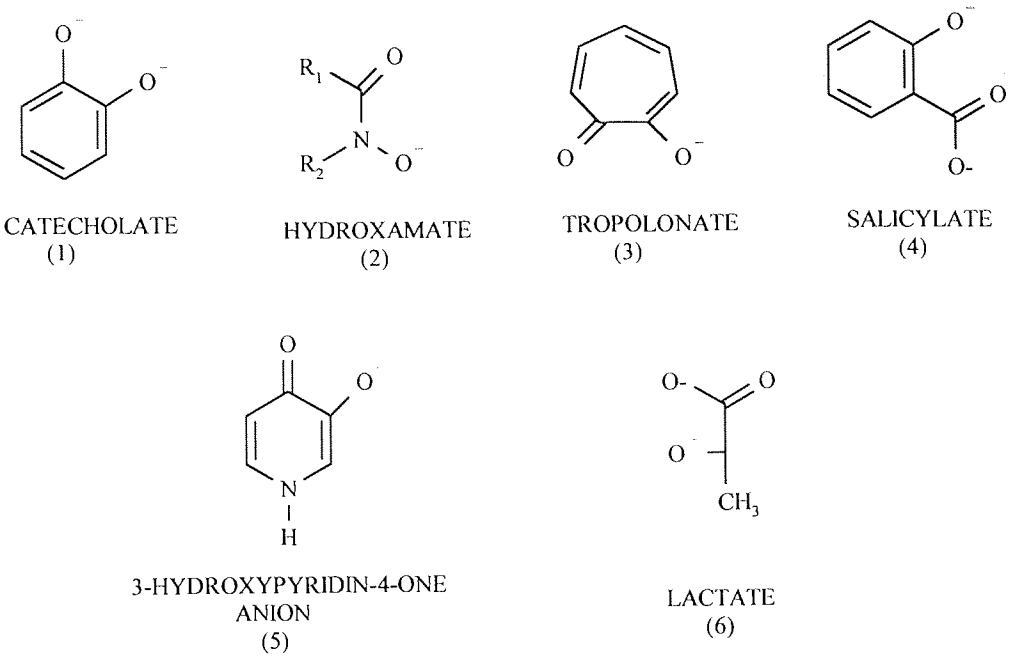


FIGURE 1.3 Structures of some typical dioxygen ligands

1.4.1 Carboxylic acids

Ionisation of the hydroxyl group of co-ordinated hydroxycarboxylate ligands starts at pH ~3. Besides monomeric species, hydroxo- and oxo-bridged polynuclear and in some cases highly polymeric complexes are also formed readily. The extent of polynuclearity seems to decrease with the increase in the denticity of the ligands (Kiss, 1994).

The $Al_2(OH)_2L^{3+}$ complexes with the monocarboxylic acetic and propionic acids form within the pH range 3-5 (Marklund, 1989).

The monocarboxylic acids, lactic and malic acid, bind Al more weakly than the simple dicarboxylates since alcoholic hydroxyl, especially in protonated form, is a weak coordination site as compared to a carboxylate. Hence besides the (COO^-,OH) co-ordinated complexes which are formed at pH < 3, various deprotonated species are the dominant complexes (Kiss, 1994). Lactic acid forms an uncharged complex, $Al_2(OH)_2(H^{-1}L)_2$ in physiological conditions, but would only bind 3% of plasma Al in the absence of citrate, and none in its presence (Marklund and Ohman, 1990).

It has been reported by several groups that citrate complexes Al at its hydroxyl and two terminal groups. This is supported by its published crystal structures (Feng, 1990).

Hue *et al.*, (1986) tested and ranked the efficacy of carboxylic acids as Al chelators, finding citric > oxalic > tartaric > malic > malonic > salicylic > succinic. They concluded that effective detoxifying agents form five and six membered ring structures through Al, with either two pairs of OH/COOH attached to two adjacent carbons or two COOH groups directly connected.

1.4.1.1 Al-citrate complexes

The nature of the complexes formed between Al and citrate is important because citrate is probably the main small molecule binder of Al in plasma and it can aid Al in crossing membranes such as the gastric mucosa (Slanini, 1986). Many stability constant measurements have been made, but these can be misleading as discussed by Findlow *et al.*, (1987). The major problem with determining stability constants of Al citrate complexes arises from the slow kinetics of ligand exchange, which was demonstatrated by Öhman (1988), who found that some solutions containing Al needed to age for 20 hours before equilibrium was reached. Jackson (1982) carried out a comparative study of the interaction of Al with citrate and its analog with a hydrogen replacing the 3–hydroxy group ionised before the central carboxylic acid. Thus, the structure of Al-citrate appears to consist of the citrate donating three ligands (the hydroxy and terminal carboxylate groups), and three water molecules to give a six co-ordinate complex (Jackson, 1982; Martin, 1986; Motekaitis, 1984).

1.4.2 Hydroxamates

The hydroxamate moiety (2) is a chelating function that has been widely adopted by bacteria and fungi for siderophore construction (Hider, 1984). The log K_1 values of hydroxamates with Group III metals are much lower than values for corresponding catechol chelates, as only one oxygen is protonated under physiological conditions (pKa = 9.35) and therefore competition with protons is less marked. The high electron density on both ligating oxygen atoms results from delocalisation of the nitrogen lone pair. The electron density of the carbonyl oxygen can be further enhanced by delocalisation of electrons from conjugated side chains, which results in an increase cation affinity. This is a strategy for siderophore design, for instance with *mycobactin* and some ferrichrome and rhodotorulic acid derivatives (Hider, 1984).

As only 3 protons are displaced from a 3:1 hydroxamate ligand, the resulting compound is neutral. Thus in principle, if the compound has a favourable octanol/water partition coefficient (K_{part}) the complex would be likely to penetrate biological membranes (Porter *et al.*, 1989).

Aliphatic hydroxamates, like amides are hydrolysed in acidic environments and consequently possess low oral activity (Summers *et al.*, 1988). Aromatic hydroxamates are capable of forming stable radicals that are likely to cause toxic effects (Hussain *et al.*, 1979).

1.4.2.1 Desferrioxamine (DFO)

To date, only the oligodentate hydroxamate ligand, DFO is used clinically for the removal of Al from the body, with a dose of 100mg DFO intravenously being able to theoretically bind with 4.1mg of Al. Approximately 50,000 patients within the UK are treated for Al overload with DFO (BNF, 1999). DFO is primarily used for the treatment of iron overload, and is known to bind as a 1:1 complex with the ferric ion, ferrioxamine (figure 1.4). It would be envisaged that an Al ion would bind in a similar fashion resulting in an aluminoxamine complex.

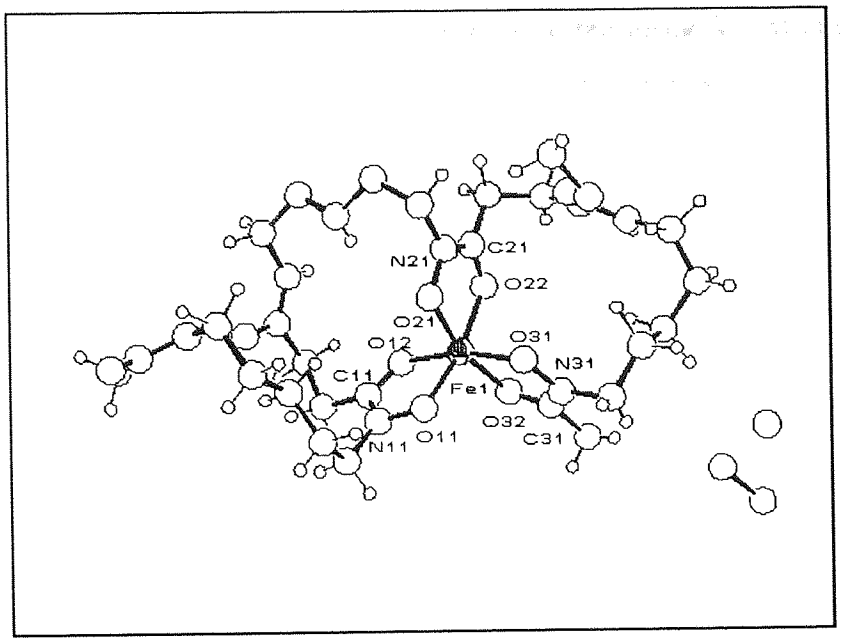


FIGURE 1.4 Structure of a 1:1 complex of Fe with desferrioxamine extracted from the Cambridge Structural Database (Hossain, 1986) (refcode DUPJON). Atoms involved in the chelate ring are labelled

DFO administration has shown excretion of both aluminoxamine and ferrioxamine in urine, showing both Fe and Al are removed with this drug. However, DFO has a greater affinity for Fe relative to Al (log stability constant of 30 and 24 respectively) (Yokel, 1994).

1.4.3 Catechols

Catechols bind Group III metals tightly resulting from the high electron density of both oxygen atoms. However, this is also associated with affinity for protons (pKa values 13.0 and 9.2) and therefore cation binding has a marked pH sensitivity. Ultimately, the competition between proton and cation leads to a range of species at neutral pH (Hider, 1991). All the complexes thought to exist at physiological pH by Fe possess a net charge, namely the 3:1 complex, charge -3, the 2:1 complex, charge -1, the 4:2 complex, charge -2, and consequently are unlikely to penetrate membranes by simple diffusion.

Catechols are also susceptible to oxidation, leading to the formation of quinones that can interact with protein thiol groups thereby causing toxic effects.

While studying the complexation of Al with catecholamines, researchers found that the high stability constants failed to give a realistic impression of the binding strengths due to the high pKa values of the catecholate ligand. Thus, a conditional stability constant was defined. (Martin, 1988).

L-Dopa is one of the few compounds with a greater logK for Al (AlL, 19.6) than Fe (FeL, 18.4). (Rajan *et al.*, 1978). However, further studies looking at 'effective logK', suggest that this catechol, as well as dopamine, noradrenaline (norepinephrine), gallic acid and tiron (effective logK values between 8.0-10.4) would not be able to compete with citrate (effective logK value of 11.7) for Al binding (Kiss, 1989).

1.5 BASIC THEORY OF COMPLEXATION TITRATIONS AND STABILITY CONSTANTS

Ionic species that can bind a hydrogen cation also have an affinity for the cations of metals. Usually, this affinity is greatest when an organic molecule is able to form at least two bonds to the metal, thus creating a ring. This ring formation is named chelation, from the Greek word for lobster's claw and the complexing species is known as a ligand.

Stability constants are the equilibrium constants for reactions between metal ions (M) and ligands (L) which take place in aqueous solution. The thermodynamic stability constant is a measure of the extent to which this species will form, or be transformed into other species under certain conditions when the system has reached equilibrium (Cotton and Wilkinson, 1980). This equilibrium can be represented as:

$$M + nL \rightleftharpoons ML_n$$

Equation 1.1

in which expression the charges on the metal ion, ligand, and the complex are usually omitted. The activities of ions in solution are strongly influenced by the total ionic concentration of the solution, thus it is necessary to maintain a constant electrolyte concentration if the equilibrium constant is to be true. The medium of choice to provide a constant ionic strength is sodium perchlorate because the perchlorate ion shows little tendency to form complexes with metal ions (Albert and Sergeant, 1984). The hydration of the species is not usually specified.

Hence, the overall stability constant (β) for the equilibrium is conventionally defined as,

$$\beta_n = \left[\frac{MLn}{[M][L]^n} \right]$$

Equation 1.2

in which the square brackets represent the concentrations in mol l^{-1}, and β is the product of the micro stability constants K_1, K_2 etc.

$$M + L \leftrightarrow ML$$
$$ML + L \leftrightarrow ML_2$$
$$ML_2 + L \leftrightarrow ML_3$$

where :

$$K_1 = \frac{[ML]}{[M][L]}$$
$$K_2 = \frac{[ML2]}{[ML][L]}$$
$$K_3 = \frac{[ML_3]}{[ML_2][L]}$$

Equations 1.3

As ligand (L) is added to the solution of metal ion (M), ML is initially formed more rapidly than any other complex in the series. As addition of ligand is continued, the ML_2 concentration rises rapidly, while the ML concentration drops, then ML_3 becomes dominant, ML and ML_2 becoming unimportant and so forth. Eventually the highest complex ML_N, where N is the maximum number of ligand molecules per metal ion, is formed to the nearly complete exclusion of all others at very high ligand concentrations.

In an aqueous solution of a metal ion, all the co-ordination positions are usually occupied by water. The reaction shown in equation (1) involves replacement of one or more molecules of water by the ligand. A chelate (or chelate complex) is formed when a multidentate ligand forms two or more co-ordinate bonds with the same metal atom thereby creating a ring structure.

The term 'chelate effect' refers to the enhanced stability of a complex system containing chelate rings as compared to the stability of a similar one which contains fewer or no rings (Bell, 1977).

The classic work of Bjerrum (1941), who developed a simple pH titration method for determining stability constants, created a surge of interest in the quantitative investigation of the many complexes furnished by weak bases (L^{n-}). At low pH, such ligands preferentially bind protons rather than metal cations. Quantitative formation of the metal chelate complex occurs only if the protons liberated by these equilibria are removed by reaction with hydroxyl ions. This is achieved in the pH titration method by the addition of a standard solution of strong alkali. Titration of the complexant, in the presence of a metal ion, results in lower pH values than are observed when the complexant is titrated alone. Analysis of the difference reveals the stability constants. Due to the length and complexity of these calculations, various computational programs have been developed such as BEST (Motekaitis, 1982), SUPERQUAD (Gans, 1985) and STABOPT (Taylor, 1996). The use of these programs permits many refinements in the calculation of stability constants from the titration data, and allows a greater flexibility in the application of the basic experimental technique. This is because a far wider range of measurements can be made in comparison with what could be contemplated if the calculation were to be investigated.

A steady decrease in K_n values with increasing n is to be expected, which may be attributed to increased steric hindrance as the number of ligands increases if they are bulkier than the water molecules they replace, and Coulombic factors, mainly in complexes with charged ligands (Cotton and Wilkinson, 1980).

TABLE 1.2 Selected log stability constants for Al complexes

Chemical family and ligand (L) with [chemical species of the complex]	Log stability constant	Reference
OH [AlL], [AlL_2], [AlL_3], [AlL_4]	8.2-9.0, 16.8-18.7, 24.7-27.0, 31.5-33.4	Martell, 1976 Smith, 1989
Ketone (acetylacetonate) [AlL], [AlL_2], [AlL_3],	8.6, 16.5, 22.3	Martell, 1977 Sillen, 1964 Smith, 1989
Catechol	17.3	Martell, 1974
Tiron [AlL], [AlL_2], [AlL_3]	16.6, 30.0, 40.0	Martell, 1977 Perrin, 1979
Dopamine [AlHL], [$Al(HL)_2$], [$Al(HL)_3$]	13.3, 24.0, 30.6	Martell, 1990
L-dopa [AlL], [AlL_2], [AlL_3]	12.7, 22.6, 28.4	Martell, 1990
Maltol [AlL], [AlL_2], [AlL_3]	8.2, 15.8, 22.5	Hedlund, 1988
Hydroxypyridinones (1,2-dimethyl-3-hydroxypyridin-2-one	34.0	Clevette, 1989
DFO	24	Yokel, 1994
AMP, ADP, ATP [AlL_2]	10.35, 12.16, 12.37	Kiss, 1991

1.6 MOLECULAR MODELLING

Over the past few years, advances in the description of the phenomena and development of more intuitive program interfaces coupled with the availability of faster, smaller and affordable computer hardware have provided experimental scientists with a new set of computational tools. These tools are being successfully used, in conjunction with traditional research techniques, to examine the structural properties of existing compounds, develop and quantify a hypothesis which relates these properties to observed activity and utilise these "rules" to predict properties and activities for new chemical entities. The development of molecular modelling programs and their application to pharmaceutical research has been formalised as a field of study known as computer assisted drug design (CADD), or computer assisted molecular design (CAMD).

Computational chemistry/molecular modelling is the science (or art) of representing structures numerically and simulating their behaviour with the equations of quantum and classical physics.

1.6.1 Molecular mechanics (MM)

MM is a mathematical formalism which attempts to reproduce molecular geometries, energies and other features by adjusting bond lengths, bond angles and torsion angles to equilibrium values that are dependent on the hybridisation of an atom and its bonding scheme (this atom description is referred to as the atom type). Rather than utilising quantum physics, the method relies on the laws of classical Newtonian physics and experimentally derived parameters (e.g. from x-ray, NMR, IR, Raman spectroscopy and *ab initio* calculations) to calculate steric energy as a function of geometry.

In a MM method, the database of compounds used to parameterise the method (a set of parameters and functions called a force field) is crucial to its success. Whereas a semi-empirical method may be parameterised against a set of organic molecules, a MM method may be parameterised against a specific class of molecules, such as

proteins. Such a force field would only be expected to have relevance to describing other proteins.

The application of the MM calculations on octahedral complexes of Al and Fe with oxygen donor atoms has been investigated by P C Yates, Dept. of Chemistry, Keele University, UK. Development of the force field was based on the experimental Al-O and Fe-O bond lengths which were used to estimate bond stretching and angle bending force constants (Yates, 1993). This force field was used in calculations on a series of ligands known to form octahedral complexes with Al based on the 'Hole Size Profile' (Drew, 1987). Of the carboxylic acids investigated, this method gives plausible predictions of the geometry of the Al and Fe complexes. However, in the very demanding application of evaluating selectivity between Al and Fe this method predicts pyruvate and lactate to be the most Al specific ligands.

The advantage of MM is that it allows the modelling of enormous molecules, such as proteins and segments of DNA, making it the primary tool of computational biochemists. The disadvantage of MM is that there are many chemical properties that are not even defined within the method, such as electronic excited states. In order to work with extremely large and complicated systems, often MM software packages have the most powerful and easiest to use graphical interfaces. Because of this, mechanics is sometimes used because it is easy, but not necessarily a good way to describe a system.

1.6.2 Quantum mechanics (QM)

QM is one of the oldest mathematical formalisms of theoretical chemistry. In its purest form, quantum theory uses well known physical constants such as velocity of light, values for the masses and charges of nuclear particles and electrons, and differential equations to directly calculate molecular properties and geometries. This formalism is referred to as *ab initio* (from first principles) quantum mechanics. The equation from which molecular properties can be derived is the Schrödinger equation,

$$H\Psi = E\Psi$$

Equation 1.4

where E is energy of the system relative to one in which all atomic particles are separated to infinite distances, Ψ is the wave function which defines the Cartesian and spin co-ordinates of the atomic particles, and H is the Hamiltonian operator which includes terms for both potential and kinetic energy. Unfortunately, the Schrödinger equation can be solved only for hydrogen. Approximations must be introduced in order to extend the utility of the method to polyatomic systems. The first approximation attempts to differentiate nuclei and electrons. It assumes that nuclei are much heavier than electrons and move much more slowly so that the molecular systems can be viewed as electrons moving around fixed nuclei (the Born-Oppenheimer approximation). Solutions to the Schrödinger equation using this assumption lead to values of effective electronic energy, which are dependent on relative nuclear co-ordinates. As the nuclei are moved to new co-ordinates and molecular energies are re-calculated, the resulting quantitative description of molecular energy in relation to geometry is referred to as the potential energy surface for the molecule. The lowest point on this surface, with respect to energy, is the ground state energy (and its associated geometry) for the molecule. The second approximation allows the wave function Ψ to be represented as the product of one electron (or spin) orbitals. The functions that are used to describe these orbitals are referred to as basis functions. This formalism is referred to as the Linear Combination of Atomic Orbitals (LCAO) theory. Once the orbitals have been derived, the orbital

coefficients (which define the energy of the system) are calculated. Hartree Fock (HF) theory is used to accomplish this goal. HF assumes that the energy of a set of molecular orbitals can be derived from the basis set functions which are used to define each orbital and a set of adjustable coefficients which are used to minimise the energy of the system. The energy calculation becomes an exercise in solving a set of (N x N) matrices to obtain optimal values for the coefficients in order to solve the equations. An iterative process is used in which an initial guess for the value of the coefficient is progressively refined until it provides consistent values. This method is referred to as the self consistent field (SCF) theory.

Quantum mechanics utilise a set of mathematical descriptions to define a theoretical model for the behaviour of molecules. The validity of these models can be gauged by comparing structures and properties derived from the model with experimental results. In general, *ab initio* methods are able to reproduce laboratory measurements for properties such as the heat of formation (ΔH_f), ionisation potential, UV/visible spectra and molecular geometry. Since quantum methods utilise the principles of atomic physics to examine structure as a function of electron distribution, their use can be extended to the analysis of molecules as yet unsynthesised and chemical species which are difficult (or impossible) to isolate. Geometry and properties of a transition state (where the electronic character of component atoms is shifting from the starting material to that of the products) and excited states (where the electronic configuration of the molecule is temporarily perturbed by adding energy to the molecule) can only be calculated using quantum methods.

Several commercial packages are available to run both semi-empirical and *ab initio* calculations. Examples include:

1. MOPAC: General purpose semi-empirical molecular orbitals package.
2. GAMESS: General Atomic and Molecular Structure System

All are capable of running the standard Hamiltonian methods, Modified Neglect of Differential Overlap (MNDO) (Dewar, 1977), Austin Method 1 (AM1) (Dewar, 1985) and Parametric Model 3 (PM3) (Stewart, 1989), which are parameterised for Al, as well as *ab initio* methods including STO-3G, 3-21G and 6-31G. They differ in their

quantum mechanical core routines. Most studies in this thesis were undertaken using GAMESS.

1.6.2.1 GAMESS

GAMESS is a program for *ab initio* and semi empirical quantum chemistry. The package is suitable for both calculations on large organic systems and accurate calculations on small molecules. This program was put together from several existing quantum chemistry programs, in particular HONDO. The GAMESS package is capable of a wide range of quantum chemical computations, some of which include:

1. calculations of SCF molecular wavefunctions
2. optimisation of molecular geometries, in terms of Cartesian or internal co-ordinates
3. calculations of molecular properties such as electrostatic potentials

An example of an input file for GAMESS calculations is listed in appendix 1.

1.6.2.2 *Ab initio* methods

The term "*ab initio*" is Latin for "from the beginning". This name is given to computations that are derived directly from theoretical principles, with no inclusion of experimental data. Most of the time this is referring to an approximate quantum mechanical calculation. The approximations made are usually mathematical approximations, such as using a simpler functional form for a function or getting an approximate solution to a differential equation.

The most common type of *ab initio* calculation is called a Hartree Fock (HF) calculation, in which the primary approximation is the central field approximation (CFA), which means the Coulombic electron-electron repulsion is not specifically taken into account, although the net effect is included in the calculation. This is a variational calculation, resulting in the approximate energies calculated being equal to

or greater than the exact energy. The energies calculated are usually in units called Hartrees (1 H = 27.2114 eV). Energies from HF calculations, resulting from the CFA, are always greater than the exact energy and tend to a limiting value called the HF limit.

The second approximation in HF calculations is that the wave function must be described by some functional form, which is only known exactly for a few one electron systems. The functions used most often are linear combinations of Slater type orbitals (STO) or Gaussian type orbitals (GTO). The wave function is formed from linear combinations of atomic orbitals (LCAO) or more often from linear combinations of basis functions. Because of this approximation, most HF calculations give a computed energy greater than the HF limit. The exact set of basis functions used is often specified by an abbreviation, such as STO-3G or 6-31G*.

A number of types of calculations begin with a HF calculation then correct for the explicit electron-electron repulsion, referred to as correlation. Some of these methods are Moller-Plesset perturbation theory (MPn, where n is the order of correction), the Generalised Valence Bond (GVB) method, Multi-Configurations Self Consistent Field (MCSCF), Configuration Interaction (CI) and Coupled Cluster theory (CC). As a group, these methods are referred to as correlated calculations (Hehre, 1985).

A method, which avoids making the HF mistakes in the first place is called Quantum Monte Carlo (QMC). This method works with an explicitly correlated wave function and evaluates integrals numerically using a Monte Carlo integration. These calculations can be very time consuming, but they are probably the most accurate methods known today.

An alternative *ab initio* method is Density Functional Theory (DFT), in which the total energy is expressed in terms of the total electron density, rather than the wavefunction. In this type of calculation, there is an approximate Hamiltonian and an approximate expression for the total electron density.

Ab initio methods eventually converge to an exact solution, once all of the approximations are made sufficiently small in magnitude. The main disadvantage of

ab initio methods is that they are expensive. These methods often take enormous amounts of computer cpu time, memory and disk space. The HF method scales as N^4, where N is the number of basis functions, so a calculation twice as big takes 16 times as long to complete. Correlated calculations often scale much worse than this. In general, *ab initio* calculations give very good qualitative results and can give increasingly accurate quantitative results as the molecules in question become smaller.

1.6.2.2.1 Basis sets

Much effort has gone into devising and comparing basis sets for *ab initio* calculations. Many types of basis set have been examined and two of these have come to dominate the area of *ab initio* molecular calculations. They are referred to as the Slater type orbital (STO) and the Gaussian basis sets. Basis sets need to satisfy essentially two important criteria:

(1) The basis set must be capable of describing the actual wavefunction well enough to give a chemically useful result.

(2) The basis set must lead to integrals F_{ij} and S_{ij} that can be evaluated inexpensively and accurately.

The basis sets used in these studies range from:

1. STO-3G - each STO approximated as linear combination of three Gaussian primitives.
2. 3-21G - each inner shell STO is represented by the sum of three Gaussians and each valence shell STO is split into inner and outer parts described by two and one Gaussians respectively
3. 6-31G – each inner shell STO is represented by the sum of six Gaussians and each valence shell STO is split into inner and outer parts described by three and one Gaussians respectively
4. 6-31G* - the 6-31G basis set is augmented with six d-type Gaussian primitives on each heavy atom to permit polarisation

Packages for *ab initio* calculations include the public domain GAMESS and the commercially available GAUSSIAN series.

Slater type orbitals resemble the orbitals obtained from an exact quantum mechanical solution for the hydrogen atom, but with a simplified radial dependence (e^{-nr}) of the wavefunction. These in turn can be approximated by a short series of Gausssian functions (such as STO-3G) with radial dependence e^{-nr^2}. These functions, which define the bell-shaped curves in statistics, are easy to integrate. Gaussian functions can also be used without reference to STOs.

There are two main considerations in the choice of a basis. The first is that one desires to use the most efficient and accurate functions possible, in the sense that the expansion will require the fewest possible terms for an accurate representation of the molecular orbitals. From this consideration, Slater functions are better than Gaussian functions. The second consideration is the speed of two electron integral evaluation. Here Gaussian functions are an advantage. By using a basis set of contracted Gaussian functions a compromise is reached.

1.6.2.2.2 Semi-empirical methods

Semi-empirical methods utilise approaches that are similar to *ab initio* methods, but several approximations are introduced to simplify the calculations. Rather than performing a full analysis on all electrons within the molecule, some electron interactions are ignored. These methods include the Huckel and Pariser-Parr-Pople approaches for aromatic compounds (in which the outer π electrons in conjugated systems are treated, but the inner, or core, electrons are ignored) and the Neglect of Differential Overlap formalisms found in the CNDO (Complete Neglect of Differential Overlap) and INDO (Intermediate Neglect of Differential Overlap). In these methods, the more complex portions of the *ab initio* calculations are ignored or set to zero. Other semi-empirical approaches replace complex portions of the calculation with parameters that are derived from experimental data. While semi-empirical methods require less computer resources than *ab initio* methods, they are still compute intensive. In general, calculations are routinely performed on

compounds that contain up to 100 atoms. The chief drawback is that its application is limited to systems for which appropriate parameters have been developed.

The advantage of semi-empirical calculations is that they are much faster than the *ab initio* calculations. The disadvantage of semi-empirical calculations is that the results can be erratic. If the molecule being computed is similar to molecules in a database (for instance the Cambridge Structural Database, CSD, where the geometry of the test crystal will be close to a minimum) used to parameterise the method, then the results may be very good. If the molecule being computed is significantly different from anything in the parameterisation set, the answers may be very poor. Semi-empirical calculations have been very successful in the description of organic chemistry, where there are only a few elements used extensively and the molecules are of moderate size. However, semi-empirical methods have been devised specifically for the description of inorganic chemistry as well.

PM3 is the latest of the Hamiltonians paramaterised for Al (although the parameters for Al are similar to those used in MNDO). It is important to note that data used for parameterisation of Al within PM3 is limited to relatively simple molecules including a series of polar compounds, mostly oxides (AlO, Al_2O) and halides (AlF, AlF_3, AlCl, $AlCl_3$, AlBr, $AlBr_3$, AlI and AlI_2) and three model complex ions of Al, namely AlO_2^-, AlF_2O^- and AlF_4^- (Stewart, 1989). These parameters are optimised to reproduce four gas phase molecular properties: ΔH_f, dipole moments, ionisation potentials, and molecular geometries. It is envisaged that these calculated molecular properties would correlate with experimentally produced stability constants. With PM3, differences in ΔH_f between predicted and experimental values are considerably reduced while errors in bond lengths are only slightly reduced (Stewart, 1989), although there are conflicting reports as to which basis set is best suited to Al complexes (Dewar, 1990). In general only small molecules (less than 10 atoms) have been published in calculations involving Al and semi-empirical basis sets, with the exception of work done by DeAlmeida (1998) who undertook AM1 calculations of anhydrotetracycline with Al to identify the most suitable binding sites of the ligand. As a result work in this thesis was dedicated to identifying the most suitable basis set for optimisations of organoaluminium complexes (Chapter five).

1.6.2.3 Thermochemistry

Thermodynamics is one of the most well developed mathematical chemical descriptions. Both semi-empirical and *ab initio* calculations tend to be very useful not only to identify an optimum geometry for a test structure but also to identify an energy term to indicate the stability of the test product.

Ab initio MO methods provide total energies, E_{eq} as the sum of electronic and nuclear-nuclear repulsion energies for molecules, isolated in vacuum, without vibration at zero Kelvin (K).

$$E_{eq} = E_{electronic} + E_{nuclear\text{-}nuclear}$$

Equation 1.5

MO parameters for MNDO, AM1 and PM3 Hamiltonians are parameterised so as to produce the experimental ΔH_f at 298°K and not E_{eq} at 0°K.

1.6.2.3.1 Heat of formation (ΔH_f)

All matter contains energy, whether it be kinetic (associated with molecular motion) or potential energy (associated with chemical bonds). These together make up the internal energy, U of matter. The heat absorbed at constant pressure is the change in enthalpy, ΔH. This can be defined by equation 1.6 below

$$\Delta H = \Delta U + P\Delta V$$

Equation 1.6

where P is a constant pressure and ΔV is the change in volume. Matter absorbing energy in solution phase at constant pressure will have negligible change in volume, ΔV, thus resulting in P and V being constant. On this assumption, ΔV would be zero, resulting in:

$$\Delta H = \Delta U$$

Equation 1.7

However QM calculations are calculated in gas phase and chemical changes in gases are likely to produce large changes in V, which can be calculated from the ideal gas equation.

$$P\,\Delta V = \Delta n\,R\,T$$

Equation 1.8

where Δn is the increase in number of moles of gas and R is the gas constant.

Ab initio calculations work out ΔU in an accurate manner, however neglect both P and V. This does not pose a problem if ΔV is zero, but in the case of gases may lead to a large discrepancy in the final value of ΔH. Semi-empirical methods on the other hand are less well suited to calculating the value of ΔU, but take into consideration the values of P and ΔV. Ultimately semi-empirical methods produce a value for ΔH that may not be as accurate as *ab initio* calculations based on ΔU, but is somewhat compensated for by its consideration of P and ΔV.

The enthalpy of a substance is quoted for the substance in its standard state (one mole of a substance in its standard state, such as solid, liquid, or gas at one atmosphere pressure). This definition can be extended for the ΔH_f, which is the heat absorbed when one mole of a substance is formed from its elements in their standard states at constant pressure. If the reaction is exothermic, the heat absorbed will be negative and consequently the ΔH_f will be negative. Consequently, the ΔH_f is a measure of how likely a product will be formed.

1.6.2.3.2 Connection between ΔH_f and stability constants

The stability constant of a product is related to the Gibbs free energy G, which is described by equation 1.2. Some endothermic reactions occur spontaneously, showing that differences in enthalpy of the reactants and products cannot be the only factor that decides whether a chemical reaction takes place. This additional factor is the entropy or degree of randomness of the system. This can be pictured by considering the dissolution of an ionic solid. As it dissolves, the regular arrangement of a crystalline lattice in solid goes to a random solution of ions. This change is termed as an increase in entropy of the system.

$$\Delta G = \Delta H - T\,\Delta S$$

Equation 1.9

where; ΔG is the change in Gibbs free energy

T is the temperature of the system (in degrees Kelvin, °K)

ΔS is the change in entropy

For a physical or chemical change to occur, ΔG for that change must be negative. The change is therefore assisted by a decrease in enthalpy (ΔH is negative) and by an increase in entropy (ΔS is positive). If the change takes place under standard conditions, that is with each reactant and product at unit concentration or pressure, then the free energy change is equal to the standard free energy change ΔG^o. When reactions take place under non-standard conditions, ΔG depends on the concentrations or pressures of the reactants and products which is not easy to compute.

Equation 1.9 shows Gibbs free energy is dependent on an enthalpy term (ΔH) and an entropy term (ΔS). Both HF and semi-empirical methods have parameters for the calculation of this enthalpy term, but neglect to consider the entropy term. This may be overcome by using free energy perturbation methods, however this method takes up a huge amount of computing time and memory and consequently would be impractical for calculations of organoaluminium complexes which are of interest in these studies.

1.7 AIMS

The ultimate aim of these studies was to obtain both a theoretical and a practical method for evaluating potential Al chelating agents. Theoretical studies will principally be undertaken using semi-empirical quantum mechanical (QM) calculations. Preliminary studies involving the geometric comparisons of the semi-empirical Hamiltonians parameterised for Al with the more powerful *ab initio* calculations were undertaken to identify the Hamiltonian of choice for optimisations of more complex structures deemed impractical for *ab initio* studies. Furthermore a search of the Cambridge Structural Database (CSD) would also identify trends and characteristics of Al complexes. CSD studies also provide a range of geometric data for organoaluminium complexes that would ultimately be the criteria for accepting subsequent QM optimisation results.

Complexes of interest within the database were to be used as starting points for QM optimisations, as crystal structures are more likely to optimise to a global minimum relative to a manually constructed structure, which had to be used, where crystals were unavailable.

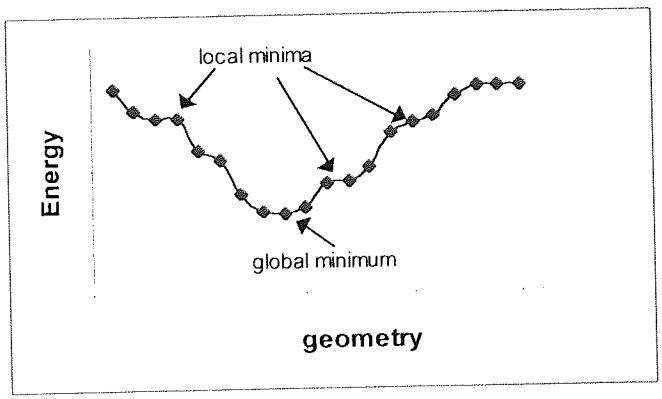


FIGURE 1.5 Diagrammatic representation showing energy profile of a hypothetical structure relative to profile outlining global and local minima

As crystal structures were a valuable part of the QM studies, as indeed they are in any drug design process, studies involving the crystal growth and determination of potential ligands of Al were undertaken.

To date, only animal models have been used to identify and investigate the efficacy of potential Al chelators. The work in this study aimed to develop and optimise a model using bacteria and cell culture as a relatively inexpensive alternative to evaluate potential ligands. Consequently, studies involving quantitative Al analysis were undertaken to allow a method of analysis of Al in these models.

CHAPTER TWO

GENERAL METHODS AND MATERIALS

The general methods and materials are described in this chapter. Specific details and variations to the standard procedures are outlined in the relevant chapters.

2.1 MATERIALS

All chemicals used were of the highest grade available from Sigma Chemical Company (Poole, UK) unless otherwise specified. All reagents were used as received without further purification.

Cell culture reagents and media were purchased from Life Technologies Inc. (Paisley, UK). Tissue culture flasks, multi-well tissue culture plates, 15mL and 50mL polypropylene tubes were purchased from Beckton Dickinson and Company (Plymouth, UK). Disposable pipettes, microcentrifuge tubes, Finnpipette tubes, Finnpipette tips and 2mL Biofreeze vials were purchased from Starstedt (Leicester, UK).

2.2 DATABASE SEARCHING

2.2.1 Instrumentation

All crystallographic searches were performed on a Silicon Graphics Iris Indigo workstation (phindigo 1), accessible by a telnet command from other workstations, with networked file storage (NFS) on a Sun server. The Cambridge Structural Database (CSD) (Allen, 1983) was used to identify polymeric species of the trivalent metal ions studied using integrated software QUEST3D and subsequent analysis using VISTA described in section 3.3.

2.2.2 Crystallographic searches

Investigations of donor atoms involved in complexation were performed in searches specifying the chelate ring length and the donor atoms as shown in Figure 2.1.

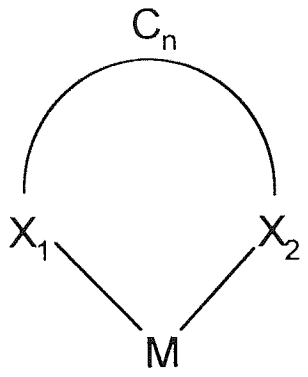


FIGURE 2.1 Basic test fragment used in QUEST3D to identify donating atoms and chelate systems involved in Al and Fe complexation. Here M is Al or Fe, X_1 and X_2 are either N,N; N,O; or O,O as donating pairs and n is either 2, 3 or 4 carbons resulting in 5, 6, or 7 membered chelate ring systems, respectively. Unspecified bonds were used to join atoms

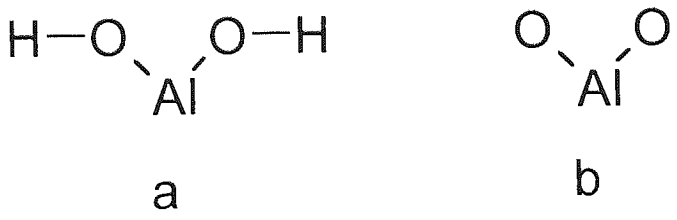
Prior to a CSD search, the following constraints were added using QUEST 3-D;

2D constraints - M was six co-ordinate with a charge of +3.

3D constraints - all Al-X bond lengths were measured, as were all Al-X-C bond angles where X represents the donor atom.

Where 2 sets of results were obtained for similar crystal structures, the crystal data with the lower discrepancy factor, (*R*) was used (see chapter four). If the *R* factors for identical crystals were similar, the data from the most recent publication was used.

2.2.3 Investigation of deprotonation of oxygen donor ligands upon complexation with Al



a b

FIGURE 2.2 QUEST fragments used to identify six co-ordinate Al complexes possessing oxygen donor atoms that are a) protonated and b) deprotonated

Prior to a QUEST search, the following 2D constraints were also added.

1. Both test fragments specified Al as 6 co-ordinate
2. Fragment (b) had the additional constraint specifying that no hydrogens were present on the oxygen donor atoms.

2.2.4 Data Analysis

Data analysis was performed using VISTA and INSTAT v2.05a.

Unpaired Student t-tests were performed using the Welch's test as the sample sizes for Al and Fe were of significant variance.

2.3 X-RAY CRYSTALLOGRAPHY

This section concentrates on crystal synthesis, and physical measurements of melting point (m.pt.). The X-ray crystallography procedure is a skilled and lengthy procedure, hence basic theory and solving of the structures are discussed separately in chapter four.

2.3.1 Synthesis of crystals

2.3.1.1 Aluminium chloride hexahydrate (ALP2XL)

10ml of 1M $AlCl_3.6H_2O$ (Aldrich) was added to 30ml of 1M pyruvic acid (Aldrich). After addition of 10mL methanol, the mixture was refluxed at 70°C for 4 hours under an argon atmosphere. Clear cube like crystals formed over a period of several days. A crystal measuring 0.525mm x 0.525mm x 0.5mm was chosen for X-ray determination.

2.3.1.2 Anhydrous DL tartaric acid (ALTAR)

10ml of 1M $AlCl_3.6H_2O$ (Aldrich) was added to 30ml of 1M DL-tartaric acid (Aldrich). The resultant mixture was placed on a hot plate and magnetically stirred for approximately 3 hours. The solution was dried *in vacuo* before freeze drying for a period of 24 hours. The resultant precipitate was redissolved in ethanol and using the liquid diffusion crystallisation technique (Orvig, 1985) small transparent colourless crystals were formed over a period of three months with a m.pt of 204.3°C. A crystal measuring 0.2mm x 0.15mm x 0.15mm was chosen for X-ray determination.

2.3.1.3 Sodium tartrate monohydrate (ALTXL)

3 parts L-tartaric acid was added to 1 part aluminium chloride hexahydrate. The mixture was refluxed at 70°C in ethanolic conditions under an argon atmosphere for 4 hours. A resultant white precipitate was filtered and redissolved using sufficient NaOH (1M). The mixture produced clear crystals over a 2 week period. A crystal measuring 0.35mm x 0.325mm x 0.225mm was chosen for X-ray determination.

2.3.1.4 Anhydrous tricarballylic acid (TRIC2XL)

10ml of 0.1M methanolic $AlCl_3.6H_2O$ (Aldrich) was added to 30ml of 0.1M methanolic tricarballylic acid (Aldrich). The resultant mixture was refluxed under argon at 70°C for 4 hours. The mixture was dried *in vacuo* before being redissolved in methanol. Transparent crystals formed over 2 weeks at 4°C. A crystal measuring 0.6mm x 0.325mm x 0.875mm was chosen for X-ray determination.

2.3.1.5 Dimethylcitrate monohydrate (CITXL)

10ml of 0.1M methanolic $AlCl_3.6H_2O$ (Aldrich) was added to 30ml of 0.1M methanolic citric acid (Aldrich). The resultant mixture was refluxed under argon at 70°C for 4hours. The mixture was dried *in vacuo* before being redissolved in methanol. Transparent crystals formed over 2 weeks at 4°C. A crystal measuring 0.2mm x 0.1mm x 0.125mm was chosen for X-ray determination.

2.3.1.6 Calix-4-arene (PYRXL)

10ml of 0.01M $AlCl_3.6H_2O$ (Aldrich) was added to 30ml of 0.01M ethanolic calix-4-arene (Aldrich). The resultant mixture was refluxed under argon at 70°C for 4hours. The mixture was dried *in vacuo* before being redissolved in methanol. Transparent crystals formed over 3 weeks at 4°C. A crystal measuring 0.15mm x 0.2mm x 0.225mm was chosen for X-ray determination.

2.3.1.7 Butylciprofloxacin (BUCIP4)

10ml of 0.1μM methanolic $AlCl_3.6H_2O$ (Aldrich) was added to 30ml of 0.1μM methanolic butylciprofloxacin (a generous gift from Professor Teresa Garrigues, Valencia, Spain). The resultant mixture was refluxed under argon at 70°C for 4 hours and then dried *in vacuo* before being redissolved in methanol. Transparent sheet like yellow crystals formed over 2 weeks at 4°C. A crystal measuring 0.25mm x 0.125mm x 0.175mm was chosen for X-ray determination.

2.3.1.8 Nalidixic acid (NAL3XL)

10ml of 0.1mM methanolic $AlCl_3.6H_2O$ (Aldrich) was added to 30ml of 0.1mM methanolic nalidixic acid (Aldrich). The resultant mixture was refluxed under argon at 70°C for 4 hours and then dried *in vacuo* before being redissolved in methanol. Transparent crystals formed over 2 weeks at 4°C. A crystal measuring 0.275mm x 0.225mm x 0.175mm was chosen for X-ray determination.

2.3.2 Density determination of crystals

A specimen of each crystal was immersed in a mixture of the miscible liquids dichloromethane (density 1.325gcm^{-3}) and iodoethane (density 1.925gcm^{-3}). The quantities were adjusted until the specimen crystal exhibited neutral buoyancy in the mixture. The density of the crystal is then calculated as follows.

$$\text{density} = \frac{[1.325 \text{ x volume of dichloromethane (ml)}] + [1.925 \text{ x volume of iodomethane (ml)}]}{\text{total volume of mixture used (ml)}}$$

Equation 2.1

2.3.3 Determination of m.pt. via Differential Scanning Calorimetry (DSC)

Thermal characteristics of the crystals were performed using a Perkin-Elmer DSC-4 system for differential scanning calorimetry, using the Thermal Analysis Data Station (TADS) for data collection. Temperature calibration of the instrument was carried out using an Indium standard. Samples (2-10mg) were sealed into aluminium pans and DSC measurements were run from 25°C to 400°C against an empty pan. All tests were run under nitrogen at a flow-rate of 25cm^3 min^{-1}, heating rate of 10°C min^{-1} , and cool rate of 320°C min^{-1}. The primary aim of DSC measurements was to establish the m.pt. of the crystal samples, although the thermal profiles also confirm crystal characteristics.

2.4 COMPUTER AIDED DESIGN

2.4.1 Instrumentation

Chem-X (Chemical Design Ltd, 1994) mounted on a Silicon Graphics Iris Indigo workstation was used as an interface to the semi-empirical quantum mechanical program Molecular Orbitals Package, MOPAC version 6, as well as for the general manipulation, visualisation and conversion of file formats of structures in the North (nth) to Crystal Structure Search Retrieval (cssr) formats and vice versa. Examples of these file formats are listed in Appendix 1.

MOPAC version 6 (Stewart 1990) was used for semi-empirical optimisations in a solvent and single point calculations. General Atomic and Molecular Electronic Structure System, GAMESS (Schmidt, 1993) was mounted on a Sun SPARC station and used for all other semi-empirical and *ab initio* calculations.

2.4.2 Molecular Orbital (MO) Calculations

All structures entered into GAMESS or MOPAC calculations were extracted from the CSD if available. Those entered from the CSD were manually edited to remove all unnecessary molecules such as solvent. Where a structure was required for GAMESS MO calculations and was not available from the CSD, then the structure was manually constructed using Chem-X 3-D build, using different templates depending on the ring chelate system to be constructed. For a 5 membered system, the 3:1 Al oxalate structure was used as the template (COKFOX) and for a 6 membered system, the 3:1 Al acetylacetonate structure was used (ALACAC02). Structures involving seven membered systems were not constructed or used for MO calculations, as the CSD work shows few structures of this type indicating that perhaps these are unlikely to be energetically favourable.

2.4.2.1 GAMESS calculations

GAMESS was used for all semi-empirical and *ab initio* calculations unless otherwise stated. An example of an input file is listed in appendix A1. The following input cards were specified:

	Group	Input card	Additional information
1	CONTRL		a free format group specifying global switches
		SCFTYP = RHF	Restricted Hartree Fock Type (this is the default for even number of electrons
		ICHARG = 0	Molecular charge of test structure which is 0 by default
		RUNTYP = OPTIMIZE	Optimise geometry using analytical energy gradient
		COORD = CART	Cartesian co-ordinates are used for the input data
2	SYSTEM		This group provides global control information for the computers operation. Default options are used.
3	BASIS		This group allows certain standard basis sets to be used
		GBASIS = PM3	Selects PM3 model Hamiltonian
4	STATPT		This is an optional group that can be used in an 'optimise runtype'
		NSTEP	Maximum number of steps to take. A default value of 20 was overidden to 100.
5	DATA		Entered in the order of atom label, atomic number and x, y, z co-ordinates

TABLE 2.1 Keywords used in a typical GAMESS input job

2.4.2.2 GAMESS output data

The GAMESS output data gave an optimised geometry in the form of x, y, z Cartesian co-ordinates, as well as a final heat of formation, ΔH_{eff} and a final energy. For comparative purposes, PM3 MO calculations were performed on the 3:1 complexes as well as on the free ligand to produce an 'effective heat of formation' ΔH_{eff} and an 'effective energy', ΔE_{eff}. These were calculated using Equations 2.2 and 2.3 respectively.

$$\Delta H_{eff} = \text{PM3 calculated } \Delta H_f \text{ for } AlL_n - \left(\frac{\text{PM3 calculated } \Delta H_f \text{ for ligand, L} \times}{\text{number of ligands in complex, n}} \right)$$

Equation 2.2

$$\Delta E_{eff} = \text{PM3 calculated E for } AlL_n - \left(\frac{\text{PM3 calculated E for ligand, L} \times}{\text{number of ligands in complex, n}} \right)$$

Equation 2.3

2.4.2.3 Generation of molecular electrostatic potential maps (MEPmaps)

MEPmaps are contour maps of a molecular electrostatic potential grid. The GAMESS program produces the grid before MEPmap is run. The following changes/additions are implemented in the GAMESS input to generate a MEPmap.

	Group	Input card	Function
1	CONTRL	MOLPLT = .TRUE.	A flag that produces an input deck for a molecule drawing program
		RUNTYP = PROP	Replaces OPTIMIZE keyword. Used to calculate properties using the VEC command
2	ELPOT	ELPLOT IEPOT= 1	replaces the STATPT input card. Used to calculate electrostatic potential
3	ELDENS		This group controls electron density
		IEDEN = 1	Compute electron density
		WHERE = GRID	Compute electron density at a given grid using the GRID option
4	VEC		Orbitals calculated from previous optimisation

TABLE 2.2 Keywords used in a GAMESS input job to generate a MEPmap

The solid lines show net positive charge, while dashed lines show net negative charge. The units of the contour lines are kcal/mol. Therefore, negative contours outline where electrophilic reagents will prefer to attack a molecule, while positive contours show the preferred sites of nucleophilic attack.

2.4.3 Tools for Structure Activity Relationships Package (Tsar) (Oxford Molecular, Oxford, UK) similarity calculations

Tsar is an integrated analysis package for Quantitative Structure Activity Relationships (QSARs). It seeks to provide all the functions required to carry out QSAR investigations. The package provides functions that can be divided into the following:

1. Record keeping: Creates and maintains numerical and structural data.
2. Database functions: Creates, maintains, and searches database of substituent properties and structures.
3. Analysis: Application of statistical techniques to numerical data to detect and exploit QSARs, and for lead optimisation.
4. Property calculation and visualisation: Derivation of numerical property information.

For the purposes of these studies, Tsar was used for similarity calculations, using a lead molecule. Similarity calculations within this software enable the user to evaluate either the Carbo (Carbo, 1980) or Hodgkin (Hodgkin, 1987; Hodgkin, 1988) indices. Carbo introduced a similarity index to compare electron densities of two superimposed molecules.

$$R_{AB} = \frac{\sum_{i=1}^{N} (P_A P_B)}{\left(\sum_{i=1}^{N} P_A^2\right)^{1/2} \left(\sum_{i=1}^{N} P_B^2\right)^{1/2}}$$

Equation 2.4

where

N = total number of grid points

P_A = property being compared (such as shape) for molecule A at the i^{th} grid point.

The numerator is a measure of the overlap between the electron densities of the two molecules, and the denominator provides the normalising factor so that the index ranges from 0 to 1. Hodgkin proposed an alternative index H_{AB}.

$$H_{AB} = \frac{\sum_{i=1}^{N} (P_A P_B)}{\sum_{i=1}^{N} P_A^2 \sum_{i=1}^{N} P_B^2}$$

Equation 2.5

Meyer (Meyer and Richards, 1991) showed that the Carbo and Hodgkin formulae may be adapted to measure similarity in terms of molecular shape by means of a simple point calculating algorithm. Each molecule is represented as a system of interlocking spheres, radius equal to the van der Waals radius, centred on the atomic nuclei. The pair of superimposed molecules is placed in a 3-D grid and a mesh of points scanned. A count is made of

O_1 - the number of grid points lying within only molecule 1.

O_2 - the number of grid points lying within only molecule 2.

B - the number of grid points lying within both molecules.

Thus, the total number of grid points in each molecule is

$T_1 = O_1 + B$ and $T_2 = O_2 + B$. The point counting analogues of the Carbo and Hodgkin indices (equations 2.4 and 2.5) are

$$S_{12}^{C} = \frac{B}{(T_1 T_2)^{1/2}}$$

Equation 2.6

$$S_{12}^{H} = \frac{2B}{T_1 T_2}$$

Equation 2.7

Prior to similarity calculations, all structures whether manually constructed or extracted from the CSD were converted into the cssr format. These were in turn used as structure input files for subsequent Tsar calculations. Using the 'rigid fit' command in ChemX-3D, all structures were superimposed on the lead structure to ensure similar starting geometries for Tsar shape calculations. The exact points of

'rigid fitting' are discussed in the relevant sections. Where Tsar was being used to analyse optimised structures from GAMESS, the individual charges calculated for each input atom were manually edited into a cssr input file. Where 3:1 complexes were being compared, bonds were drawn between the central Al ion and the donating atoms to ensure Tsar accepted the structure as a single fragment.

2.5 OPTIMISATION OF MORIN AL ASSAY

Glassware has been found to contribute Al in samples probably by leaching Al as aluminosilicates, (McDermott, 1976) therefore all glassware was soaked in 2M nitric acid, and then rinsed with d/d water prior to use.

Reagents including acids used in subsequent studies involving Al analysis, were passed through an acid form Chelex 100 column (BioRad) to minimise possible Al contamination.

2.5.1 Calibration

100μL samples of varying concentrations (0.283 – 11.333μg mL^{-1}) of Al as lactate or chloride samples were mixed thoroughly with 3mL of a 10% stock morin (figure 2.3). The resultant mixture was left for 30 minutes before fluorescence measurements were taken on a Perkin Elmer Luminescence spectrophotometer LS50 as described in section 2.5.2.

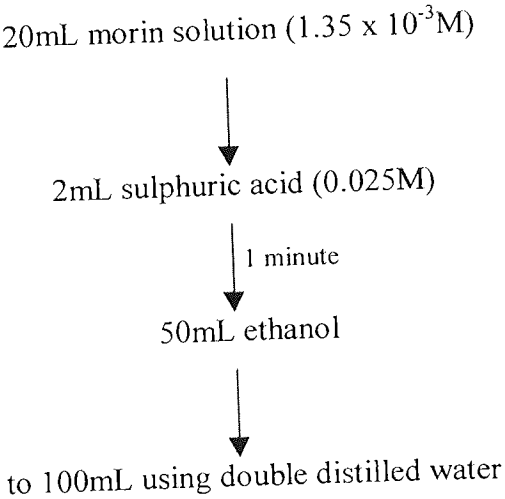


FIGURE 2.3 Diagrammatic representation of reagents used to make up morin stock solution prior to fluorescence measurement

The morin solution was stored in an amber bottle and stored for a maximum of 72 hours.

2.5.2 Quantitative fluorescence measurements

100μL Al samples were thoroughly mixed with 3mL of 10% morin stock solution. The mixture was allowed to stand at room temperature in the dark for one hour prior to fluorescence measurements. All quantitative fluorescence measurements were performed on a Perkin Elmer Luminescence spectrophotometer LS50 using 'the fluorescence data manager manual' (FLDMM) interface. 3mL samples of Al:morin were placed in fluorescence quartz cuvettes prior to insertion in the spectrofluorimeter (section 2.5.1). Default values were used for measurement except for the excitation and emission wavelengths that were set at 421 and 510nm, values established to be the optimum in prior scans of Al free and Al:morin solutions.

2.5.3 Atomic absorption spectroscopy (AAS)

All AAS work was undertaken on a Varian SpectrAA 300/400 graphite furnace spectrometer (Toxicology Dept, City Hospital, Birmingham, UK) purged with nitrogen gas. Samples were made up using a matrix consisting of 50% Al sample and 50% 2M nitric acid. 5μL aliquots of the resultant matrix samples were injected into the spectrometer and each sample was measured three times at a wavelength, λ of 309.3nm.

The furnace parameters listed in Table 2.3 were found to give optimal analysis.

TABLE 2.3 Furnace parameters used for Al analysis via AAS

Step number	Temperature (°C)	Time (sec)
1	90	5
2	100	25
3	140	10
4	700	15
5	1000	17
6*	2500	1.8
7	2500	3

* absorption reading taken at this step

2.6 MICROBIOLOGY

2.6.1 *Escherichia coli* W3110 (*E. coli*) and storage

E. coli was obtained from the Aston Microbiology Research Group culture collection. This strain does not produce the siderophores, enterobactin and aerobactin which may complicate studies involving Al transport. Long term storage of this strain was at -70°C. Short term storage involved the plating *of E. coli* onto nutrient agar (NA) (Oxoid Ltd) plates and storing at 4°C for a maximum of 4 weeks.

2.6.2 Determination of growth curves of *E. coli*

Growth experiments were conducted using an *E. coli* inoculum taken from a culture stored at 4°C. This inoculum was suspended in 50mL of nutrient broth (NB) (Oxoid Ltd) and allowed to grow to stationary phase at 37°C. 1mL of this culture was resuspended in 50mL of NB in culture flask at 37°C and shaken at 120 throws per minute. The optical density (OD) of this culture was taken at relevant time intervals.

The growth of a culture can be determined by measuring the turbidity of the inoculum using OD measurements. Koch (1961) showed that the total amount of light scattered is directly proportional to the ratio of cell size to the wavelength of incident light. Accordingly, a wavelength of 470nm was chosen for OD measurements (OD_{470nm}).

2.6.3 Measurement of OD

OD measurements were undertaken using two different measurements dependent on the experimental conditions. Studies utilising 96 well ELISA plates involved the use of an Anthos 2001 plate reader, and all other OD measurements were undertaken on a Pye Unicam SP6-400 spectrometer using 1mL plastic cuvettes. All OD studies involved the measurement of a sterile reference that was subsequently subtracted from sample OD values.

Correlations were achieved by seeding *E. coli* at varying concentrations with measurement OD at 470nm relative to a sterile blank reference.

2.6.4 Influence of Al on antibiotic loaded neo-sensitabs

200mL of NA was sterilised via autoclave. Whilst warm and liquid, varying amounts of sterile $AlCl_3.6H_2O$ was added ranging from 0-10mM (sterilised by passage through a 0.47μm cellulose acetate filter) to each sample plate. This Al doped NA was allowed to set on a 243 x 243 x 18mm bioassay dish (BioRad) prior to surface inoculation with *E. coli*. Neo-sensitabs doped with antibiotics were placed on the surface in a Latin square pattern. These plates were incubated at 37°C, after which the zones of inhibition were measured.

2.6.5 Determination of minimum inhibitory concentration (MIC) for ciprofloxacin on *E. coli*

Varying volumes of ciprofloxacin resulting in final concentrations ranging from 0.1 to 100μM were made up in sterile NB. 200μL was added to each well in a 96 well plate. This was placed in the plate reader described in section 2.6.3 pre-programmed to maintain temperature at 37°C, and to take OD measurements every 15 minutes following vigorous shaking.

2.6.6 Determination of Al in microbial cells

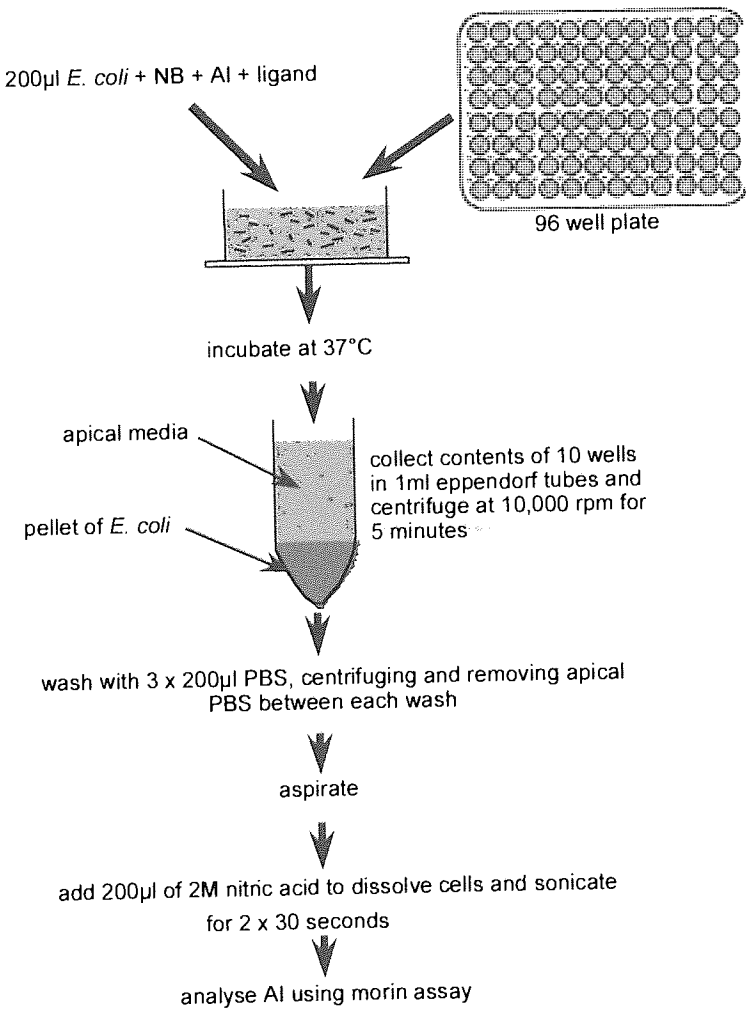


FIGURE 2.4 Schematic representation of procedure used to scavenge pre-treated *E. coli* cells ready for Al analysis

2.6.7 Microscopy and photography

A Jenamed fluorescence microscope (Jena Instruments, Oberkochen, Germany) and a high pressure mercury HBO-50 light source (C-Z Scientific, Basingstoke, UK) were used to visualise cell associated fluorophores. For fluorescence microscopy, a filter mounted in a mechanical cube positioned above the objective lens of the microscope to permit rapid switching of the filters and allow images of the fluorescence.

The technique of fluorescence microscopy was used to investigate the influx of Al into *E. coli* cells. After the required incubation period of the *E. coli* in 100μM Al doped NB, a 1mL sample was extracted and centrifuged at 10,000 rpm for 52 minutes. The resultant pellet of *E. coli* was washed three times in double distilled water as described in previous sections. A sample was placed on a slide and fixed by passing over a flame. An ethanolic 2mM morin solution was added dropwise onto the microscope slide ensuring all the *E. coli* were coated. The sample was left in the dark for 5 minutes before being washed by a stream of d/d water. The slide was then examined by fluorescence microscopy.

Cells were photographed using an Olympus camera with a Jenamed adaptor and Kodak Gold (colour), or a Konika (colour) 35mm film.

2.7 CELL LINE AND CULTURE TECHNIQUES

2.7.1 U87-MG Cell line

U87-MG human glioblastoma cells, derived from a grade 3 malignant glioma by the explant technique (Ponten and McIntyre, 1968), were obtained from the European Collection of Animal and Cell Cultures (ECACC), Porton Down, UK. U87-MG cells were maintained at 37°C, in a 5% CO_2 atmosphere, in Dulbecco's Modified Eagle's medium (DMEM) containing 10 % v/v *mycoplasma*-screened Foetal Calf Serum (FCS), 1% v/v penicillin / streptomycin and 2mM L- glutamine (All supplied by Life Technologies Inc, UK). Cells were maintained in 75 cm^3 flasks (Falcon, UK) containing 30mL maintenance media. Cells were passaged every 4 days by diluting 1 to 5 with fresh maintenance media. To passage, the cells were washed with sterile PBS and trypsinised with 2% trypsin PBS/EDTA (all abbreviations are listed in list of abbreviations).

Where U87-MG cells were grown on cell culture plates, the cell number was first determined as described in section 2.7.1.2 and 2.7.1.3. Cells were diluted to the appropriate count per millilitre using maintenance media. U87-MG cells were seeded at 5.0 x 10^4 cells per 2mL per well in 24 well plates when used for cell viability studies via the trypan blue exclusion assay (section 2.7.1.3). This produced 70-80% confluent cell cultures after 24 hours, when cells were used for association studies.

The number of cells seeded in multiwell cell culture plates was determined using a Neubauer haemocytometer as described in sections 2.7.1.2 to 2.7.1.4, and diluting to the required concentration. For cell association studies, U87-MG cells were seeded at 5.0 x 10^4 cells/mL in 96 well plates (Costar, Cambridge, MA, USA) unless otherwise stated, resulting in 70-80% confluent cell cultures after 24 hours.

2.7.1.1 Long Term Storage of Cells

All cell lines were prepared for long time storage by trypsinising a semi-confluent culture in a 75cm^2 flask with 2ml trypsin (2% v/v) in PBS / EDTA (0.2% w/v EDTA in PBS, pH 7.2) and neutralising with 10ml DMEM. The cells were pelletted by centrifugation at 1,000 rpm for 3 minutes (Mistral 3000 1 centrifuge, Sanyo MSE, Leicester, UK). The supernatant media was removed and the cell pellet was re-suspended in 1ml DMEM containing 90% v/v FCS, and 10% DMSO in a 2ml screw capped cryo-vial (Costar, Cambridge, MA, USA). The cells were frozen slowly at –70°C before transfer to a liquid nitrogen storage vessel at –196°C. Rapid thawing at 37°C and gradual dilution recovered the cells with media. The cells were pelletted and resuspended in media before seeding in 25cm^2 flasks.

2.7.1.2 Determination of Cell Number

The cell density was determined using the counting chamber of a Neubauer haemocytometer (Weber Scientific International Ltd, UK). Cells were removed from culture flasks with 2ml trypsin (2% v/v) in PBS / EDTA (0.2% w/v EDTA in PBS), pH 7.2) and diluted to 10ml with PBS. The cells were immediately pelletted by centrifugation at 1,000rpm for 3 minutes in Mistral 1 centrifuge tubes (MSE Ltd, Crawley, UK). The supernatant was removed and the cell was re-suspended in 10ml of media. The counting chamber of the haemocytometer was filled with a small aliquot of cell suspension. The hemocytometer was placed under the light microscope and the cell number was determined by obtaining the mean count per large square on the haemocytometer. The mean count value indicated the number of cells x 10^4 present in the sample per mL.

2.7.1.3 Determination of viable cell number by trypan blue exclusion assay

Cell viability was measured using a trypan blue exclusion assay. Cells were washed with PBS and 100µl of trypan blue (4mg/ml) was mixed with 400µl of re-suspended, trypsinised cells and counted as described in Section 2.7.1.2. Live cells exclude trypan blue, whereas non-viable cells are stained by trypan blue, hence can be identified when viewed under the microscope.

The mean total amount count of viable cells per square and the total mean cell count (viable and non-viable) can be used to calculate the number of viable cells per mL and the percentage of viable cells:

Viable cells per mL = mean viable count per square x 10^4 x 1.25 (dilution factor)

Equation 2.6

% Viable cells = mean viable cell count / total cell count x 100

Equation 2.7

2.7.1.4 Determination of Viable Cell Number by the MTT Assay

Traditionally, the *in vitro* determination of toxic effects of unknown compounds has been performed by counting viable cells after staining with a vital dye such as trypan blue. The MTT system is a means of measuring the activity of living cells via mitochondrial dehydrogenase. The key component is 3-[4,5-dimethylthiazol-2-yl]-2,5-diphenyl tetrazolium bromide (MTT). Solutions of MTT, dissolved in medium without phenol red are yellowish in colour. Mitochondrial dehydrogenase of viable cells cleaves the tetrazolium ring, yielding purple formazan crystals that are insoluble in aqueous solutions. The crystals can however be dissolved in dimethylsulphoxide (DMSO). The resulting purple solution is spectrophotometrically measured at a wavelength of 570nm (OD_{570nm}). An increase or decrease in cell number results in a concomitant change in the amount of formazan formed, indicating the degree of cytotoxicity caused by the test material.

MTT was at a concentration of 5mg/mL in PBS and stored at 4°C and kept for no longer than two weeks. Prior to use, the apical medium in each well was aspirated and 200µL of 5% MTT solution (made up using serum free/phenol red free media) was added to the monolayer of each well, which was then incubated for 4 hours at 37°C. Again the apical medium was aspirated and discarded and 100µL of DMSO was added to dissolve the crystals formed. The plate was vibrated on a Dynex Revelation 3.04 plate reader prior to reading the OD_{570nm}.

The principal advantage of the MTT assay is that the method of monitoring is well suited for use with a 96 well plate.

2.7.2 Al delivery studies in U87-MG cells

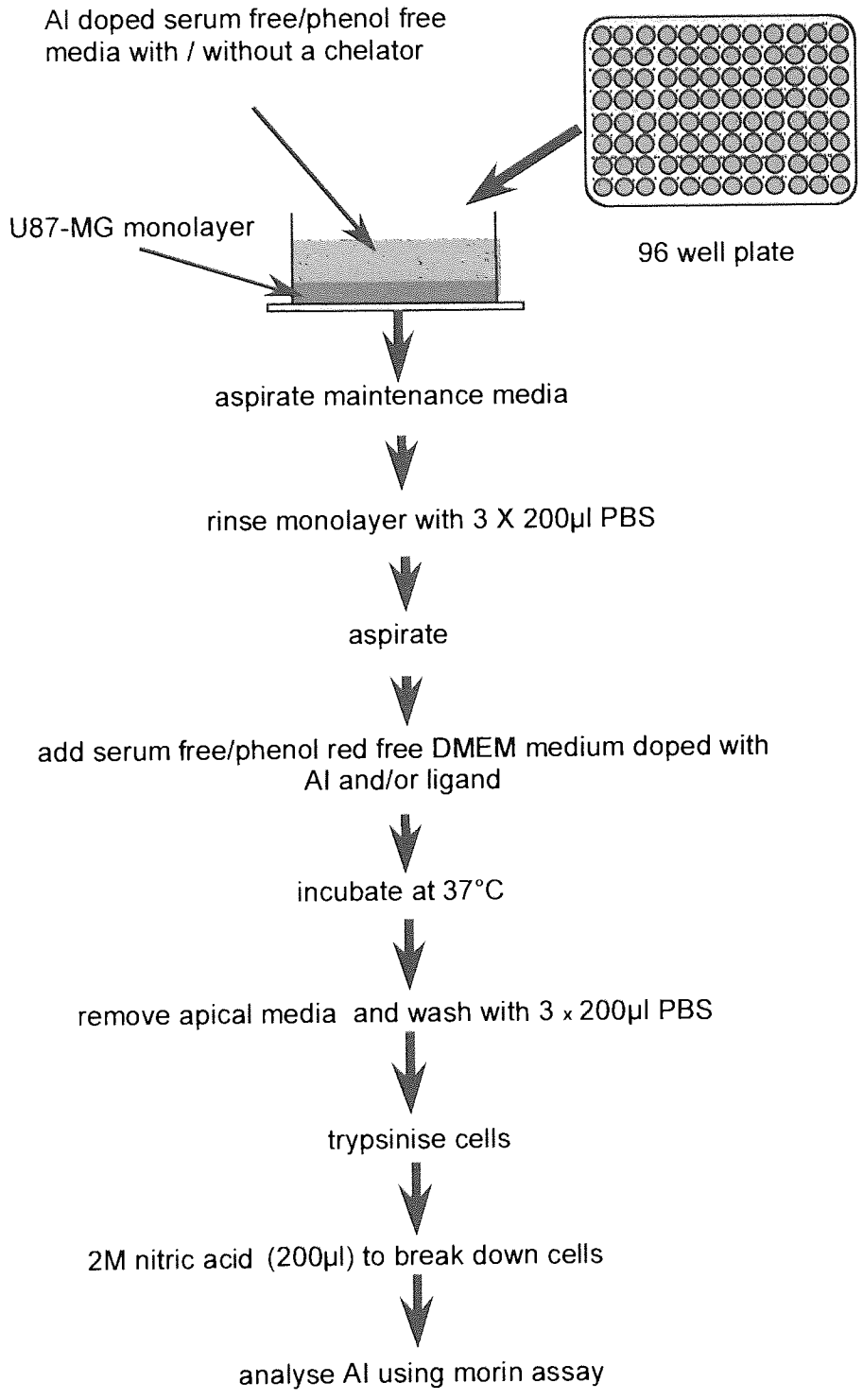


FIGURE 2.5 Schematic representation of procedure used to scavenge pre-treated U87-MG cells ready for Al analysis

2.7.3 Assessment of the effect of temperature on cell delivery of Al lactate

To assess the effect of temperature on the delivery of Al into cells, studies were performed as described in section 2.7.2 at 37°C, in parallel with additional experiments at 4°C. For the low temperature experiments the method was amended as follows: After the required growth period, cells in 96 well plates were washed three times with 200μL sterile PBS (at 4°C) for 15 minutes. The media was removed and Al lactate (100μM) in serum free/phenol red free medium (at 4°C) was added to each well and incubated for the required time period at 4°C.

2.7.4 Assessment of the effect of metabolic inhibitors on cell delivery of Al

To assess the effect of metabolic inhibition on the delivery of Al lactate into U87-MG cells, the cells were pre-treated with sodium azide and 2'-deoxyglucose, which reduce cellular adenosine tri-phosphate (ATP) production by more than 60%, as described by Wu-Pong *et al.*, (1992). Serum free/phenol red free media containing 10mM sodium azide and 50mM 2-deoxyglucose were prepared and warmed at 37°C. Following initial washing of the cells with sterile PBS as described in section 2.7.2, cells were pre-treated for 30 minutes at 37°C with media containing the metabolic inhibitors. The medium was removed and 200μL of 100μM Al lactate doped serum free/ phenol red free medium containing inhibitors was added to the wells and the cell delivery experiments were continued as in section 2.7.2.

CHAPTER THREE

THE CAMBRIDGE STRUCTURAL DATABASE

3.1 INTRODUCTION

3.1.1 Overview of the Cambridge Structural Database (CSD)

The Cambridge Crystallographic Data Centre (CCDC) builds and maintains the Cambridge Structural Database (CSD), the largest searchable database of experimentally determined crystal structures. To date there are 190,000 entries with approximately 10,000 new entries being added each year, comprising of organic, organometallic compounds, and metal organic complexes. Proteins and inorganic structures are held in the Protein Databank (PDB) and the Inorganic Crystal Structural Database (ICSD). In general, the structures discussed in this thesis (Chapter 4) are organic with the exception of aluminium chloride hexahydrate, hence this chapter will be concerned with the CSD.

All information submitted to the CSD is subject to computerised check, evaluation procedures and thorough visual proofing to ensure it is of the highest possible factual standard. Table 2.1 shows the quality of crystal data within the CSD.

TABLE 3.1 Quality of data within the CSD

R value (discrepancy factor)	Description	% abundance
1-3	Exceptional	6.6
3-4	Very high	16.5
4-5	High	20.0
5-7	Good	28.7
7-9	Average	13.1
9-10	Fair	3.5
10-15	Poor	6.3
>15	Bad	1.6
Not reported	-	3.0

Thus, some 72% of the CSD entries would be judged as of good precision or better in terms of crystallographic data ($R < 7\%$). A further 17%, making a total of 89% with $R < 10\%$, would be judged as adequate for most molecular modelling applications.

A reference code (refcode), which identifies the chemical compound (the first 6 letters) and its publication history (last two digits) describe each entry in the CSD. The 1st digit refers to the publication history of each study by a given research group, 0 indicates the initial paper, 1 and 2 would indicate later publications. The 2nd digit identifies supplementary studies of the compound, such as those undertaken by a different research group, in a different polymorph, using different radiation, temperatures etc.

The information content of each entry can be conveniently summarised by the 3 major subdivisions:

1. 1-D information which consists of bibliographic and chemical text strings and individual numerical items.
2. 2-D chemical connectivity comprising a complete representation of the formal chemistry of the molecule(s) and ion(s) that constitute the crystal structure.
3. 3-D molecular and crystal structure in the form of x, y, z co-ordinates, space group symmetry, cell parameters etc., that provide geometrical and visual representations.

In these studies, crystal structures are cited using the refcodes allowing easy access via the CSD. Where a particular crystal structure is deemed particularly of interest, citations in the usual way as well as the refcodes are noted.

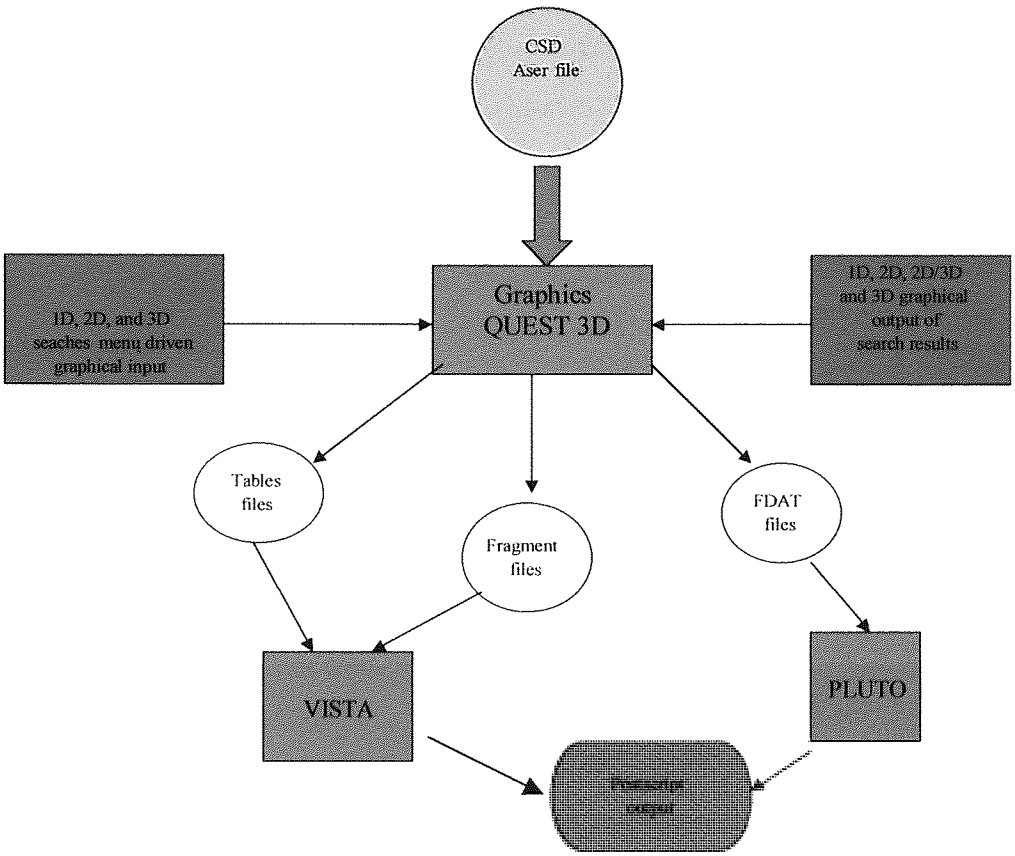


FIGURE 3.1 CSD graphics software system

3.1.2 3-D Database searching in Drug Design

Molecular modelling and protein structure determination are now a major part of any medicinal chemistry investigation (Cohen, 1990). Since 1980, 3-D quantitative structure activity relationship (QSAR) methods for the prediction of potency based on 3-D properties have been developed (Hopfinger, 1980; Kati, 1987; Cramer, 1988; Doweyko, 1988; Boulu, 1990). Additionally, 3-D searching allows design or recognition of potential bioactive molecules (Martin, 1990) and identifies existing molecules that match a hypothesis of the 3-D requirements for bioactivity. It thus can be used to validate such pharmacophores and to suggest other existing compounds for testing to find a new lead. Database searching is complementary to 3-D quantitative structure activity relationships (QSAR) (Cramer, 1988) since it can be used to design series for 3-D QSAR analysis and 3-D QSAR can be used to rank compounds suggested for synthesis or testing by 3-D searching. (Lin, 1988).

Typical geometric parameters calculated from the 3-D structure of a database molecule include:

1. Points located at a) the nucleus of an atom or centre of a lone pair, b) centre of mass of several atoms, c) projected binding points such as charged groups.
2. Lines either between two points or produced as a least squares line calculated from more than two points.
3. Planes calculated from three points or produced as a least squares plane calculated from more than three points.

3.2 AIM

To review the trends in binding characteristics between ligands with Al and other trivalent metal ions, especially the ferric ion, Fe^{3+}, as it has been reported that all ligands that bind Fe will also bind Al (Yokel, 1994). Al is essentially a 'hard' Lewis acid (section 1.4), thus it is expected that preferential binding would be to the relatively hard donor atoms, although binding to borderline or even 'softer' donor atoms also occurs, such as hydrogen, sulphur and phosphorus. Of the harder donor atoms, the halogens will only form monodentate complexes, consequently only the possibilities of N and O as donor atoms will be considered in this study. Ultimately binding trends of Al can be used as the basis for validation of semi-empirical and *ab initio* calculations performed in the following chapters.

3.3 CO-ORDINATION CHARACTERISTICS OF Al AND OTHER TRIVALENT CATIONS

A metal ion was constructed in QUEST3-D and using the 2D constraints a co-ordination number and charge of +3 was specified (in the case of Fe, Co and Cr where more than one oxidation state is possible) as described in section 2.2.

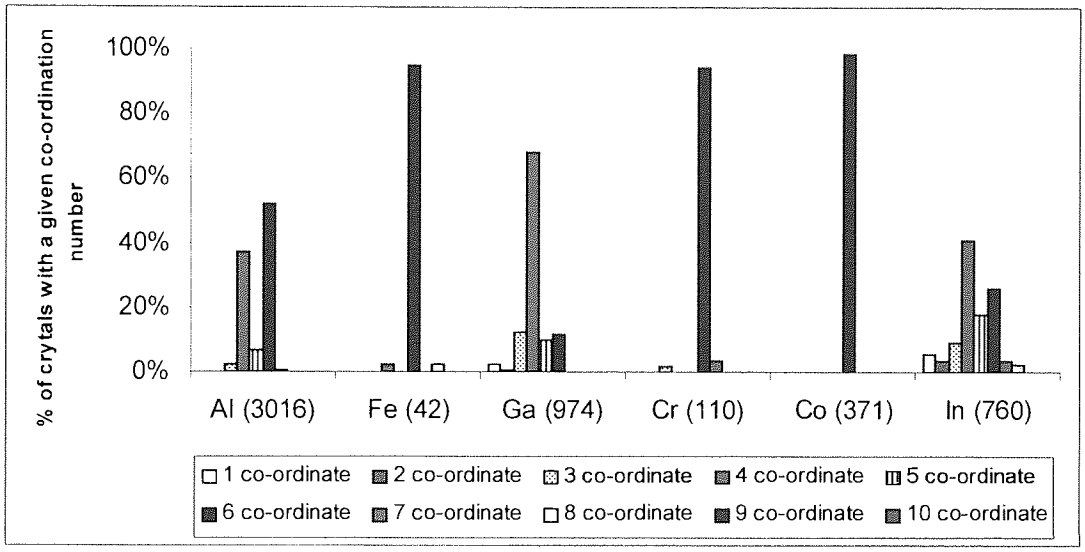


FIGURE 3.2 Range of co-ordination numbers for crystal structures of various trivalent metal cations found within the CSD. Figures in parentheses show total number of hits

A wide range of co-ordination was found for the trivalent metal ions, six being the preferred coordination number, with the exception of Ga and In. Al has co-ordination numbers ranging from 3 to 9, with co-ordination numbers of 4 (sp^3 hybridised) and 6 (d^2sp^3 hybridised) making up 88% of all 3016 Al crystals within the CSD. Fe is dominated by a co-ordination of 6 (d^2sp^3 hybridised), with single hits being found for Fe crystals with a co-ordination number of 4 (KENZAE) and 8 (ZOYYIV).

3.4 POLYMERIC SPECIATION OF Al AND Fe CRYSTALS WITHIN THE CSD

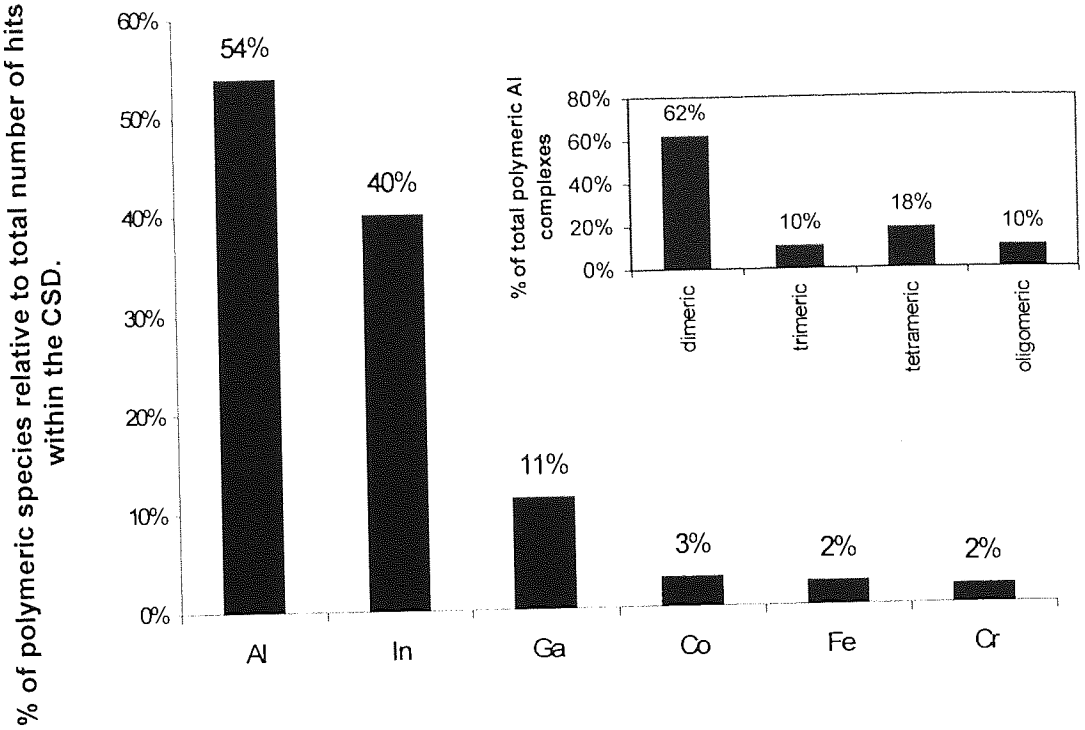


FIGURE 3.3 Percentage polymeric species relative to total number of crystals within the CSD for trivalent metal ions. Inset shows relative abundance of polymeric species for Al. (The term oligomeric within the inset is used to describe pentameric species and above)

Al shows a higher degree of polymerisation relative to the other trivalent metal ions studied. This fact has already been attributed to the Al ion (Motekaitis, 1984) and put forward as a reason for the lack of stability constants measured for these types of complex. The inset in figure 3.3 shows a classification of the polymeric species for Al, showing dimeric and tetrameric species to be the most common. Several types of bridging occur within the Al compounds that exhibit dimerisation. This may be due to direct Al-Al binding as in $[Al(II)Br_2]_2$ (Mocker, 1994) which possesses an unusually small Al-Al distance of 2.527(6)Å. There are also examples where the Al

atoms are bridged by single oxygen atoms (Gurian, 1991; Kliebisch, 1986; Eley, 1961; Wynne, 1985), single bromide ions (Rytter, 1975; Rytter, 1973) and single chloride ions (Couch, 1972; Troyanov, 1995; Stollmaier, 1981).

As previously mentioned (section 1.4), Fe and Al have similar ionic radii, and tend to bind to similar ligands. Hence the remainder of this chapter concentrates on these two metal ions as hexa co-ordinated species, the most common co-ordination found within the CSD for both metal ions (Figure 3.2).

3.5 DONOR ATOMS INVOLVED IN COMPLEXATION OF HEXA CO-ORDINATED Al AND Fe CHELATES

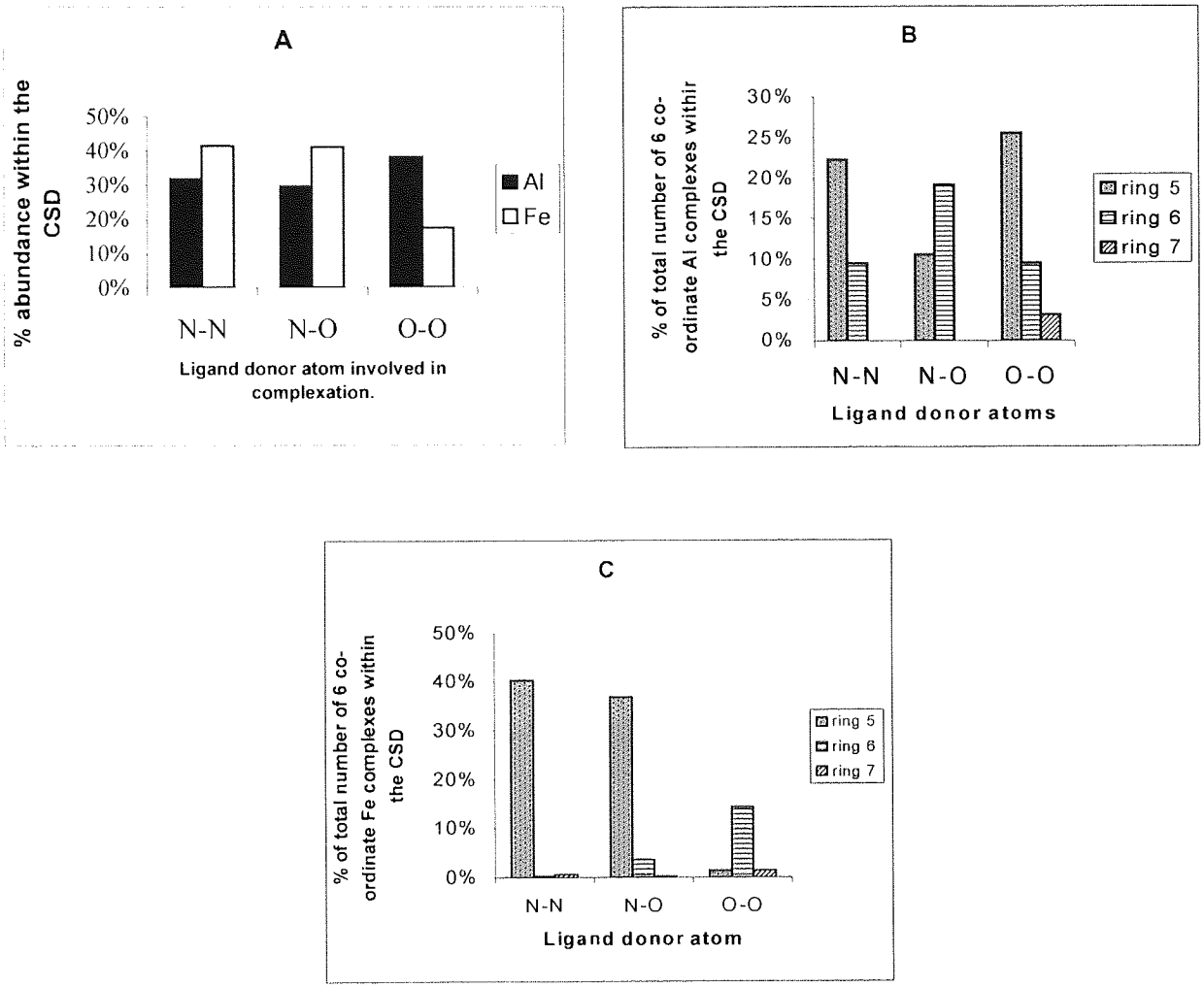


FIGURE 3.4 Abundance of Al and Fe hexa co-ordinated complexes within the CSD (A). Speciation of hexa co-ordinated complexes into 5, 6, and 7 membered chelate ring systems for Al (B) and Fe (C)

When oxygen is the exclusive donating atom Al predominates as a 5 membered chelate system as opposed to a 6 membered chelate system that is the most abundant for Fe. Where nitrogen atoms are the exclusive donors, Fe predominates as a 5 membered system. Figure 3.4A shows Al preferentially binds to bidentate ligands where oxygen are the exclusive donating atoms with approximately 40% of all CSD

hits. Fe on the other hand, clearly has a preference for binding with bidentate ligands possessing at least one nitrogen atom at the ligating site.

3.6 GEOMETRIC COMPARISON OF IDENTICAL COMPLEXES OF Al AND Fe WITHIN THE CSD

To ensure differences in geometry were a result of the central cation, and not merely to differences in ligand structure, studies using isomorphous complexes of desferrichrome and acetylacetonate were undertaken. This study was conducted using identical complexes of alumichrome A and ferrichrome A (van der Helm, 1981), differing only by their central ion. Complexes of Al and Fe acetylacetonate (Rahman, 1990; Kabak, 1996) were also compared to illustrate that the trend seen is independent of the chelate ring size.

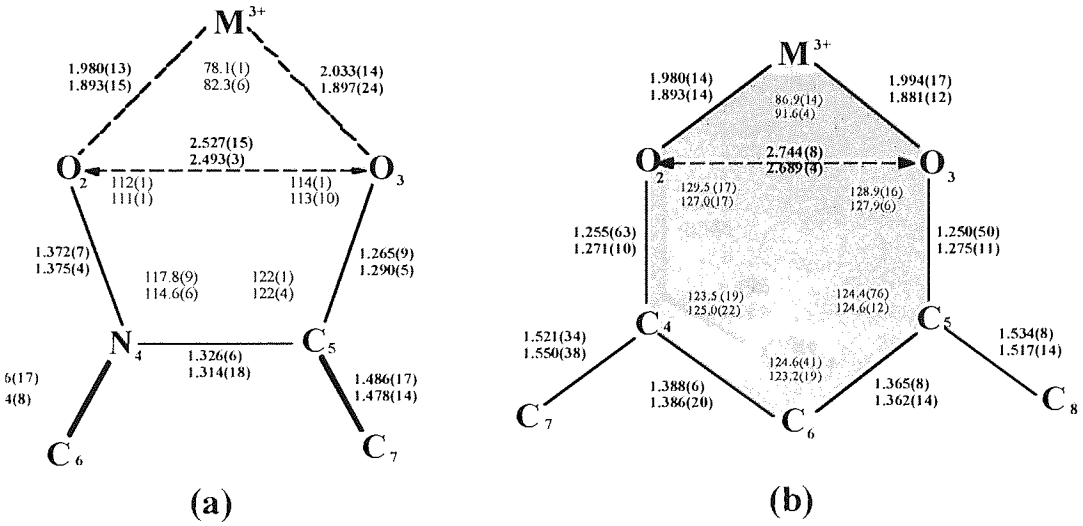


FIGURE 3.5 5 and 6 membered chelate systems of identical complexes of Al and Fe highlighting the geometric differences (a) alumichrome A (ALUMIC10), ferrichrome A (ALFECB) and (b) Al and Fe acetylacetonate (ALACAC02 and FEACAC02 respectively). Mean bond distances (Å) are shown in bold. Upper and lower numbers represent Fe and Al geometries respectively (n = 3, ±SD)

Complexation involving desferrichrome occurs in a hexadentate manner, forming three chelate rings within the complexes as depicted in figure 3.5a. Acetylacetonate binds in a bidentate fashion resulting in a 3:1 complex possessing 6 membered chelate rings (3.5b). Both structures (figures 3.5a and 3.5b) were chosen for this analysis, as both left and right sides of the metal ions within the complex are chemically equivalent. The Fe-O bond distance is significantly larger than the Al-O bond distance resulting in a lower bite angle for the Fe complex. Statistically significant differences ($P < 0.05$) can also be seen in N-C and O-C distances.

3.7 Al COMPLEXATION INFLUENCE ON BOND LENGTHS OF LIGAND

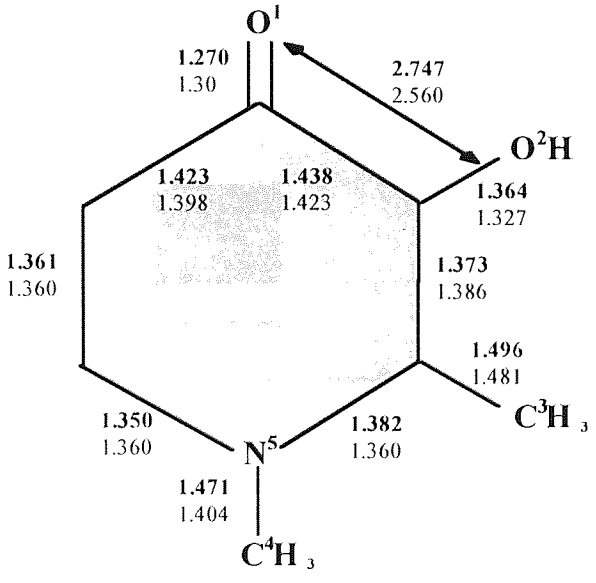


FIGURE 3.6 Bond lengths of crystal structures of 3-hydroxy-1,2-dimethylhydroxypyridinone (FIMLOC10) (Nelson, 1988) and its 3:1 Al complex (GALDEC01) (Hider, 1990).Top and bottom numbers shows distances in Å of free ligand and complex (n = 3, mean) respectively

Figure 3.6 shows the influence of the tripositive Al ion on the ligand. Complexation significantly reduces most of the bond distances, in particular the exocyclic bonds. The distance O_1-O_2 is reduced from 2.747Å on the free ligand to 2.560Å in the 3:1 complex, a bite distance typical of Al complexes.

3.8 EFFECT OF Al ON PROTONATED LIGANDS

To establish if the highly charged Al ion would cause a ligand to become deprotonated upon complexation, a CSD search was undertaken as described in section 2.2.3.

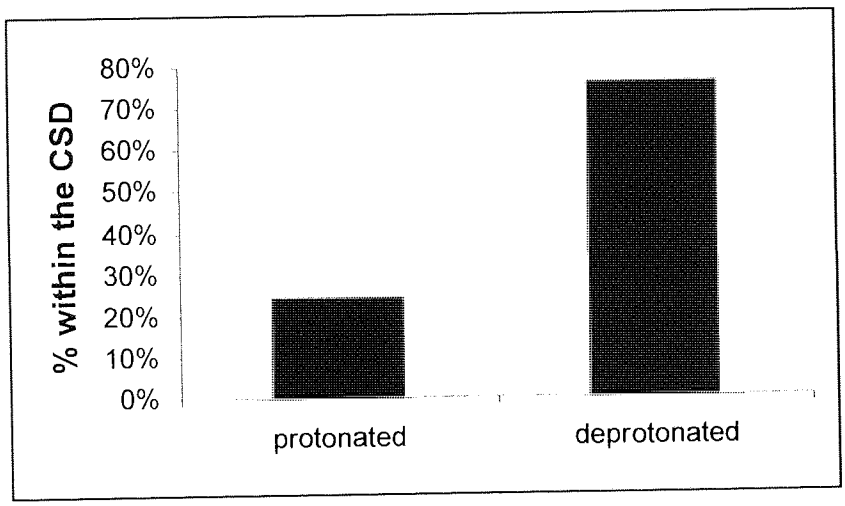


FIGURE 3.7 Six co-ordinate Al complexes with oxygen donor atoms showing protonated and deprotonated species

Of the total of 161 Al complexes investigated, 39 (24%) were protonated in at least one of the donating sites, the remaining 122 (76%) structures were deprotonated. Al ions possess a charge of +3 and a relatively small ionic radius of 0.54Å, consequently exhibit a high positive charge density. As a result any positively charged species such as protons will be strongly repelled which may in the majority of cases result in dissociation of the proton from the ligand..

3.9 OVERVIEW OF GEOMETRIES OF Al AND Fe CRYSTALS WITHIN THE CSD

Geometric differences between identical complexes of Al and Fe have been discussed in the previous section (3.6). This study aims to illustrate that this trend is followed throughout crystals of these metal ions.

3.9.1 Metal-donor (M-D) distances for hexa co-ordinated complexes of Al and Fe

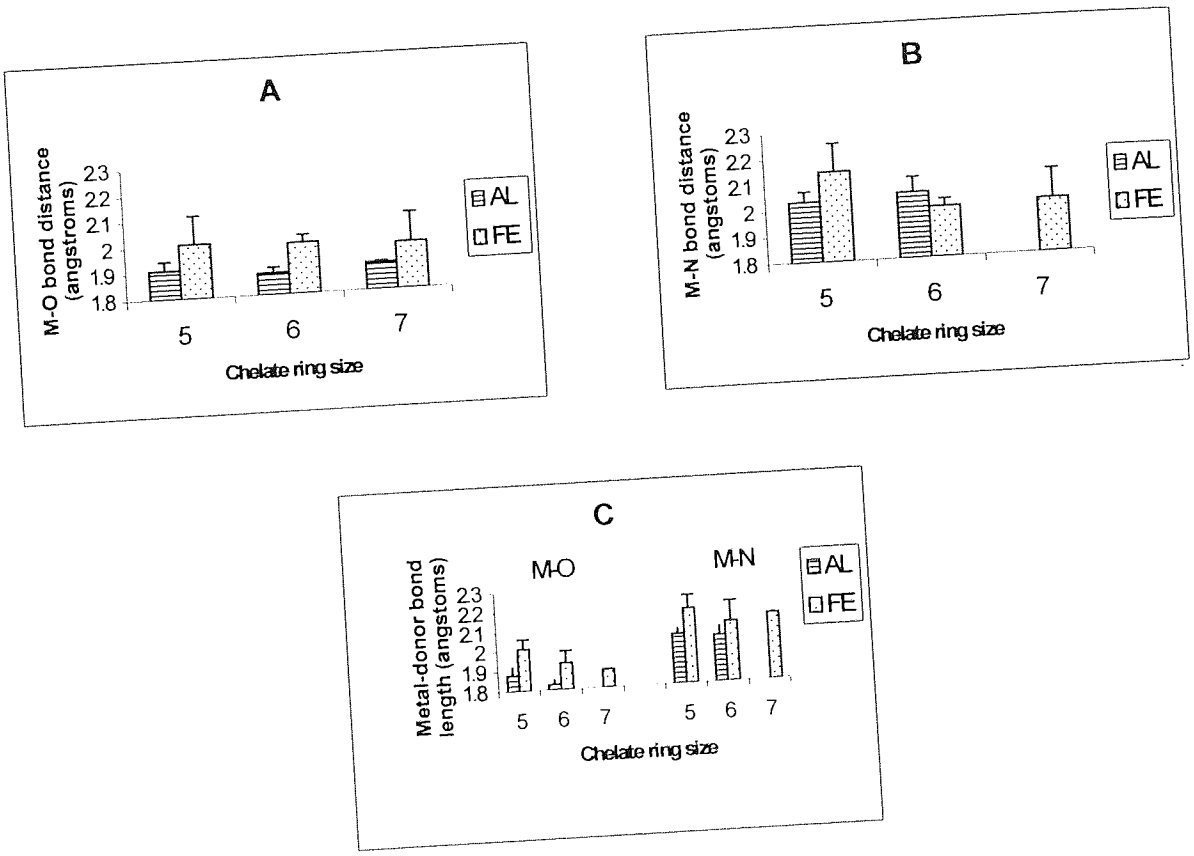


FIGURE 3.8 Bond distances for hexa co-ordinated Al and Fe complexes extracted from the CSD. (A) with O as donor atoms, (B) with N as donor atoms and (C) with N and O as the donating atoms

M-D distances tend to be minimal when a 6 membered chelate system is formed for Al complexes when O is the sole donor atom and N is the exclusive donor for Fe complexes. Complexes involving both O and N donor atoms (represented as D) show no apparent trend with the exception of the M-O distance decreasing with increasing chelate ring size for Fe complexes.

3.9.2 Bite angles and distances for hexa co-ordinated Al and Fe complexes

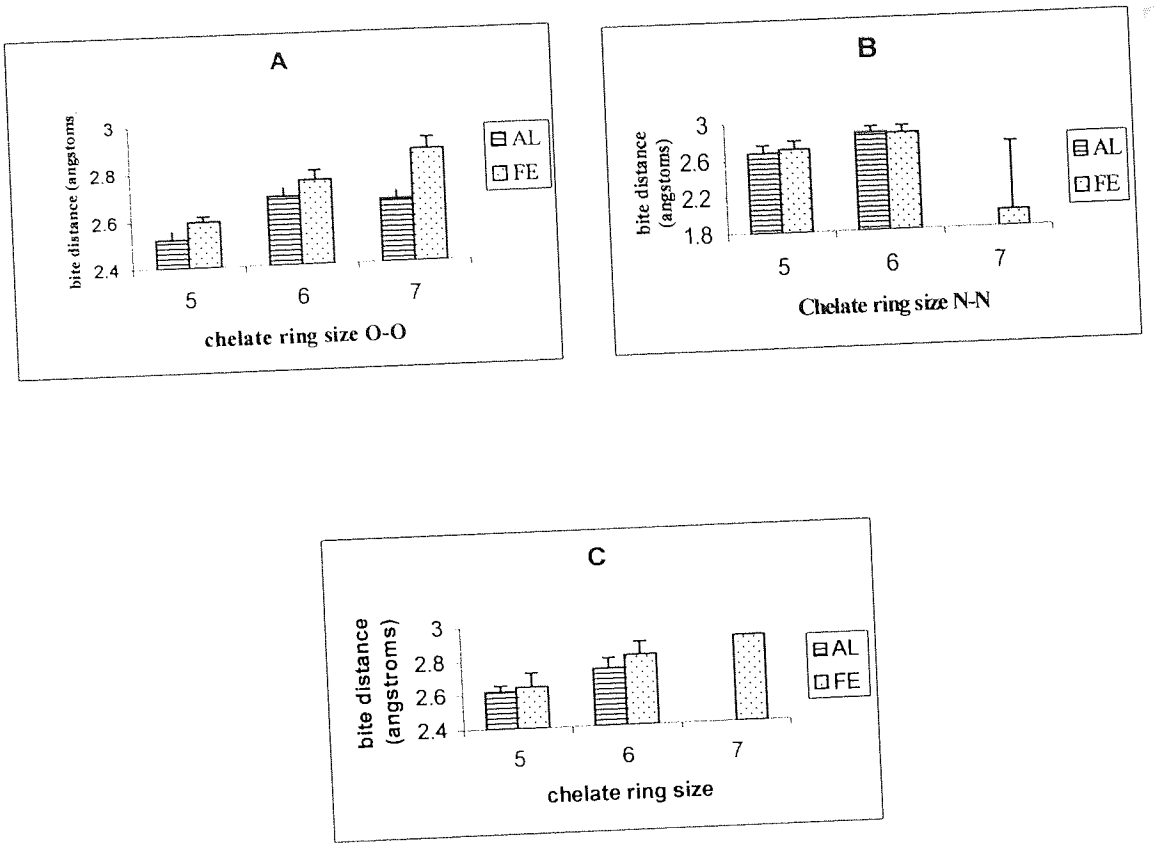


FIGURE 3.9 Bite distances for hexa co-ordinated Al and Fe complexes extracted from the CSD. (A) with O as donor atoms, (B) with N as donor atoms and (C) with N and O as the donating atoms

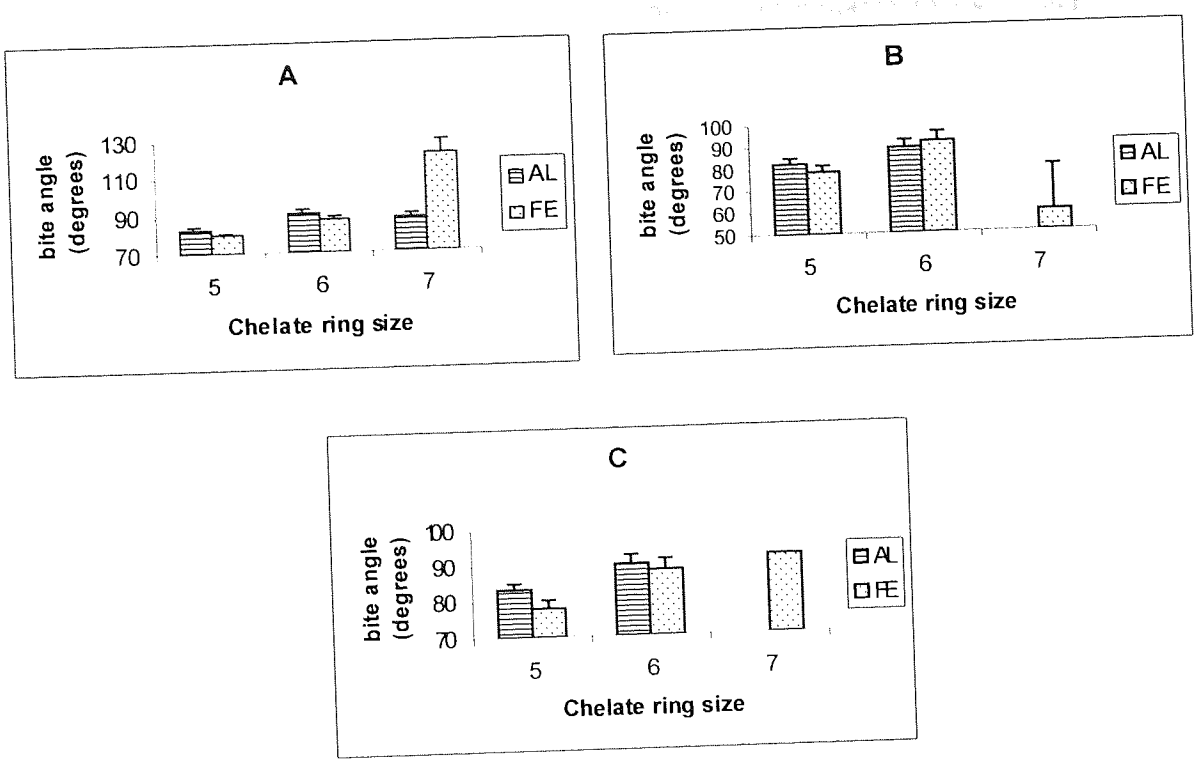


FIGURE 3.10 Bite angles of hexa co-ordinated Al and Fe complexes extracted from the CSD. (A) with O as donor atoms, (B) with N as donor atoms and (C) with N and O as the donating atoms

Figures 3.8 and 3.9 highlight differences in trends of bite angles and distances exhibited by Al and Fe complexes. Fe complexes involving O donor atoms show that as the chelate ring size increases, an increase in bite distance and consequently bite angle also occurs. In all cases 6 membered chelate systems produce bite angles closest to 90°, the ideal angle for octahedral geometry (Cotton and Wilkinson, 1980).

Figures 3.7(B) and 3.8(B) show an abnormally low bite distance and angle for the 7 membered chelate complexes of Fe with N as the donor. This is due to the donor N's on two of the complexes, AZHPFE10 (Little and Doedens, 1972) and BCINFE (Doedens, 1970), being bonded directly to one another, forming a three membered chelate ring as well as being involved in the larger chelate ring system, consequently leading to distortion of the geometry. Excluding these two structures would lead to a mean bite distance of 2.90Å and a mean bite angle of 85.3°.

Bite distances are significantly larger for Fe complexes, attributable to the larger ionic radius of the Fe ion and Fe-D distance (figure 3.9).

3.9.3 D-C distances and M-D-C angles for hexa co-ordinated Al and Fe complexes

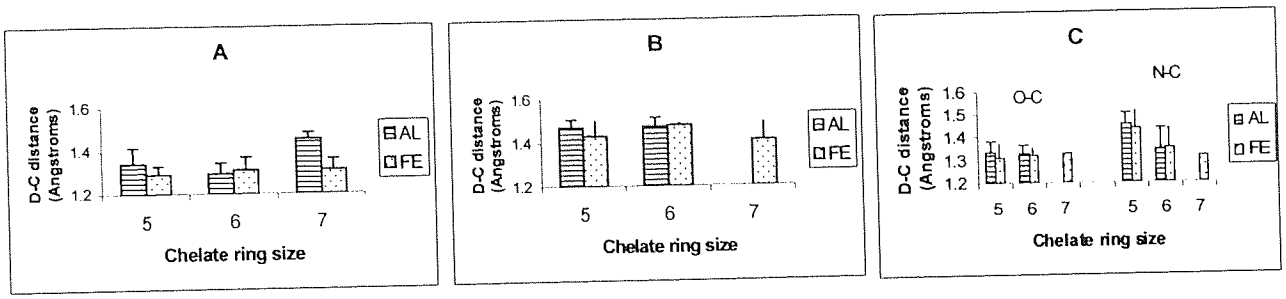


FIGURE 3.11 D-C distances of hexa co-ordinated Al and Fe complexes extracted from the CSD. (A) with O as donor atoms, (B) with N as donor atoms and (C) with N and O as the donating atoms

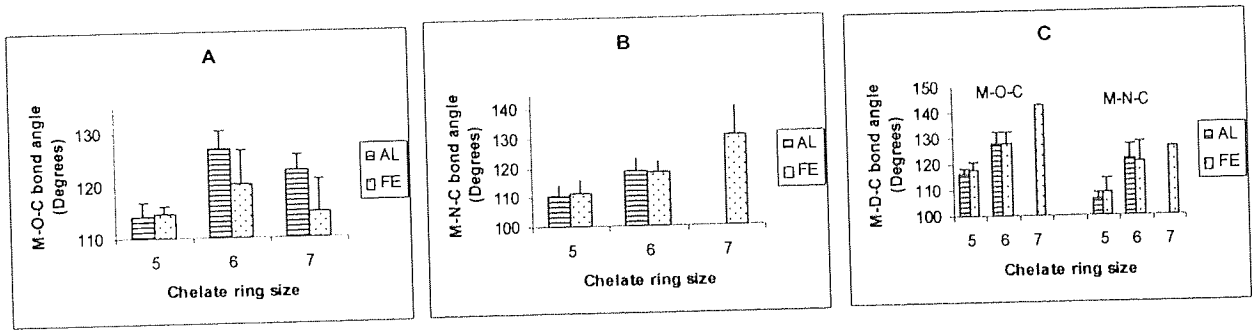


FIGURE 3.12 M-D-C angles of hexa co-ordinated Al and Fe complexes extracted from the CSD. (A) with O as donor atoms, (B) with N as donor atoms and (C) with N and O as the donating atoms

3.10 CONCLUSION

This chapter summarised the published crystal structures of some 3,000 Al co-ordinated compounds. Except for two examples, one which is in a +1 oxidation state and the other in the +2 oxidation state (Mocker, 1994), both of which are tetrahedral, Al is found in the +3 oxidation state. The octahedral and tetrahedral arrangements are the most common, utilising monodentate to hexadentate ligands. The predominant ligand in tetrahedral Al chemistry is the chloride ion, while the oxygen donor atom predominates the 6 co-ordinate octahedral species. There is a tendency for the bond to lengthen with covalent radius of the donating atom and with increasing co-ordination number of the Al atom.

The database study has shown that both Al and Fe exist predominantly as six co-ordinate which ideally would lead to octahedral complexes. Both metal ions bind to N and O donor atoms, although Al clearly has a preference for oxygen and Fe for nitrogen as both are capable of donating lone pairs of electrons. In general the majority of oxygen donor ligands tend to deprotonate upon complexation to Al. Al tends to show the greatest tendency for polymerisation resulting in difficulty in undertaking complexometric titrations. The tendency of polymerisation and the fact that Al salts are poorly soluble in aqueous solution makes the measurement of stability constants more difficult, hence the limited amount of stability data for Al complexes relative to other metal ions.

Al-O and Al-N bond distances are statistically significantly shorter than mean Fe-O and Fe-N distances at the 95% confidence limit tested. This may be attributed in part to the higher charge density of Al relative to Fe, and the physical fact that the ionic radius of Al is shorter than that of Fe. M-O-C and M-N-C angles show no significant difference between the two trivalent ions.

CHAPTER FOUR

X-RAY CRYSTALLOGRAPHY

4.1 INTRODUCTION

Single crystal X-ray crystallography is a highly specialised technique that is now used almost routinely as a method of determining the 3D structure and molecular dimensions of organic molecules. X-ray crystallography independently confirms the structural formulae of crystalline compounds, reveals the crystal structure, and enables the evaluation of molecular conformation and configuration. Well refined structures provide unambiguous information on the connectivity of molecules in the solid state and as such, the technique is often used to confirm or refute structures proposed on the basis of synthetic pathways, or analytical procedures such as MS, NMR and IR.

For this work, the technique is used for structural analysis of one inorganic and six organic crystals. With the exception of aluminium chloride hexahydrate (ALP2XL), all the crystals studied were organic possessing hard oxygen atoms, which in theory are capable of complexation with Al via electron donation. Chapter three has discussed in detail the information that can be utilised from crystallographic databases such as the CSD. These studies are concerned with structural analysis of crystals of ligands that potentially bind to Al. X-ray crystallography is a skilled procedure and consequently the underlying principles and procedures will be discussed further within this chapter.

4.1.1 Basic principles and theory of X-ray crystallography

4.1.1.1 X-rays

X-rays lie in the electromagnetic spectrum between ultraviolet light and gamma radiation and have an approximate range of wavelengths of 0.1 to 100Å. They are usually produced by rapidly decelerating fast moving electrons and converting their energy of motion into a quantum of radiation.

Both a copper (Cu) (λ = 1.54184Å) and a molybdenum (Mo) (λ = 0.71073Å) source for radiation were used in these studies. Cu was used for the data collection of the anhydrous tartaric acid discussed later, while Mo was used for all other structures. Cu X-ray tubes produce a higher flux of incident photons (for the same power settings) relative to Mo tubes, and these are diffracted more efficiently. Thus Cu radiation is particularly useful for small or otherwise weakly diffracting crystals. Mo radiation allows collection of data to a higher resolution and the data has minimal absorption.

4.1.1.2 Crystal Geometry, Symmetry and Space Groups

4.1.1.2.1 The Unit Cell

In 3-D, the imaginary parallelepiped containing one unit of a translationally repeating pattern, which displays the full symmetry of the lattice, is termed the unit cell. The distances a, b and c, are its primitive translations; α being the angle between the b and c axes, β the angle between a, c and γ the angle between a and b (Figure 4.1).

4.1.1.2.2 The Miller Indices

The resulting assembly of regularly stacked unit cells, each possessing identical contents, enables reduction of crystal analysis to spatial arrangement determination of those atoms within a single unit cell, or those within the asymmetric unit, if the unit cell possesses a degree of internal symmetry. In turn, the lattice of a crystal is a regular array of regularly repeating imaginary points, to reproduce the regularly repeating crystal structure.

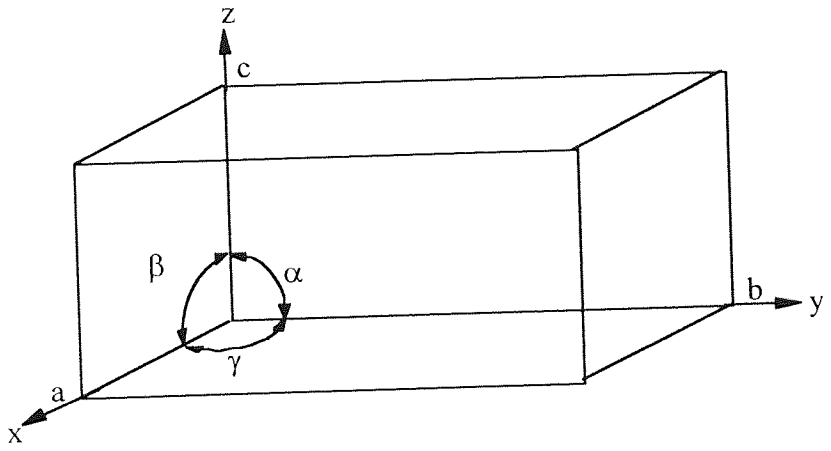


FIGURE 4.1 Unit cell dimensions of a crystal

This network of points constitutes the formation of a stack of planes of which the orientation may be defined by the ratio of the intercepts of its reference plane; *a/h*, *b/k*, *c/l*, where the *h*, *k* and *l* integers used to define the plane are the designated Miller Indices, to which a symbol (*hkl*) may be given.

Also known as the parametral plane of the crystal, the reference plane can be any plane which has an intercept on the three crystal axes *a*, *b* and *c* (Figure 4.2).

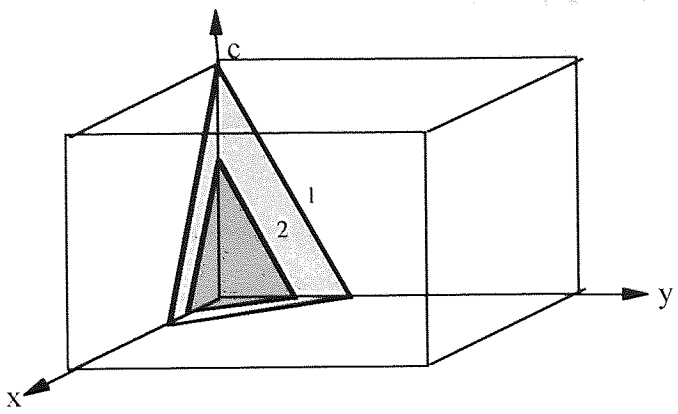


FIGURE 4.2 Example of a lattice plane and an interleaving plane. Plane 1 has intercepts ½, ½, 1 on the *x*, *y*, and *z* axes, respectively, and have the indices (2, 2, 1) (the reciprocals of the intercepts)

For all planes parallel to a given direction, the ratio of the intercepts on the axes is the same. For a given value of the ratio *a*, *b*, and *c*, the Miller indices of a plane are inversely proportional to its intercepts on the axes, and thus fundamental to modern-day mathematical resolution of the crystal structure. The geometrical reason for their use arises from the fact that *h/a*, *k/b*, and *l/c* are proportional to the direction cosines of the normal to the plane (*hkl*), which is used for crystallographic definition.

4.1.1.2.3 Geometry of X-ray diffraction and Bragg's Law

In any particular direction, the radiation scattered by the row of points will have zero intensity by destructive interference of the individual scattered rays unless they are all in phase. Since, except in the straight through direction, individual rays have different path lengths, these path differences must be equal to whole numbers of wavelengths to keep the rays in phase. Thus, for rays scattered by two adjacent points in the row (i.e. diffraction in one dimension);

$$\text{Path difference} = a \sin \varphi_I + a \sin \varphi_d = h\lambda$$

Equation 4.1

where: φ_I = angle of incident beam in a given direction

φ_d = angle of diffracted beam in a given direction

For a given value of φ_i (a fixed incident beam), each value of h corresponds to an observed diffraction maximum, and equation 4.1 can be used to calculate the permitted values of φ_d, the direction in which intensity is observed.

For diffraction by a 3-D lattice there are 3 such equations and all have to be satisfied simultaneously. Equation 4.1 contains the lattice a spacing, angles relative to this a axis of the unit cell and the integer h. The other two equations, correspondingly, contain the unit cell axes b and c and integers k and l respectively. Thus each allowed diffracted beam (each spot seen in an X-ray diffraction pattern) can be labelled by three integers, or indices h, k, l, which uniquely specify whether the unit cell geometry is known.

W. L. Bragg derived an alternative but equivalent description in 1913 (Bragg, 1968).

$$2d\sin\theta = n\lambda$$

Equation 4.2

where: λ = radiation wavelength

d = lattice plane spacing

θ = angle of incidence of the X-ray beam

n = integer (analogous to the order of the diffraction grating).

From Bragg's equation (equation 4.2), it may be derived that the angles of incidence and reflection are equal, and that the incoming and outgoing beams, and the normal to the reflecting planes all lie in one plane (Figure 4.3).

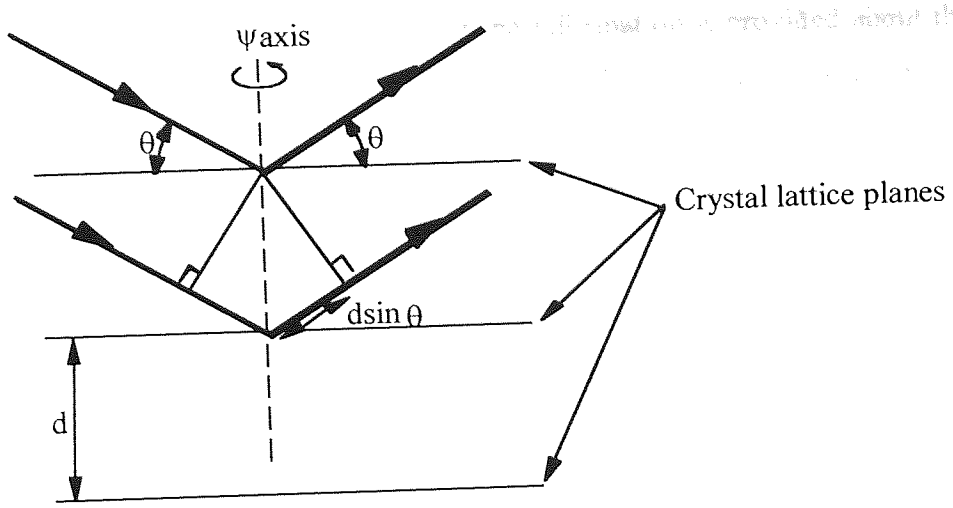


FIGURE 4.3 Schematic representation of the Bragg equation

The path difference, d between waves scattered from adjacent parallel lattice planes must consequently be an integral number of wavelengths, *n*, thus enabling derivation of the position of diffraction maxima for values of the angle of incidence. For a significant diffraction effect, the spacing must be comparable to the wavelength, which is the reason X-rays are used.

The Bragg equation allows each observed diffracted beam (reflection) to be uniquely labelled with its three indices and for its net scattering angle (2θ from the direction of the beam) to be calculated from the unit cell geometry, of which each d spacing is a function.

Rearrangement of the Bragg equation gives:

$$\sin\theta = \left(\frac{\lambda}{2}\right)\left(\frac{1}{d}\right)$$

Equation 4.3

Thus, the distance from each spot to the centre of an X-ray diffraction pattern is proportional to sinθ, mathematically demonstrating the reciprocal nature of the geometrical relationship between a crystal lattice and the angular spread of the scattering. Hence, each reciprocal lattices point (section 4.1.1.2.4) within a diffraction

pattern represents a Bragg reflection. However, no information is provided about the intensities of diffraction maxima that are observed when Bragg's equation is satisfied.

4.1.1.2.4 The Reciprocal Cell

There also exists a second related lattice, termed the reciprocal lattice whose unit cell lengths are denoted as a^*, b^* and c^*, and the interaxial angles as α^*, β^* and γ^*. The relationship between the two correlates the fundamental translations of one lattice in a perpendicular orientation to the other. For orthogonal axes, the fundamental translations and dimensions of the reciprocal lattice are parallel and inversely proportional respectively, to those of the crystal lattice. Consequently, the geometry of the diffraction pattern attained from crystal analysis is related to the lattice and unit cell geometry of the crystal structure. Reciprocal cell parameters are used in diffractometer control programs to manipulate the diffraction geometry, in order to derive the cell and crystal orientation parameters from selected observed reflections, and with subsequent prediction of the positioning of all reflections for intensity measurements.

$$a^* = \frac{b \times c}{V} \qquad b^* = \frac{c \times a}{V} \qquad c^* = \frac{a \times b}{V}$$

Equation 4.4

Each of these equations remains valid if all quantities marked with an asterisk become unmarked and vice versa.

4.1.1.2.5 Crystal Systems and Their Symmetry

In the most general system, triclinic, all six lattice parameters can assume any value. In other crystal systems, symmetry decreases the number of independent parameters to the values given in column two of Table 4.1 (section 4.1.2.2.1). Certain simple conventions follow, for instance in the monoclinic system, one of the axes is unique in the sense that it is perpendicular to the other two. This axis is conventionally taken as b so that $\beta \neq 90°$. A further convention required that the a and c axes be chosen so that $\beta > 90°$.

There are 14 types of Bravais lattices (Figure 4.4).

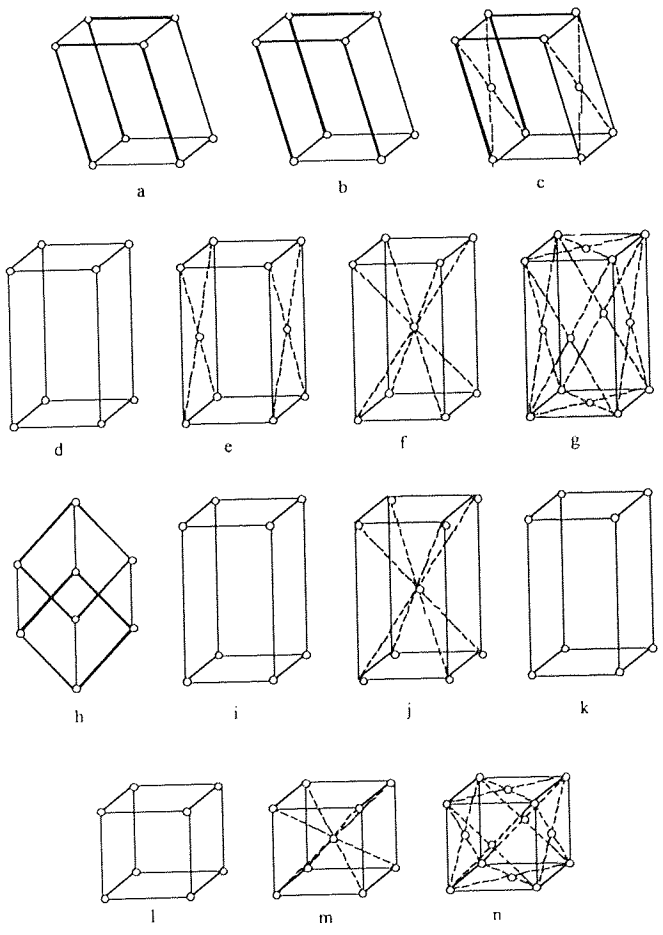


FIGURE 4.4 The 14 Bravais lattices (adapted from Stout and Jensen, 1989)

Each crystal system is characterised by a specific minimum number of symmetry elements, and referable to certain characteristic axes (Table 4.1).

TABLE 4.1 Characteristics of the seven crystal systems

Crystal System	Axial Length	Axial Angle	Symmetry Characteristics
Triclinic	$a \neq b \neq c$	$\alpha \neq \beta \neq \gamma$	–
Monoclinic	$a \neq b \neq c$	$\beta > 90°$; $\alpha = \gamma = 90°$	Two-fold rotation axis parallel to b
Orthorhombic	$a \neq b \neq c$	$\alpha = \beta = \gamma = 90°$	Three mutually perpendicular two-fold rotation axes
Tetragonal	$a = b \neq c$	$\alpha = \beta = \gamma = 90°$	Four-fold rotation axis parallel to c. Two-fold rotation axes perpendicular
Trigonal (rhombohedral lattice)	$a = b = c$	$\alpha = \beta = \gamma \neq 90°$	–
Hexagonal	$a = b = c$	$\alpha = \beta = 90°$; $\gamma = 120°$	Six-fold axis parallel to c. Two-fold rotation axes perpendicular to c.
Cubic	$a = b = c$	$\alpha = \beta = \gamma = 90°$	Three-fold rotation axes along all four body-diagonals. Four-fold axes parallel to each crystal axis. Two-fold axes

Other lattices possess additional centring; monoclinic with centring on one face, orthorhombic with centring on one face, or on all faces, or with body centring and tetragonal with body centring. The symmetry of the lattice shows as metric symmetry (special values of unit cell axial ratios and angles). Conversely, special values of unit cell dimensions are a guide to lattice symmetry but sometimes a misleading value may occur resulting in incorrect determination.

4.1.1.2.6 Point Groups and Space Groups

Molecular materials only occasionally pack so that molecular symmetry coincides with lattice symmetry. The analysis of intermolecular interactions such as H-bonding and base stacking, shows that they frequently make use of the unit cell symmetry for efficient packing. The symmetry of unit cell contents may be derived from the symmetry of the diffraction pattern and from systematically absent reflections, with subsequent derivation of the Bravais lattice and the probable space group which may also reveal information on unit cell content and molecular packing prior to structure determination. Space group determination also vastly simplifies the analysis of the diffraction pattern as different regions of the pattern are known to be identical. The presence of a lattice restricts the possibilities of rotational symmetry to a total of five types. Point symmetry operations which have at least one point of an object unmoved, comprise:

a) *n*-fold rotation axes (2,3,4,6): a rotation of $(360/n)°$ results in self-coincidence of the structure.

b) *n*-fold rotatory-inversion axes (2 or m, 3, 4, 6): application of this inversion operation with the origin of co-ordinates as the 'centre of inversion' implies that every point x, y, z becomes $-x, -y, -z$. An n-fold rotation-inversion axis implies a rotation of $(360/n)°$ followed by inversion through a point on the axis produces no apparent change in the structure.

c) mirror planes (*m*): application of this operation produces a reflection of the structure into self-coincidence.

It is characteristic of point groups that there is a point in space about which, or through which, the symmetry elements may be considered to operate and which remains unmoved by the operations. These point symmetry operations can be combined in 32 distinct ways with the 14 Bravais Lattices to give the 3-D crystallographic point groups. Translation symmetry becomes possible as it is no longer necessary for successive applications of a symmetry operation to bring a point back to its original position. Subsequently, combinations of point-symmetry operations with their translations enables the derivation of the following space-symmetry operations:

a) *n*-fold screw axes n_r: the corresponding symmetry operation is a rotation about the axis by 360°/*n*, followed by a translation parallel to the axis by *r*/*n* of the identity period along that axis (*r* = an integer less than *n*, where *n* = 2, 3, 4, 6 is the fold of the axis) of the unit cell length in that direction. For example, a 2-fold screw axis translates by 1/2 the repeat distance to the axis.

b) glide planes: the combination of reflection across a plane with a translation parallel to the reflecting plane. The translation in such a plane occurs along an edge or face diagonal of the unit cell. A point equivalent by a simple translational symmetry operation, a lattice vector, must be reached after two glide translations; these translations may be half of the repeat distance along a unit cell edge, where the glide plane is referred to as an a-, b-, or c-glide depending upon the edge parallel to the translation.

From the combination of pure rotations, rotatory inversions, screw axes and glide planes, 230 combinations of symmetry elements are acquired for crystal symmetry description; each combination is termed a space group and may be found in the International Tables (1996).

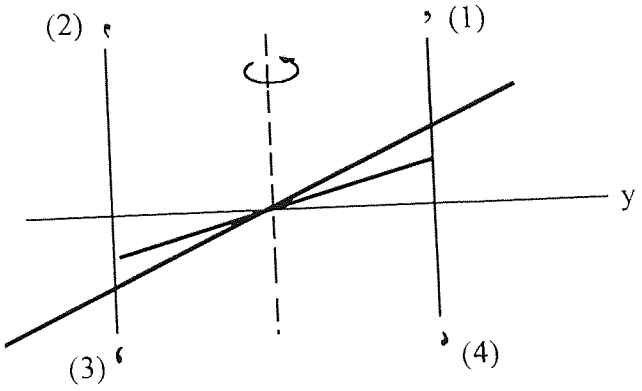


FIGURE 4.5 A point symmetry operation; a centre of symmetry produced by 2-fold axis combined with reflection

4.1.2 The Crystal Analysis Procedure

4.1.2.1 Crystal growth, evaluation and mounting

The quality of the crystal on which the diffraction data is acquired is generally the main determinant of the final quality of the structure. The effects of poor crystals propagate through the data collection, structure solution, and refinement stages to affect the quality of the final structure, in which unsatisfactorily high uncertainties may limit useful comparison and discussion.

4.1.2.1.1 Crystal growth

The aim was to produce relatively large single crystals between 0.1 to 0.5mm. To obtain this, crystals were generally grown slowly, taking from minutes to months depending on the system. There are 4 well used methods for crystal growth:

1. Solution methods are by far the most widely used and flexible. Ideally a solvent in which the crystal is only sparingly soluble should be used.
2. Sublimation is the direct conversion of a material from the solid to the gas without passing into the intermediate liquid phase. This method has been harnessed to produce solvent free crystals.
3. Fluid phase growth encompasses both high temperature growth from melts and low temperature growth from compounds that melt below ambient temperature.
4. Solid state synthesis may in some favourable circumstances produce adequate single crystals, but microcrystalline samples are more typical.

4.1.2.1.2 Evaluation

There are a number of procedures, which can provide an indication of whether it is worthwhile proceeding with a particular crystal or batch of crystals once synthesised.

1. Microscopy: Using a microscope with a polarising attachment, the crystal shape can be scrutinised to ascertain that it is indeed single with straight edges. The extinction of the crystal upon rotation between crossed polarisers is the best optical indication of the quality of the crystal, with an extinction over a change in angle of less than 1° implying a good quality crystal.
2. X-ray photography: can be used to establish the unit cell dimensions and diffraction symmetry of the crystal.
3. Differential Scanning Calorimetry (DSC): This technique was conducted prior to mounting a crystal on the diffractometer to determine melting point. The method used is described further in section 2.3.3.
4. Diffractometry: The ultimate test of a crystal is how it behaves on the diffractometer. Reflections must possess sufficient intensity, be well shaped (not split or extremely broadened) and index to give a sensible unit cell.

4.1.2.1.3 Mounting

For crystals that are stable to ambient conditions of air, moisture and light, the requirements are simple. The crystal is fixed securely with an amorphous glue such as epoxy resin onto a glass fibre, which in turn is fitted usually with wax to a goniometer head. Once fixed, the crystal should be centred so the x-ray beam would pass through the centre of the crystal and completely bathe it in radiation.

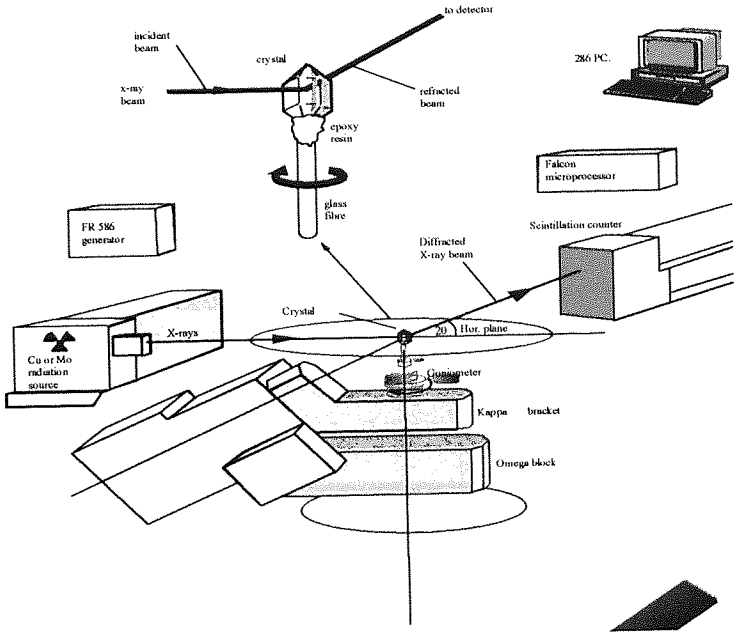


FIGURE 4.6 Overview of the CAD-4 crystallography apparatus

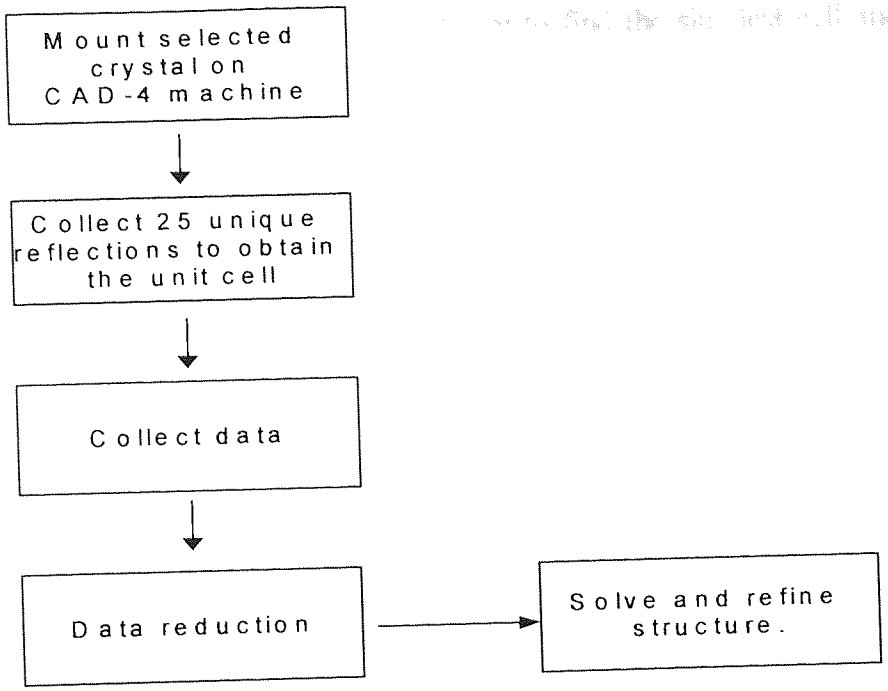


FIGURE 4.7 Overview of procedures involved in solving a crystal structure

4.1.2.2 Stages in Structure Determination

4.1.2.2.1 Reflection searching to obtain an orientation matrix and unit cell dimensions

The first objective once a crystal has been mounted would be to obtain the unit cell dimensions. This is essentially a blind searching procedure. 25 unique reflections are normally collected, although a recommended minimum of 12 unique reflections are required for indexing. The initial matrix and cell may not be sufficiently precise for data collection unless reflections with high Bragg angles are within the unique list. Orthodox 2θ angles around 30° for Mo and 50° for Cu are high enough to give good resolution without incurring problems due to splitting of the α_1/α_2 doublet.

As each reflection in the unique list is collected, it is centred using the 'SETANG' routine in the CAD-4 software, ensuring the diffracted beam passes the centre of the detector. Once all the unique reflections are collected, indexing, a mathematical

procedure is performed by the CAD-4 software to find the simplest cell and matrix that allows integral indices to be assigned to all reflections.

Ideally one would have 25 unique reflections with similar strong intensities with similar narrow scan widths. The 'SETANG' routine in the CAD4 software is then repeated to accurately centre these 25 unique reflections.

Once a primitive cell is found, the next step would be to establish the correct Bravais lattice (crystal system and lattice type). This is done solely on metric considerations of a, b, c and the angles α, β, γ.

For the first steps, the lowest symmetry should be considered first, which is guided by inspection of the morphology or physical properties of the crystals, or from knowledge that the crystals must be chiral. Size, shape, and density determination of the unit cell to determine how many formula units per unit cell exist follow this. Diffraction symmetry and Bravais lattice (P, A, B, C, I, F or R) determination is followed by data measurement. Diffraction or Laue groups provide the minimum symmetry information, which may be determined from the diffraction pattern. Assuming anomalous data are not obtained, the symmetry of the diffraction point group, determined from the diffraction pattern, is used to determine the necessary data required. Comparison between the symmetry equivalent intensity data and the possible crystal symmetries yields Laue symmetry. Each ray, reflected from a given set of planes in a crystal, possesses an inherent intensity dependent upon the electron distribution. As each reciprocal lattice point corresponds to one such ray, each has its own associated intensity. A reciprocal lattice in which each point has been assigned a weight equal to the intensity of the diffracted ray is termed the intensity-weighted reciprocal lattice. The possible symmetries of such lattices, the Laue symmetries, are just those of the 11 centrosymmetric point groups that result when a centre is added to each of the 32 point groups.

Once the lattice has been assigned, the space group remains to be determined (Glusker and Trueblood, 1972). A method that allows the reconstruction of the reciprocal lattice, enables observation of the systematic presence or absence of specific groups of

reflections which thus imply the presence or absence of certain symmetry elements. The systematic absence conditions, appropriate for the given Laue group, are tested to determine cell centring, glide planes and screw axes, with performance of a statistical test to detect a centre of symmetry. For many of the more common space groups, systematic absences uniquely determine the space group. Unfortunately, the information provided by systematic absences is not complete; only translational symmetry elements can be detected and there are many space groups not fully defined by these elements. As such, for this large set of less common space groups, two or more possible space group choices exist, and hence each of these is tested in turn to give the most probable solution. Initially, the highest possible symmetry space group is considered towards symmetry reduction, where the cell parameters are tested for possible higher metric symmetry.

Symmetry operations involving translation are indicated by special conditions for certain classes of data, which are listed in Volume A of the International Tables (1996) to provide confirmation for the successful determination of a space group. If ambiguity still exists and symmetry operations not involving translations are indicated, statistical tests on intensity distribution are applied to indicate the presence of such symmetry. Finally, if this fails and a conjecture must be made, it is helpful to take account of the relative frequency of the possible space groups. Up to this point, the process is geometrically reliant. However, it is the task of X-ray crystallography to locate the exact positions of atoms, and this depends upon a knowledge of the intensities of the spectra, and the measurement and subsequent interpretation of these.

4.1.2.2.2 Data collection

The aim is the efficient (in terms of time) measurement of intensity data to the maximum possible precision whilst avoiding errors which could degrade the quality of the data set. Once started, data collection is a fully automated procedure so it is particularly important that the parameters controlling it are optimally set before commencing. Such parameters include:

1. **Scan type and width**: Scanning a reflection involves the movement of the crystal (ω) with movement of the detector (2θ). A pure ω scan reduces the overlap between neighbouring reflections and is ideal where long cell axes or wide reflection profiles are present. An $\omega/2\theta$ scan is generally used to record reflections when the mosaic spread is very low and was the method of choice in these studies. The scan width is set based on the profile found during the scan of the unique reflections used in obtaining the unit cell dimensions. Setting too wide a scan width wastes diffractometer time, but too narrow a scan is worse because it will truncate reflections and introduce systematic errors into the data.
2. **Detector and collimator aperture**: This should be narrow enough to reduce background radiation and thereby increase precision, but wide enough to avoid truncating reflections, which would lead to systematic errors. The collimator aperture should be adjusted to allow the whole crystal to be bathed in the main X-ray beam, thus collimator aperture is dependent on the size of the crystal.
3. **Weak reflections**: Can be valuable in solving and refining structures. Intensity measurement done using a 'prescan' method. Each reflection is scanned relatively rapidly, before a triage is carried out by comparing the resulting $I/\sigma(I)$ ratio with pre-set upper and lower thresholds. A reflection that exceeds the upper threshold is deemed to be 'strong' and the measurement is accepted, while one below the lower threshold is deemed to be 'weak' and no further measurements are made. Those between the limits are scanned for an estimated additional time in an attempt to reach the upper threshold, subject to a time limit per reflection.
4. **Intensity standards – checking and reorientation**: Intensity standards consist of three reflections well distributed in reciprocal space from the unique reflection list. These should be intense, although not too strong at low angles (as these are the most likely to change due to an irradiation-induced increase in mosaic spread).

These standards are measured at two hour intervals. If any standards drop or move (by more than the limits set) the crystal is reorientated by re-centring a list of reflections.

5. **Choosing the reflections to measure**: A 'zigzag' method is usually employed, as this tends to be efficient with respect to moving from one set of reflection indices to the next. The time required for data collection also depends on the upper 2θ limit. The number of reflections is proportional to $\sin^3\theta$. For a given crystal, a data set (collected using Mo radiation) with $2\theta_{max} = 60°$ has more than twice as many reflections as one with $2\theta_{max} = 45°$. The minimum upper 2θ limits recommended by *Acta Crystallographica* are 50° for Mo radiation and 134° for Cu radiation, both of which are equivalent to a resolution of 0.84Å.

In all the structure studies within this chapter, these criteria were met.

An azimuthal (ψ) scan follows data collection. The crystal is rotated about the scattering vectors of a number of reflections. As a reflection remains in a diffracting position throughout, the variation of its intensity as a function of crystal orientation can be measured. At $\kappa = 90°$ the movement corresponds to rotation about ϕ. The CAD-4 geometry does not allow κ to exceed 100°, thus angles >80° are used. The ψ increments are 10° over the whole 360°.

4.1.2.2.3 Data Reduction

The process of data reduction requires the application of a number of corrections. Some of these (Lorentz and polarisation corrections) must be applied to every set of data. No operator input is required as both CADABS (Gould and Smith, 1986) and DATREDXL (Brookhaven National Laboratory; Univ. of Birmingham, 1986), use the appropriate correction factors. Both DATREDXL (output format: 3F4.0, 2F8.2) and CADABS (output format: 3F4.0, 2F8.0) are used for the purpose of converting the intensities obtained from the CAD-4 diffractometer to a form that can be read by structure solving programs such as MULTAN84 (Main *et al*, 1984), and SHELXS92 (Sheldrick, 1992) an automatic crystal structure solution program.

Other corrections such as absorption need not be applied in every case.

4.1.2.2.3.1 Applied Corrections to Intensity Data

The intensity data collected from the diffraction process constitutes the raw material from which crystal structures are derived. The data consists of a set of indices, diffractometer setting angles, background count before the scan, peak count accumulated during the scan and background count after the scan. These physical measurements on the crystals provide the information required for construction of the structural model. The preliminary manipulation of these intensities, that is the conversion of the raw material intensities to a corrected, more generally usable form, is referred to as data reduction. This process is usually undertaken by the data reduction program DATREDXL or CADABS to correct for background, geometrical and possibly absorption factors, which may manifest as physically meaningless values of important factors such as anisotropic atomic vibration parameters, in the ensuing structure refinement process.

The steps applied to the raw data for the purpose of data correction include total background subtraction, Lorentz-polarisation and intensity correction. The most widely used technique in carrying out a scan is to scan through the whole reflection (usually over a 2θ range of 1.5-2.5°) in a fixed period of time. The corresponding background is then obtained from the sum of the two counts, each for half the scan time, taken with the apparatus stationary at the beginning and end of the scan range [background-peak-background method (BPB)].

4.1.2.2.3.2 The Lorentz-Polarisation Correction

The intensities of the diffraction maxima show a variation in different directions and vary significantly with the angle of scattering. The X-rays scattered by a group of atoms, specifically within one unit cell of a structure in any direction in which there is a diffraction maximum, possess a specific combination of amplitude and phase, measured relative to the scattering by a single electron. This is the structure factor, symbolised by F or $|F_{hkl}|$ and is the most important quantity derived from the intensities.

The intensity of the scattered radiation is proportional to the square of the amplitude and hence the intensity of the diffracted beam corresponding to the diffraction maximum, where I_{hkl} is proportional to $|F|^2$ divided by geometric factors.

$$|F| \propto \sqrt{I}$$

Equation 4.5

where:

|F| = structure factor;

I = background corrected intensity.

The structure factor amplitude is calculated theoretically once the positions of the atoms in the cell are known. Furthermore, structure factors are used in the calculation of electron density maps from which the positions can be determined, thus it is customary to convert the intensities into 'observed' structure amplitudes $|F_o|$. The relationship between $|F_o|$ and I depends upon a number of factors, primarily geometric, that are related to the individual reflection and to the apparatus used to measure its intensity.

$$|F_{hkl}| = (KI_{hkl}/Lp)^{1/2}$$

Equation 4.6

where p, the polarisation factor, is given as

$$p = \frac{(1 + \cos^2 2\theta)}{2}$$

Equation 4.7

The minimal input to the data reduction program consists of raw intensity data, each reflection identified by its indices h, k and l and the cell parameters. Coded information with the method of data measurement is often able to provide the correct form for application of the Lorentz expression. The Lorentz factor (L), dependent on the Bragg angles and measurement technique used, is a correction factor accounting for the time and place the rotating crystal spends in the reflection position to diffract the beam. The polarisation term arises as a consequence of the nature of the X-ray beam and the manner in which its reflection efficiency varies with the reflection angle. The partial polarisation of an X-ray beam, when scattered by electrons from a crystal monochromator must be taken into account as it affects the subsequent reflection from the crystal under study.

4.1.2.2.3.3 Absorption and extinction

To obtain greatest accuracy it is necessary to calculate the absorption for the actual path length travelled within the crystal by the beam reflecting from each infinitesimal portion of the crystal and to integrate these results over the volume of the crystal. The severity of absorption is dependent upon the radiation source, the number of heavy atoms and the crystal morphology. Two crystal-based methods may be used for absorption correction. The first is based upon accurate indexing of crystal faces and measurement of their distances from a common reference point. The second is based upon ψ scans where the crystal is rotated about the scattering vectors of a number of reflections as described in section 4.1.3.1.2. This data is utilised and corrected for by the CADABS program. Extinction correction must also be applied. This is an expression for attenuation of the primary beam passing through the rotating crystal, dependent upon the distance of the reciprocal lattice point from the origin. Extinction predominantly affects strong, low-angle reflections and is corrected by a single

correction factor as a variable of structure refinement. Thermal-diffuse scattering artificially enhances high-angle reflection intensity.

4.1.2.2.3.4 Crystal Deterioration and Percentage Decay

Data collection also involves the periodic measurement with ensuing merger of a set of six standard reflections, three intensity reflections (collected every two hours) and three orientation reflections (collected every two hundred reflections) to monitor any decomposition or slippage of the crystal. To ensure that reliable, relative intensities are attained, repeated checks for calibration of standard reflections are made. As data collection proceeds, the integrated intensities of those reflections measured may significantly change with time where a monotonic decrease in diffraction intensity indicates possible crystal deterioration which is most likely initiated by crystal exposure to X-rays. This enables a comparison between intensity values with subsequent calculation of the extent of radiation damage. Once data collection has proceeded without any overall trend in the intensities of the check reflections, the spread of measurements may be used to estimate the parameter if used in the beam correction. The purpose of decay correction is to place intensity measurements at different stages of the data collection on the same scale. Both DATREDXL and CADABS account for application of a simple linear intensity corrector to the measured data.

4.1.2.2.4 Data Conversion

4.1.2.2.4.1 Scaling

Once the necessary corrections have been applied to the individual reflections, it is often necessary to bring various sets of reflections to a common basis in order to attain a uniform data set, where the output from the data reduction program consists of a set of records, one to a reflection, containing the necessary information for subsequent calculations.

4.1.2.2.4.2 Absolute Scaling and Temperature Factors

Useful information may be obtained via statistical comparison of the observed intensity data with the theoretical predictions for a crystal composed of a random assemblage of atoms. Following from Bragg's Law, if a particular set of lattice planes coincide in orientation and position with a densely populated planar set of atoms in a crystal, an intense diffraction maximum is detected as scattering from corresponding atoms occurs in phase. The amplitude for scattering electromagnetic radiation from a single atom, as a function of angle, is given by the scattering factor (f) expressed in terms of the power of an equivalent number of electrons located at the position of the atomic nucleus. The variation of the scattering factor is a consequence of the finite size of the atom, which is regarded as the scattering source. Hence, the amplitude measured from the entire crystal reveals the type of atoms in the crystal and the phase angle between path lengths. Thermal motion also has an effect on the X-ray intensities which causes the scattering of the real atom to fall off more rapidly than that of the ideal, stationary model.

4.1.2.2.4.3 Preliminary Stages to the Final Structure

The practical approach for advancing from the observed structure magnitudes to the final structure comprises of three stages. The first and most critical of these is;

1. the development of a phase set and associated structural model sufficiently close to correct for the application of Fourier methods. This phasing model is a poor representation of the entire chemical structure due to its incompleteness.
2. successive cycles of structure factor and Fourier calculation are continually elaborated such that all the atoms in the molecule are located and placed in reasonably correct positions; only distinctions regarding atom types and bond orders should necessitate additional detail at this stage. The phases should be fairly well fixed, with little variation in detail required during the final stage.
3. Subsequent refinement is undertaken to attain the best fit between F_o and F_c, and the best approximation to the true structure where atomic positions and temperature factors are adjusted.

4.1.2.2.5 The Phase Problem

In determining an unknown structure, a Fourier summation needs to be performed to attain a 3-D image of the scattering matter. If the structure factors |F| and phase angles α (for each h, k, l) are known, the electron density distribution ρ of the unit cell can be calculated and plotted for all values of x, y and z, to give a 3-D electron density map. The electron density at a point x, y, z in a unit cell of volume V_c, is

$$\rho(x,y,z) = \frac{1}{V}\sum_{h}\sum_{k}\sum_{l}\left|F_{hkl}\right|\cos 2\pi(hx+ky+lz-\alpha_{hkl})$$

Equation 4.8

If the electron density is known, assuming atoms to be at the centres of peaks, the entire structure may be derived. Structure solutions would thus be superfluous in computation except for the principle difficulty that the available data consist only of the structure factor magnitudes and not of the phases. The necessity to supply these missing data: the problem of attaining estimates of the phase angles so that an image of the scattering matter can be calculated constitutes the phase problem.

4.1.2.2.6 Determination of Atomic Parameters

Approximations to true electron density maps for solving the phase problem can be calculated by two approaches. The first is by a direct calculation of initial phases which allow the deduction of an atomic model from a Fourier map and the second by the direct location of enough atoms in the cell to yield approximate but adequate phases for F_c calculation. The first uses direct methods to find values of α directly. The second method derives a trial structure via use of the Patterson, heavy atom, or isomorphous replacement methods, and calculates approximate values of α for each reflection.

4.1.2.2.6.1 Direct Methods

Of the available methods for solving the crystal structure of a small molecule, the most commonly applied is the direct method. Crystal structures may be solved using SHELXS, which is particularly effective if a large proportion of the data is observed in the 1.0Å region of reciprocal space and if no significant problems regarding the choice of space group exist.

Direct methods require that the structure factors be placed on an absolute scale. The magnitude of the structure factors depends upon the extent to which atoms co-operatively scatter and also upon the scattering angles themselves, where scattering occurs with decreased strength at high angles. Contributions from reflections with high structure factor amplitude tend to dominate any map calculated, including those with phases corresponding to the correct structure. Hence, only these high-value terms normalised with respect to all reflections with similar scattering angles, need to be initially considered in an attempt to obtain an approximation to the correct map.

Direct methods for both centrosymmetric and non-centrosymmetric structures are most successful when care is taken, initially, to find the first few phases, and to observe that reflections with indices related to those of many other strong reflections are used in the early stages. It is possible to derive relations among the phases of different reflections as there are limits to the possible phase angles for individual reflections even in non-centrosymmetric structures, but especially in centrosymmetric structures, where the phase angle of a structure factor F(*hkl*) is either 0° or 180°. These relations arise as a consequence that the electron density can never be negative and that it is near zero except for isolated resolved peaks at atomic positions. Hence, from their relationships it is often possible to derive phases for almost all strong reflections and thus determine the structure from the resulting approximate electron density map. For centrosymmetric structures, relations can be found amongst these structure factors which involve the magnitudes of the larger structure factors normalised in a certain way. The calculation of normalised structure factors from F_o values affords the distribution of intensities (which are technically related to F^2). For a non-centrosymmetric structure, this should follow the theoretical values for an

acentric distribution, and for a centrosymmetric structure it should be centric. However, the presence of other symmetry elements may shift the distribution to centric and hypercentric respectively.

If the atoms can be located, the phase angle may approximate closely to the real value. Subsequently, an approximate electron density map can be calculated and interpreted using observed structure amplitudes and approximate phase angles, to yield a blend of the true structure with the trial structure.

4.1.2.2.6.2 Structural Refinement

Repetitive refinement is necessary as the initially estimated phases may give a poor image of the scattering matter and because the least squares equations are not linear. Refinement has thus been extended to the problem of fitting the observed diffraction intensities with those calculated. Refinement of the structure can be initiated once approximate positions have been determined. Atomic parameters are systematically varied to yield the best possible agreement of the observed structure factor amplitudes with those calculated for the proposed structure, to afford a 3-D structural model with significantly improved bond angles and lengths. Many successive iterative refinement cycles are usually needed before the structure reaches convergence as shifts in the atomic parameters from cycle to cycle become negligible with respect to the expected experimental errors. There are two common refinement techniques used: Fourier syntheses and the least squares method.

4.1.2.2.6.2.1 Fourier Syntheses

The purpose of the Fourier Series is to calculate electron density over the whole unit cell starting from previously unscaled data in the form of h, k, l, F, and α. However, the input amplitudes and phases of the structure factors possess a certain degree of inaccuracy, rendering the process only an approximation. The solution of the crystal structure results from successive approximations, and is reliant upon the relation of the repeating structure and diffraction pattern, via Fourier summations.

Although Fourier syntheses are less suitable for refinement than other techniques and cannot be used to refine scale and thermal parameters, if atoms are resolved, then fairly accurate positional parameters for the atoms can be determined. Subsequently, once the approximate positions and identities of all the atoms in the asymmetric unit are known, the amplitudes and phases of the structure factors can be readily calculated. The amplitudes and phases of the structure factors *calculated* from an approximation method will be to some degree incorrect, but at least a crude approximation is obtained, where the amplitudes can be replaced with measured values. Hence, an approximation to the true electron density can be calculated by a 3-D Fourier summation of the experimentally observed structure factor amplitudes with the calculated phases that hold increased importance.

If the positions of the atoms in the structure are known, the calculated phase angle may be nearly correct. Subsequently, an approximate electron density map calculated with observed structure amplitudes and computed phase angles will contain a blend of the true structure with the trial structure used to compute the phase angles. If the trial structure contains most of the atoms of the true structure, at or near their true positions, the resulting electron density map will contain peaks near sites representing atoms which were omitted from the trial structure, in addition to those that were previously located.

In centrosymmetric structures, as the phase angles are either 0° or 180°, a slight error in the structure may not have any effect upon most of the phase angles. A map computed with observed |F| and computed phase angles may be correct even if the original model possessed some slight error. However, with non-centrosymmetric structures, for which the phase angles may have any values from 0° to 360°, there will be at least some errors in most of the phases. Consequently the calculated electron density map will be weighted more in the direction of the model used to calculate the phases than with a centrosymmetric structure. Once most of the known structure has been derived, difference maps rather than electron density maps are computed, where the coefficients for the calculation are the differences between F_O and F_C with the computed phase angle. This affords a map in which the positive region is representative of an area where too few electrons were included, a negative region

represents the converse. If possible, H atoms are located from electron difference maps. Any remaining H atoms are assumed to ride on attached atoms and are placed in calculated positions.

The main uses of Fourier syntheses in crystal structure determination are:

1) Patterson functions – analysis of intensity distributions
2) Initial maps for a few data phased by direct methods
3) Difference maps to expand partially solved structures
4) Location of hydrogen atoms
5) Final checking of a structure

The major problem with Fourier sums is that the phases, which are vital to the summations, are at best only approximately known. As a Fourier synthesis is the best way of knowing whether a crystal structure has been solved, variations try to maximise useful data. During the refinement of the structure, if the magnitude of the observed structure factor, F_o, is markedly lower than calculated structure factor F_c, the correction for extinction and refinement is carried out by least squares. An excellent determination of attainment of a good structure is a flat difference map at the end of refinement.

4.1.2.2.7 Least Squares

The success of least squares method originally proposed by Légendre the availability at the start of a reasonably good set of phases, that is a good trial structure, where it makes the sum of the squares of the errors a minimum. A cyclic process ensures an improved value for the individual parameters, until no further improvement is observed. Any anomalies in molecular geometry or packing should be scrutinised with great care and regarded with some scepticism. As there are many more observations than parameters to be determined, statistical methods are used to fit an appropriate equation expressing the errors in |F| that result from errors in the trial structure.
At the conclusion of any least squares refinement process, calculation of a difference Fourier synthesis is recommended. After the structure has been fully refined,

parameters are obtained from the least-squares refinement as a set of co-ordinates and displacement parameters for each atom from which geometrical parameters, including bond lengths and angles, torsion angles, intermolecular and other non-bonded distances and least-squares planes with angles between can be calculated. Movements of atoms are calculated and corrections of apparent geometrical values applied to every derived result, an estimated standard deviation as a measure of its precision or reliability applied. As the technique is so suitable for high-speed computation, least squares refinement is the most common method used in structure improvement.

SHELXL93 refinement is based on full-matrix least-squares which calculates structure factors and accumulated least square totals solved later for parameter changes. Further refinement of parameters includes atomic co-ordinates, anisotropic displacement parameters (non-hydrogen atoms) and atomic isotropic vibration parameters (hydrogen atoms), scale factor for $|F_o|$, and an extinction parameter. Small variations in these parameters are made on each cycle to produce a test agreement between F_o and F_c.

4.1.2.2.8 Weighting Scheme

The functions minimised in the least squares method carry a weighting factor for each observation. The weighting should be a measure of the reliability of each observation. If chosen correctly, the weighting factor is able to adjust the contribution of each observation to the normal equations such that the most reliable results are produced.

A useful index often output by least squares refinement programs is the 'goodness of fit' (GOF), also termed the standard deviation of an observation of unit weight. It is a measure of the degree to which the found distribution of differences between $|F_o|$ and $|F_c|$ fits the distribution expected from the weights used in the refinement. If these weights are correct, which implies that the errors in the data are strictly random and correctly estimated, and if the model properly represents the structure that gives rise to the data, the value of GOF is 1.0

4.1.2.2.9 Determination of Structure Correctness

The general criteria for assessing the likely correctness of a structure, that is, if the experimentally observed data are reasonably precise and the model is appropriate, depend upon:

1. The agreement of the individual observed structure factor amplitudes $|F_o|$ with those calculated for the refined model $|F_c|$, which should be comparable to the estimated precision of the experimental measurements of the structure factors.
2. The electron density difference map phased with the final parameters of the refined model which should reveal no fluctuations in electron density greater than those expected on the basis of the estimated precision of the electron density.
3. Anomalies in the molecular geometry and packing or other derived quantities which should be scrutinised.

4.1.2.2.9.1 The Discrepancy Factor (R)

The agreement index known as the R factor depends on the type and complexity of the structure, and on the quality of the experimental data. It is a measure of the precision of the derived structure, denoting how well the calculated model fits the observed data. The lower the R factor, the greater the confidence placed in the quality of the refined model. As stated in chapter three, R values below 7% indicate a good quality structure.

$$R = \frac{\sum |\Delta F|}{\sum |Fo|} = \frac{\sum \left| |Fo| - |Fc| \right|}{\sum |Fo|}$$

Equation 4.8

If initial phases are poor, the first approximations to the electron density will contain significant incorrect detail with peaks near, but isolated from the correct location and

the R factor will initially be large. The reliability is assessed by checking the estimated standard deviations of the derived results and inspection of those measures regarding the agreement for the values of $|F_O|$ with the values of $|F_C|$, as indicated by the absence of any unexplained peaks in a final difference map, together with chemical integrity of the resulting structure.

4.1.3 ORTEP diagrams

The model attained by least squares refinement is displayed using the ORTEP-III version 1.0.2 program designed for Windows 95 (32 bit version) (Johnson *et al*, 1998). Atoms in a molecule are represented as ellipsoids whose size is related to the displacement parameters. If any ellipsoids are large or elongated, they may indicate atoms undergoing large thermal vibration. Alternatively, they may warn of undetected disorder or errors in the data. Use of these ORTEP drawings also involves symmetry application for model assignment of the unit cell, thus enabling determination of molecular packing and intermolecular bonding.

ORTEP-III has the advantage over its predecessors in that it can directly read in SHELX instruction files and incorporates a graphical use interface (GUI) allowing manual labelling and manipulation of plots.

4.2 AIM

These studies were conducted to establish the definitive 3-D structures of ligands possessing oxygen donor groups. Some of these structures are novel in that crystallographic determinations have not previously been reported such as the anhydrous DL tartaric acid (ALTAR), dimethylcitrate (CITXL) and butylciprofloxacin (BUCIP). Others such as sodium tartrate (ALTXL) and the inorganic structure aluminium chloride hexahydrate (ALPXL) have improved *R* factors relative to previously reported counterparts. Tricarballylic acid (TRIC2XL), nalidixic acid (NAL3XL) and oxalic acid dihydrate (MEOXAL) have also been included for comparative purposes, although their final *R* values are poorer than previously reported structures.

Only selected geometric parameters are listed in the relevant sections within this chapter; additional information including co-ordinates, structure factors and selected anisotropic displacement parameters are listed in appendix two.

4.3 ALUMINIUM CHLORIDE HEXAHYDRATE (ALP2XL)

Aluminium chloride hexahydrate is of interest medicinally in that it is a potent antiperspirant and is the main ingredient for hyperhidrosis preparations such as Anhydrol Forte, (Dermal), and Driclor, (Stiefel) (BNF, 1999).

4.3.1 Crystal data

A single crystal (0.525mm x 0.525mm x 0.5mm) of ALP2XL, [$AlCl_3.6(H_2O)$] crystallised in the rhombohedral space group number 161, R3c, Z = 6. Al and Cl are both in special positions (Wyckoff's notation a and b, respectively). At 293 K, the geometric parameters were a = 7.893(1) Å, b = 7.893(2) Å, c = 7.893(2) Å, α = 96.99(2)°, β = 96.99(2)°, γ = 96.99(1)° and V = 479.76 Å^3. The formula weight was 482.85, the calculated density was 1.671 Mgm^{-3}, agreeing well with the experimentally determined density of 1.657 Mgm^{-3} as determined using the flotation method described in section 2.3.2. The absorption coefficient was μ = 1.58 mm^{-1}, $R(F)$ = 0.0184; $wR(F^2)$ = 0.0433.

Unit cell dimensions were obtained from least squares analysis of setting angles of 25 unique reflections with $9.3° \leq \theta \leq 14.1°$. Intensity data were collected by the ω-2θ scan technique with ω scan range of 1.35 + 0.35 tanθ and a ω scan speed of 0.41 to 2.75deg min^{-1} with graphite monochromated Mo-Kα radiation. Significant alterations in the intensity and orientation standards did not occur, but by the end of the data collection the intensity standards had reduced by approximately 5.6%. These were compensated using a linear and isotropic decay estimate. A total of 4294 reflections were collected $-10 \leq h \leq 10$, $-10 \leq k \leq 10$, $-10 \leq l \leq 10$ in the range $2 < \theta < 27°$ and were merged to give 705 unique reflections (R_{int} = 3.58%) of which 353 were deemed observed with Fo > 4σ (Fo). Data reduction was performed by CADABS, allowing an empirical absorption correction to be made based on the ψ scan giving minimum and maximum reciprocal absorption corrections of 0.9671 and 1.0374, respectively. All non-hydrogen atoms were located by direct methods using the SHELXS-86 program.

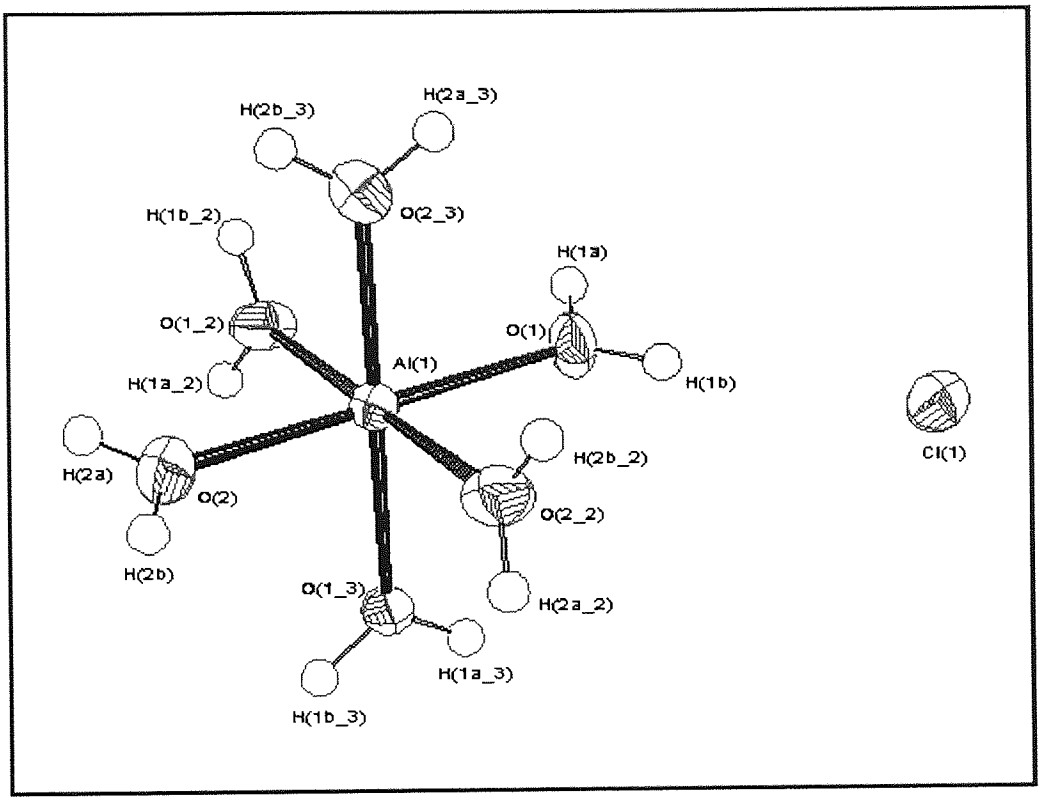


FIGURE 4.8 ORTEP III view of aluminium chloride hexahydrate (ALP2XL) showing labelling scheme. Thermal ellipsoids drawn at the 50% probability level and H atoms shown as 0.1Å spheres

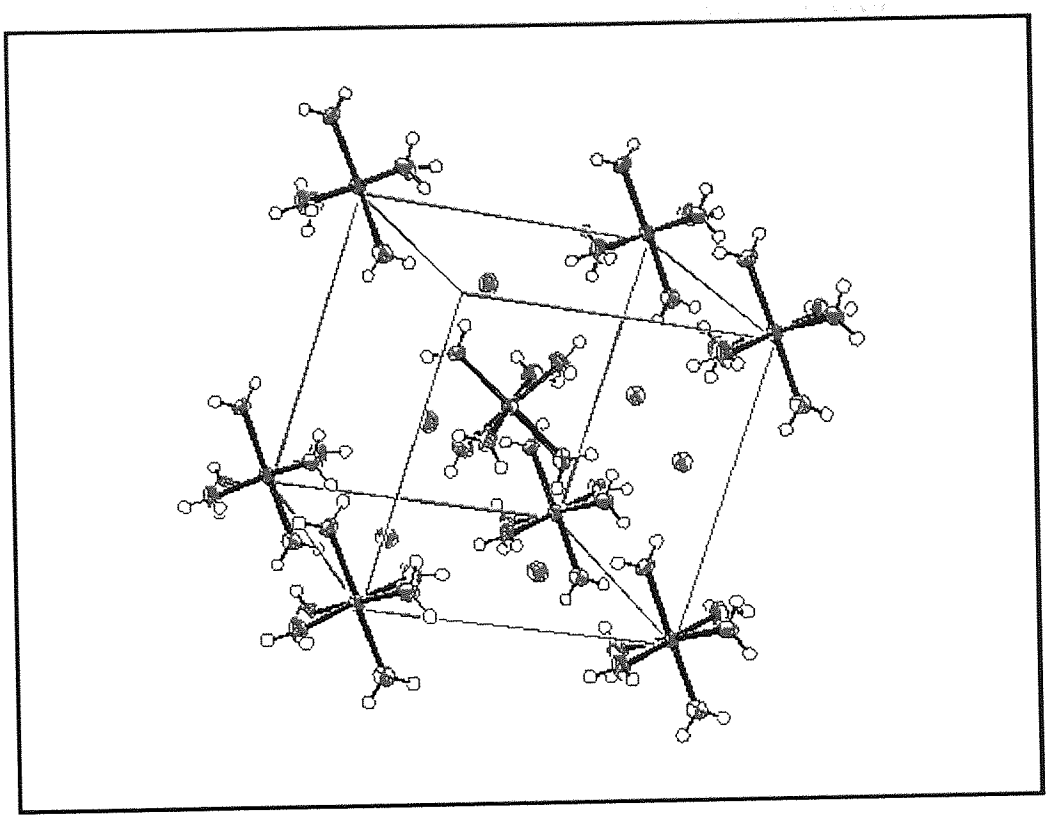


FIGURE 4.9 ORTEP III generated diagram showing unit cell of ALP2XL viewed normal to the 001 plane

TABLE 4.2 Selected bond lengths (Å) and bond angles (°) for ALP2XL

	Bond length
Al(1)-O(2)#2	1.847(3)
Al(1)-O(2)#3	1.847(3)
Al(1)-O(2)	1.847(3)
Al(1)-O(1)#2	1.895(3)
Al(1)-O(1)#3	1.895(3)
Al(1)-O(1)	1.895(3)

	Bond angle
O(2)#1-Al(1)-O(2)#3	90.09(12)
O(2)#1-Al(1)-O(2)	90.09(12)
O(2)#2-Al(1)-O(2)	90.09(12)
O(2)#1-Al(1)-O(1)#2	179.9(2)
O(2)#2-Al(1)-O(1)#2	89.87(13)
O(2)-Al(1)-O(1)#2	89.95(14)
O(2)#1-Al(1)-O(1)#3	89.78(14)
O(2)#2-Al(1)-O(1)#3	179.9(2)
O(2)-Al(1)-O(1)#3	89.89(13)
O(1)#1-Al(1)-O(1)#3	90.16(12)
O(1)#1-Al(1)-O(1)	90.09(13)
O(1)#2-Al(1)-O(1)	89.87(13)
O(2)-Al(1)-O(1)	179.9(2)
O(1)#1-Al(1)-O(1)	90.09(13)
O(1)#2-Al(1)-O(1)	90.09(11)

Symmetry transformations used to generate equivalent atoms:

#2 z, x, y #3 y, z, x

4.3.2 Discussion

To date, only two structures of $Al_2Cl_6.6H_2O$ have been found in the ICSD. The initial determination was done in 1934 (Andress, 1934), although the hydrogen atoms were not located. The second and more recent study was done in 1982 (Buchanan, 1982) arriving at a final *R* of 8.7%. Hence this structure has been redetermined. ALP2XL was found to solve as both a centrosymmetric and a non-centrosymmetric structure resulting in wR values of 4.70 and 4.33% respectively. Using Hamilton's hypothesis (International Tables for X-ray crystallography, IV), it was found that the non-centrosymmetric structure was the better. The structure finally refined to an *R* of 1.84%, showing a high quality set of data. Al-O bond lengths are in the range of 1.848Å to 1.896Å, lengths typical as described in the previous chapter. O-Al-O angles are 90° and 180°, angles typical of the most favoured octahedral arrangement for Al complexes involving oxygen donor atoms.

4.4 ANHYDROUS DL TARTARIC ACID (ALTAR) AND SODIUM (+) TARTRATE MONOHYDRATE (ALTXL)

4.4.1 Crystal data for ALTAR

A single crystal (0.2mm x 0.15mm x 0.15mm) of anhydrous DL tartaric acid [$C_8O_{12}H_6$] crystallised in the triclinic space group number 2, $P\bar{1}$, Z = 2. At 293 K, the geometric parameters were a = 4.888(1) Å, b = 6.574(1) Å, c = 9.177(1) Å, α =74.77(1)°, β = 88.464(9)°, γ = 76.554(9)° and V = 276.55 Å^3. The formula weight was 300.18, the calculated density was 1.802 mg m^{-3} and the absorption coefficient was μ = 1.58 mm^{-1}, $R(F)$ = 0.0481; $wR(F^2)$ = 0.144.

Unit cell dimensions were obtained from least squares analysis of setting angles of 25 unique reflections with 18° ≤ θ ≤ 32.8°. Intensity data were collected by the ω-2θ scan technique with ω scan range of 1.35 + 0.35 tanθ and a ω scan speed of 0.55 to 2.75 deg min^{-1} with graphite monochromated Cu-Kα radiation. Significant alterations in the intensity and orientation standards did not occur, but by the end of the data collection the intensity standards had reduced by approximately 4%. These were compensated using a linear and isotropic decay estimate. A total of 1249 reflections were collected -6 ≤ h ≤ 6, -8 ≤ k ≤ 8, 0 ≤ l ≤ 11 in the range 2 < θ < 75° and were merged to give 1129 unique reflections (R_{int} = 4.34%) of which 940 were deemed observed with Fo > 4σ (Fo). Data reduction was performed by CADABS, allowing an empirical absorption correction to be made based on the ψ scan giving minimum and maximum reciprocal absorption corrections of 0.9293 and 1.0679, respectively. All non-hydrogen atoms were located by direct methods using the MULTAN program.

4.4.2 Crystal data for ALTXL

A single crystal (0.35mm x 0.35mm x 0.25mm) of ALTXL [$C_{16}H_{28}O_{28}Na_4$] crystallised in the orthorhombic space group $P2_12_12_1$, Z = 4. At 293 K, the geometric parameters were a = 3.452(1) Å, b = 3.987(1) Å, c = 10.337(5) Å, α = 95.56(2)°, β = 96.34(2)°, γ = 106.769(9)° and V = 760.34 Å^3. The formula weight was 482.85, the calculated density was 1.898 mg m^{-3}, agreeing well with the experimentally determined density of 1.894 mg m^{-3}. The absorption coefficient was μ = 0.24 mm^{-1}, $R(F) = 0.0253$; $wR(F^2) = 0.0705$.

Unit cell dimensions were obtained from least squares analysis of setting angles of 25 unique reflections with $10.2° \leq \theta \leq 16.3°$. Intensity data were collected by the ω-2θ scan technique with ω scan range of 1.35 + 0.35 tanθ and a ω scan speed of 0.41 to 2.75 deg min^{-1} with graphite monochromated Cu-Kα radiation. Significant alterations in the intensity and orientation standards did not occur, but by the end of the data collection the intensity standards had reduced by approximately 1.6%. These were compensated using a linear and isotropic decay estimate. A total of 1,628 reflections were collected $-9 \leq h \leq 9$, $-11 \leq k \leq 11$, $-13 \leq l \leq 0$ in the range $3.04 < \theta < 27°$ and were merged to give 1446 unique reflections (R_{int} = 1.46%) of which 1216 were deemed observed with Fo > 4σ (Fo). Data reduction was performed by CADABS, allowing an empirical absorption correction to be made based on the ψ scan giving minimum and maximum reciprocal absorption corrections of 0.9221 and 1.0599, respectively. All non-hydrogen atoms were located by direct methods using the SHELXS-86 program.

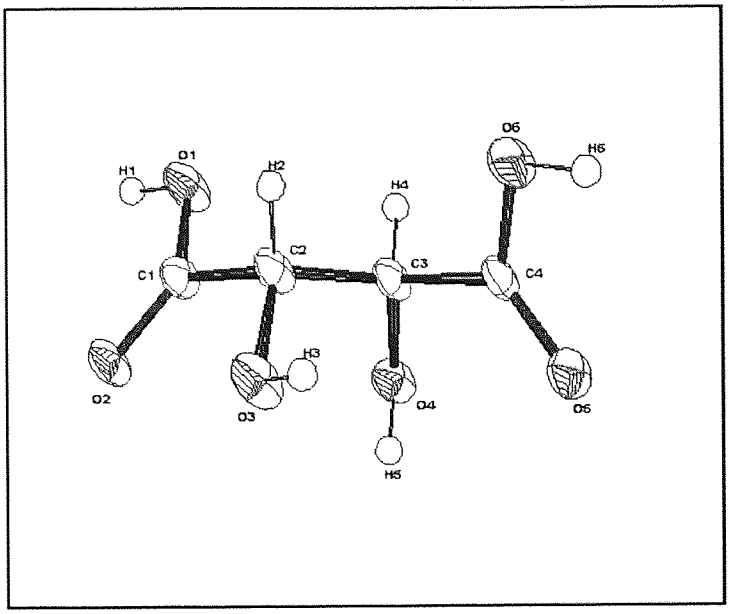


FIGURE 4.10 ORTEP III view of anhydrous DL tartaric acid (ALTAR) showing labelling scheme. Thermal ellipsoids drawn at the 50% probability level and H atoms shown as 0.1Å spheres

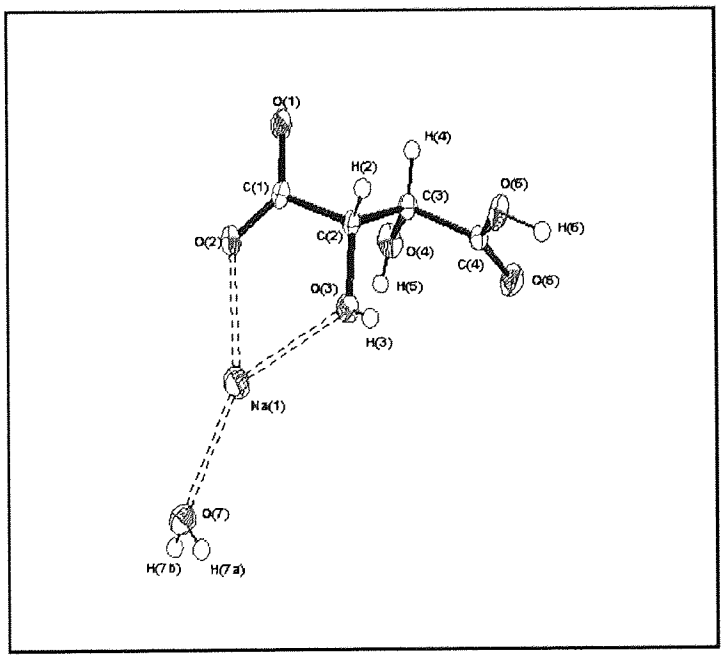
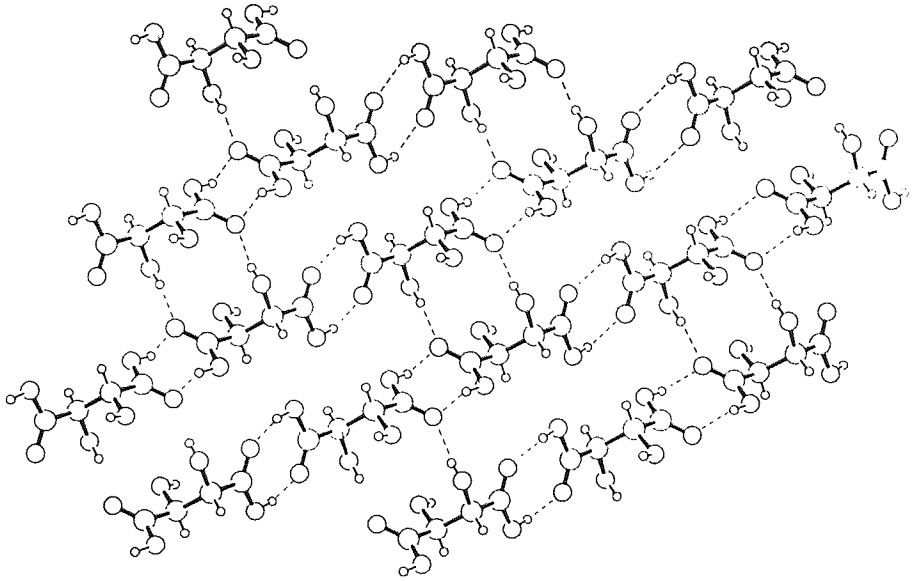


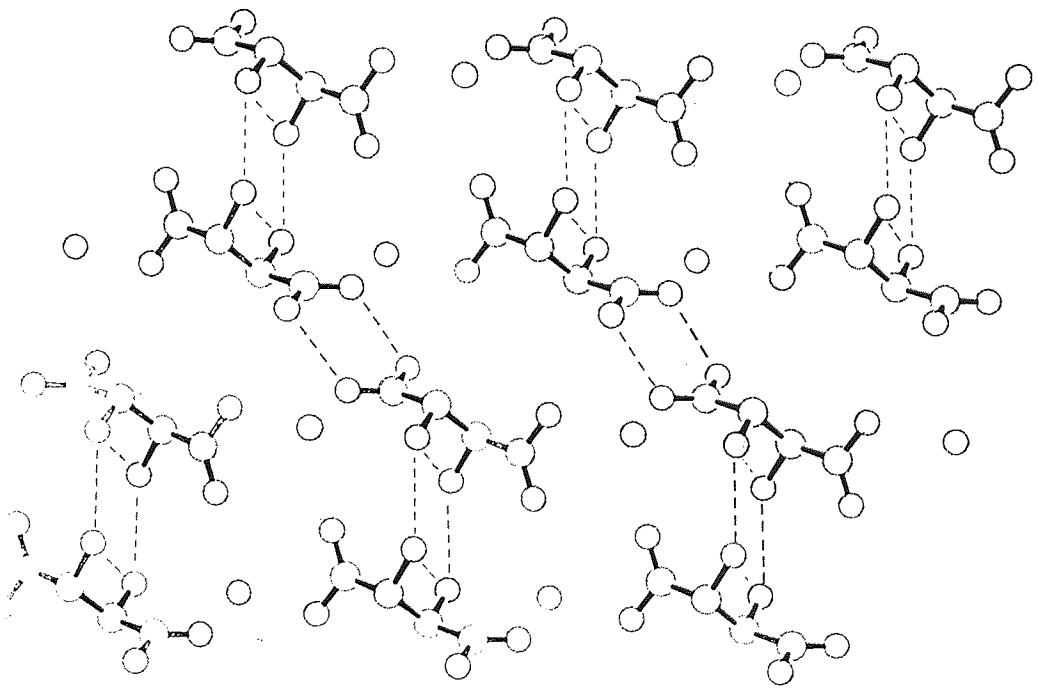
FIGURE 4.11 ORTEP III view of sodium tartrate monohydrate (ALTXL) showing labelling scheme. Thermal ellipsoids drawn at the 50% probability level and H atoms shown as 0.1Å spheres. Dashed lines indicate non covalent bonding

TABLE 4.3 Selected bond lengths (Å), bond angles and bond torsion angles (°) for ALTAR and ALTXL

Geometrical parameter	ALTAR	ALTXL
C1-C2	1.518(2)	1.542(2)
C2-C3	1.547(3)	1.525(2)
C3-C4	1.521(2)	1.529(2)
C1-O1	1.303(2)	1.272(2)
C1-O2	1.222(2)	1.225(2)
C2-O3	1.403(2)	1.407(2)
C3-O4	1.404(2)	1.419(2)
C4-O5	1.215(2)	1.210(2)
C4-O6	1.310(2)	1.308(2)
O3...O4	2.974(2)	2.922(2)
NA1-O2	-	2.431(2)
NA1-O3	-	2.413(2)
NA1-O7	-	2.415(2)
H7A-O7-H7B	-	110.7(6)
O2-NA1-O7	-	65.09(5)
O3-NA1-O7	-	141.72(7)
O1-C1-O2	112.16(14)	126.2(2)
O5-C4-O6	125.4(2)	125.7(2)
C1-C2-C3-C4	-177.7	-176.7
O2-C1-C4-O5	19.8	56.4
O3-C2-C3-O4	65.3	66.6



(a)



(b)

FIGURE 4.12 Packing diagrams of DL tartaric acid a: anhydrous form (ALTAR) b: monohydrate form (TARTDL) (Parry, 1951)

TABLE 4.4 Distances and angles of intermolecular hydrogen bonds involved in packing of ALTAR

Hydrogen bonds	H...O	O...O	O-H...O
O_1-H_1...O_2^{i}	1.73(4)	2.656(2)	168(3)
O_3-H_3...O_4^{ii}	1.92(4)	2.835(2)	178(3)
O_6-H_6...O_5^{iii}	1.74(4)	2.672(2)	169(4)
O_4-H_5...O_2^{iv}	2.12(3)	2.962(2)	171(3)
O_4-H_5...O_3^{iv}	2.47(3)	2.974(2)	119(2)

i -x, 2-y, 1-z; ii 1+x, y, z; iii 2-x, 1-y, -z; iv 1-x, 1-y, 1-z

4.4.3 Discussion

Data analysis shows crystallisation of the racemate in the anhydrous form, a structure that has only previously been solved as a hydrated crystal (DLTART). The distance of the C2-C3 bond (1.5472 Å) is slightly larger than the distance accepted for sp^3-sp^3 bonds (1.533 $Å^2$). The mean value of the other C-C length (C1-C2 and C3-C4) (1.520 Å) is larger than the value suggested for sp^2-sp^3 bonds (1.505 $Å^2$) (Lide, 1962). G.S. Parry crystallised this material in 1951 as the monohydrate, and deduced that the water molecule held sheets of tartaric acid together via hydrogen bonding (O-O distances in the range of 2.61Å to 3.39Å). ALTAR shows hydrogen bonding between the two terminal carboxyl groups of two adjacent carboxylic groups, one D- isomer and one L-isomer. Hydrogen bonding between adjacent carboxylic acid groups creates centrosymmetric dimers on both ends of the molecule forming ribbons. Similar dimers occur with Parry's DL tartaric acid solved in 1951 (TARTDL). Parry also suggested that the two hydroxyl groups hydrogen bond to two hydroxyl groups of an adjacent tartaric acid molecule so that a square is formed from the four hydroxyl groups involved in H bonding, thus forming parallel columns (Figure 4.12(b)). *Meso* tartaric acids, which differ from DL tartaric acids via an asymmetric carbon atom also show dimerisation via the carboxylic group. The triclinic anhydrous *meso* tartaric acid

triclinic anhydrous *meso* tartaric acid (TARTAM) shows dimerisation in this way on both ends of the molecule, whereas the triclinic hydrate (TARTMM) and the monoclinic hydrate (TARTMM01) dimerise on one carboxyl group only, the other being involved in hydrogen bonding with water molecules. Whilst the two hydroxyl groups are involved in hydrogen bonding in ALTAR, they bond to hydroxyls of two adjacent tartaric acid molecules. The packing diagram generated by ORTEP III shows closer packing of neighbouring tartaric acid molecules via hydrogen bonding compared to the monohydrate (O-O distances in the range 2.656Å to 2.974Å: Table 4.4), hence a higher relative density.

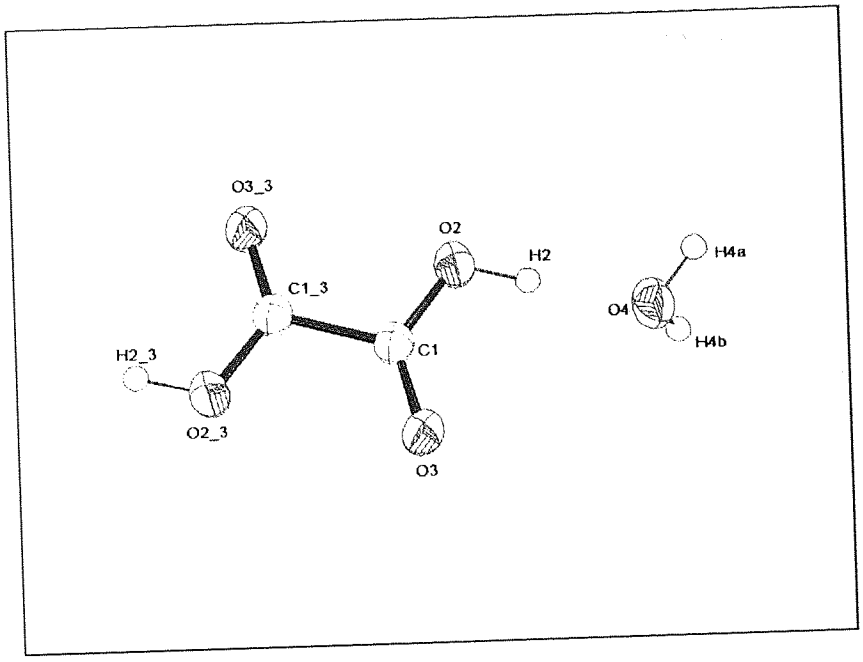
The structure of ALTXL has been reported on two previous occasions resulting in final *R* values of 3.3% (ZZZSSS01; Kubozono, 1993) and 2.1% (ZZZSSS02; Bott, 1993), both of which were solved in the orthorhombic space group $P2_12_12_1$. As shown in Figure 4.11, the O_2 position is deprotonated due to the electrostatic interaction with the sodium ion. In general, all geometric parameters of ALTXL compare well with those reported by Bott (1993).

4.5 OXALIC ACID DIHYDRATE (MEOXAL)

4.5.1 Crystal data for MEOXAL

A single crystal (0.7mm x 0.525mm x 0.475mm) of MEOXAL $[(C_1H_1O_2.H_2O)_2]$ crystallised in the monoclinic space group $P2_1/c$, space group number 14, Z = 2. At 293 K, the geometric parameters were a = 6.118(1) Å, b = 3.607(1) Å, c = 11.84(2) Å, β = 103.25(1) and V = 255.25 Å^3. The formula weight was 142.07, the calculated density was 1.64 Mgm^{-3}, agreeing well with the experimentally determined density of 1.631 Mgm^{-3} as determined using the flotation method described in section 2.3.2. The absorption coefficient was μ = 0.17 mm^{-1}, $R(F) = 0.0337$; $wR(F^2) = 0.0880$

Unit cell dimensions were obtained from least squares analysis of setting angles of 25 unique reflections with $10.3° \leq \theta \leq 15.4°$. Intensity data were collected by the ω-2θ scan technique with ω scan range of 1.35 + 0.35 tanθ and a ω scan speed of 0.39 to 2.75 deg min^{-1} with graphite monochromated Mo-Kα radiation. Significant alterations in the intensity and orientation standards did not occur, but by the end of the data collection the intensity standards had reduced by approximately 1.8%. These were compensated using a linear and isotropic decay estimate. A total of 1200 reflections were collected $-7 \leq h \leq 7$, $-4 \leq k \leq 4$, $-15 \leq l \leq 0$ in the range $2 < \theta < 25°$ and were merged to give 555 unique reflections (R_{int} = 3.13%) of which 522 were deemed observed with Fo > 4σ (Fo). Data reduction was performed by CADABS, allowing an empirical absorption correction to be made based on the ψ scan giving minimum and maximum reciprocal absorption corrections of 0.9620 and 1.0442, respectively. All non-hydrogen atoms were located by direct methods using the SHELXS-86 program.



A

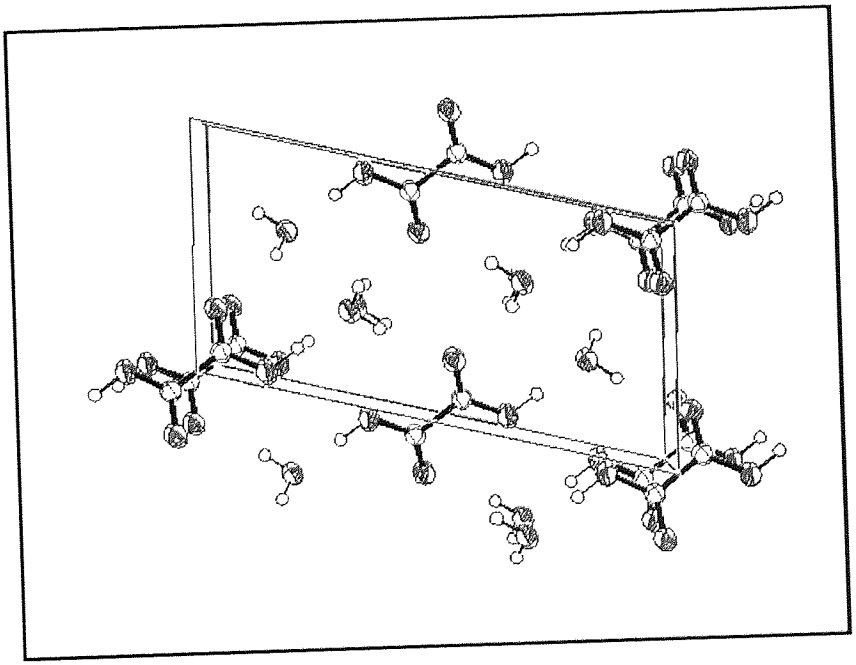


FIGURE 4.13 ORTEP III view of oxalic acid dihydrate (MEOXAL) (A) showing labelling scheme and (B) packing arrangement. Thermal ellipsoids drawn at the 50% probability level and H atoms shown as 0.1Å spheres

TABLE 4.5 Bond lengths (Å) and angles (°) for MEOXAL

	Bond length
C(1)-O(3)	1.2111(13)
C(1)-O(2)	1.2851(13)
C(1)-C(1)#3	1.548(2)

	Bond angle
O(3)-C(1)-O(2)	127.18(9)
O(3)-C(1)-C(1)#3	120.84(11)
O(2)-C(1)-C(1)#3	111.98(11)

Symmetry transformations used to generate equivalent atoms:

#3 -x+2,-y,-z+2

4.5.2 Discussion

Numerous studies have been carried out on oxalic acid in the anhydrous form and as a dihydrate. Of the dihydrate structures that solved by Ahmed (1969; OXACDH11) had the lowest *R* value of 2%. Geometric parameters of this structure tend to be similar to those previously reported (Derissen, 1974).

4.6 DIMETHYLCITRATE MONOHYDRATE (CITXL) AND TRICARBALLYLIC ACID (TRIC2XL)

4.6.1 Crystal data for CITXL

A single crystal (0.2mm x 0.125mm x 0.1mm) of CITXL [$C_8H_{14}O_8$] crystallised in the triclinic space group $P\bar{1}$, Z = 2. At 293 K, the geometric parameters were a = 7.886(2) Å, b = 8.114(1) Å, c = 9.587(1) Å, α = 94.45(1)°, β = 110.21(2)°, γ = 106.65(2)° and V = 541.66 Å^3. The formula weight was 476.38, the calculated density was 1.460 Mgm^{-3}, agreeing well with the experimentally determined density of 1.453 Mgm^{-3} as determined using the flotation method described in section 2.3.2. The absorption coefficient was μ = 0.1 mm^{-1}, $R(F)$ = 0.0674; $wR(F^2)$ = 0.1958.

Unit cell dimensions were obtained from least squares analysis of setting angles of 25 unique reflections with $5.1° \leq \theta \leq 13.4°$. Intensity data were collected by the ω-2θ scan technique with ω scan range of 1.35 + 0.35 tanθ and a ω scan speed of 0.46 to 2.75 deg min^{-1} with graphite monochromated Mo-Kα radiation. Three intensity standards were measured every two hours and in every 200 experimental reflections 3 orientation monitor reflections were located. Significant alterations in the intensity and orientation standards did not occur, but by the end of the data collection the intensity standards had reduced by approximately 2.2%. These were compensated using a linear and isotropic decay estimate. A total of 3137 reflections were collected $-10 \leq h \leq 10$, $-10 \leq k \leq 2$, $-12 \leq l \leq 12$ in the range $2 < \theta < 27°$ and were merged to give 2346 unique reflections (R_{int} = 3.56%) of which 992 were deemed observed with $Fo > 4\sigma(Fo)$. Data reduction was performed by CADABS, allowing an empirical absorption correction to be made based on the ψ scan giving minimum and maximum reciprocal absorption corrections of 0.9748 and 1.0235, respectively. All non-hydrogen atoms were located by direct methods using the SHELXS-86 program.

4.6.2 Crystal data for TRIC2XL

A single crystal (0.875mm x 0.6mm x 0.325mm) of TRIC2XL [$C_6H_8O_6$] crystallised in the orthorhombic space group 61, Pbca, Z = 8. At 293 K, the geometric parameters were a = 11.749(2) Å, b = 23.76(1) Å, c = 5.319(2) Å, $\alpha = \beta = \gamma = 90°$ and V = 1484.51 Å^3. The formula weight was 1408.99, the calculated density was 1.576 Mgm^{-3}, agreeing well with the experimentally determined density of 1.568 Mgm^{-3} as determined using the flotation method described in section 2.3.2. The absorption coefficient was μ = 0.14 mm^{-1}, $R(F) = 0.0603$; $wR(F^2) = 0.1933$.

Unit cell dimensions were obtained from least squares analysis of setting angles of 25 unique reflections with $10.6° \leq \theta \leq 14.1°$. Intensity data were collected by the ω-2θ scan technique with ω scan range of 1.35 + 0.35 tanθ and a ω scan speed of 0.46 to 2.75 deg min^{-1} with graphite monochromated Mo-Kα radiation. Three intensity standards were measured every two hours and in every 200 experimental reflections 3 orientation monitor reflections were located. Significant alterations in the intensity and orientation standards did not occur, but by the end of the data collection the intensity standards had reduced by approximately 3.3%. These were compensated using a linear and isotropic decay estimate. A total of 3267 reflections were collected $-14 \leq h \leq 1$, $-30 \leq k \leq 20$, $-6 \leq l \leq 1$ in the range $2 < \theta < 27°$ and were merged to give 1620 unique reflections (R_{int} = 7.06%) of which 1298 were deemed observed with Fo > 4σ (Fo). Data reduction was performed by CADABS, allowing an empirical absorption correction to be made based on the ψ scan giving minimum and maximum reciprocal absorption corrections of 0.8247 and 1.2692, respectively. All non-hydrogen atoms were located by direct methods using the SHELXS-86 program.

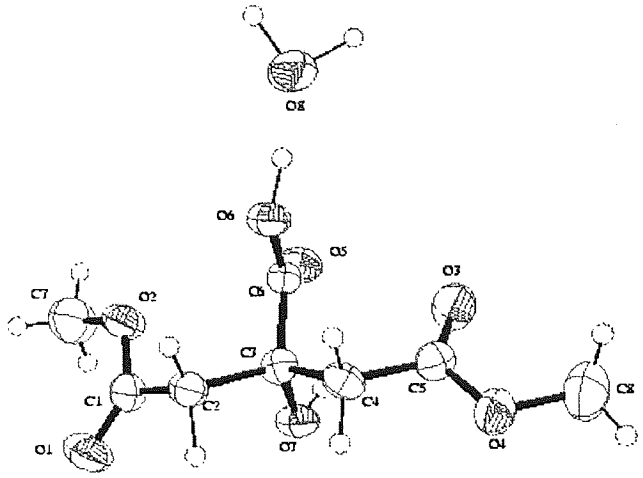


FIGURE 4.14 ORTEP III view of dimethylcitrate monohydrate (CITXL) showing labelling scheme. Thermal ellipsoids drawn at the 50% probability level and H atoms shown as 0.1Å spheres

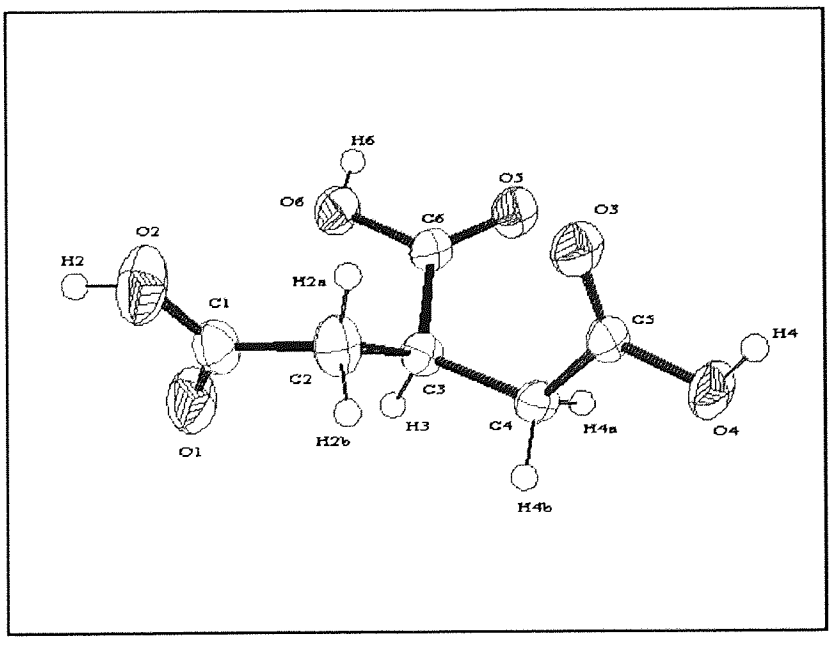


FIGURE 4.15 ORTEP III view of tricarballylic acid (TRIC2XL) showing labelling scheme. Thermal ellipsoids drawn at the 50% probability level and H atoms shown as 0.1Å spheres

TABLE 4.6 Selected bond lengths (Å), bond and torsion angles (°) for CITXL and TRIC2XL

Bond length/torsion angle	CITXL	TRIC2XL
O(1)-C(1)	1.208(6)	1.215(4)
O(2)-C(1)	1.318(6)	1.300(4)
O(2)-C(7)	1.463(7)	-
O(3)-C(5)	1.194(6)	1.217(3)
O(4)-C(5)	1.334(6)	1.314(3)
O(4)-C(8)	1.457(8)	-
O(5)-C(6)	1.209(5)	1.210(3)
O(6)-C(6)	1.315(6)	1.318(3)
O(7)-C(3)	1.417(6)	-
C(1)-C(2)	1.497(8)	1.505(4)
C(2)-C(3)	1.548(7)	1.539(4)
C(3)-C(6)	1.518(6)	1.508(4)
C(3)-C(4)	1.518(7)	1.523(4)
C(4)-C(5)	1.497(7)	1.499(4)
O(1)-C(1)-C(2)-C(3)	120.8(6)	34.5(5)
O(2)-C(1)-C(2)-C(3)	-60.0(6)	-147.2(3)
C(1)-C(2)-C(3)-C(6)	67.6(6)	76.0(4)
C(1)-C(2)-C(3)-C(4)	-169.4(4)	-155.5(3)
C(6)-C(3)-C(4)-C(5)	-56.5(6)	70.2(3)
C(2)-C(3)-C(4)-C(5)	-179.9(4)	-58.3(4)
C(3)-C(4)-C(5)-O(3)	33.8(8)	-2.0(4)
C(3)-C(4)-C(5)-O(4)	-149.2(4)	178.2(2)
C(4)-C(3)-C(6)-O(5)	120.6(6)	3.8(4)
C(2)-C(3)-C(6)-O(5)	-118.2(5)	133.7(3)
C(4)-C(3)-C(6)-O(6)	-58.0(6)	-178.1(2)
C(2)-C(3)-C(6)-O(6)	63.1(6)	-48.2(3)
C(7)-O(2)-C(1)-O(1)	-2.5(8)	-

Bond angle	CITXL	TRIC2XL
C(1)-O(2)-C(7)	116.1(4)	-
C(5)-O(4)-C(8)	115.5(5)	-
O(1)-C(1)-O(2)	124.0(5)	123.9(3)
O(1)-C(1)-C(2)	124.2(5)	122.3(3)
O(2)-C(1)-C(2)	111.8(5)	113.8(3)
C(1)-C(2)-C(3)	113.0(4)	112.8(2)
O(7)-C(3)-C(6)	108.8(4)	-
O(7)-C(3)-C(4)	109.6(4)	-
C(6)-C(3)-C(4)	111.4(4)	111.8(2)
O(7)-C(3)-C(2)	107.0(4)	-
C(6)-C(3)-C(2)	111.9(4)	111.9(2)
C(4)-C(3)-C(2)	108.1(4)	114.5(2)
C(5)-C(4)-C(3)	114.3(4)	115.9(2)
O(3)-C(5)-O(4)	123.4(5)	123.6(3)
O(3)-C(5)-C(4)	124.7(5)	124.4(2)
O(4)-C(5)-C(4)	111.8(5)	112.1(2)
O(5)-C(6)-O(6)	124.8(4)	124.0(3)
O(5)-C(6)-C(3)	123.0(4)	123.9(2)
O(6)-C(6)-C(3)	112.1(4)	112.1(2)

TABLE 4.6 continued

C(7)-O(2)-C(1)-C(2)	178.3(5)	-
C(1)-C(2)-C(3)-O(7)	-51.5(6)	-
O(7)-C(3)-C(4)-C(5)	63.9(6)	-
C(8)-C(4)-C(5)-O(3)	1.8(8)	-
C(8)-O(4)-C(5)-C(4)	-175.2(5)	-
O(7)-C(3)-C(6)-O(6)	-178.9(4)	-

TABLE 4.7 Distances of intermolecular hydrogen bonds involved in packing of CITXL and TRIC2XL

Hydrogen bonds	CITXL	TRIC2XL
O_2-H_2...O_1^{i}	-	1.762
O_6-H_6...O_3^{iii}	-	1.963
O_4-H_4...O_5^{ii}	-	1.899
O_4-H_4...O_2^{iii}	-	1.899
C_5-H_6...O_3^{ii}	-	1.963
O_6-H_6...O_8	1.567	-
O_8-H_{8A}...O_5^{iv}	1.676	-
O_8-H_{8B}...O_7^{v}	1.593	-

Symmetry operators:

(i) 2 - x, 1 - y, -1 - z (ii) –0.5 + x, y, 0.5 – z (iii) 0.5 + x, y, 0.5 – z (iv) –x, -y, -z

(v) x, -1 + y, z

4.6.3 Discussion

To date, no structure has previously been reported for CITXL, while only one has been reported for TRIC2XL (Barnes, 1988; GEMXEB), although this structure produced a lower final *R* value of 6.2%. Comparisons of TRIC2XL with CITXL, which differs only in the presence of a hydroxyl group on C_3, show very similar bond lengths and angles, but differ somewhat in terms of torsion angles. In particular, the 5-carbon chain of CITXL is fully extended, while the chain of TRIC2XL has one trans and one gauche torsion angle. The carbon-carbon bonds adjacent to the terminal carboxyl groups for both structures are significantly shorter than those around the central carbon atom. The carboxylic group on TRIC2XL at the C_1 position is linked to the same group on an adjacent molecule forming a dimer similar to that discussed in section 4.4.3. The presence of the methyl groups at the O_2 and O_4 positions sterically hinders hydrogen bond formation, although its free acid counterpart, anhydrous citric acid shows similar hydrogen bond dimer formation as above (Glusker *et al* (1969, CITRAC10).

4.7 CALIX-4-ARENE (PYRXL)

4.7.1 Introduction

Calixarenes are a class of synthetic macrocycles having phenolic residues in a cyclic array linked by methylene groups at positions *ortho* of the hydroxyl groups. The central phenyl groups of calixarenes produce π clouds (Schneider, 1988) making them suitable candidates for possible inclusion of Al. Indeed two crystal structures of calix-4-arenes with Al have been solved (Gardiner, 1996), whereby Al is bound *endo* and *exo* cavity (TOFYIW and TOFYES, respectively). On this basis, the structure of unsubstituted calix-4-arene was determined.

4.7.2 Crystal data for PYRXL

A single crystal (0.625mm x 0.35mm x 0.275mm) of PYRXL crystallised in the hexagonal $P6_3/m$ space group (number 176), $Z = 6$. At 293 K, the geometric parameters were $a = 14.473(1)$ Å, $b = 14.473(4)$ Å, $c = 18.80(1)$ Å, $\alpha = \beta = 90°$, $\gamma = 120°$ and $V = 3411.5$ Å^3. The formula weight was 2546.83, the calculated density was 1.240 Mgm^{-3}, agreeing well with the experimentally determined density of 1.231 Mgm^{-3} as determined using the flotation method described in section 2.3.2. The absorption coefficient was $\mu = 0.08$ mm^{-1}, $R(F) = 0.0589$; $wR(F^2) = 0.1816$.

Unit cell dimensions were obtained from least squares analysis of setting angles of 25 unique reflections with $9.63° \leq \theta \leq 13.98°$. Intensity data were collected by the ω-2θ scan technique with ω scan range of 1.35 + 0.35 tanθ and a ω scan speed of 0.33 to 2.75deg min^{-1} with graphite monochromated Mo-Kα radiation. Significant alterations in the intensity and orientation standards did not occur, but by the end of the data collection the intensity standards had reduced by approximately 3.7%. These were compensated using a linear and isotropic decay estimate. A total of 7898 reflections were collected $-6 \leq h \leq 6$, $-8 \leq k \leq 8$, $0 \leq l \leq 11$ in the range $2 < \theta < 27°$ and were merged to give 2545 unique reflections (R_{int} = 10.91%) of which 1412 were

deemed observed with Fo > 4σ (Fo). Data reduction was performed by DATREDXL. All non-hydrogen atoms were located by direct methods using the SHELXS-86 program.

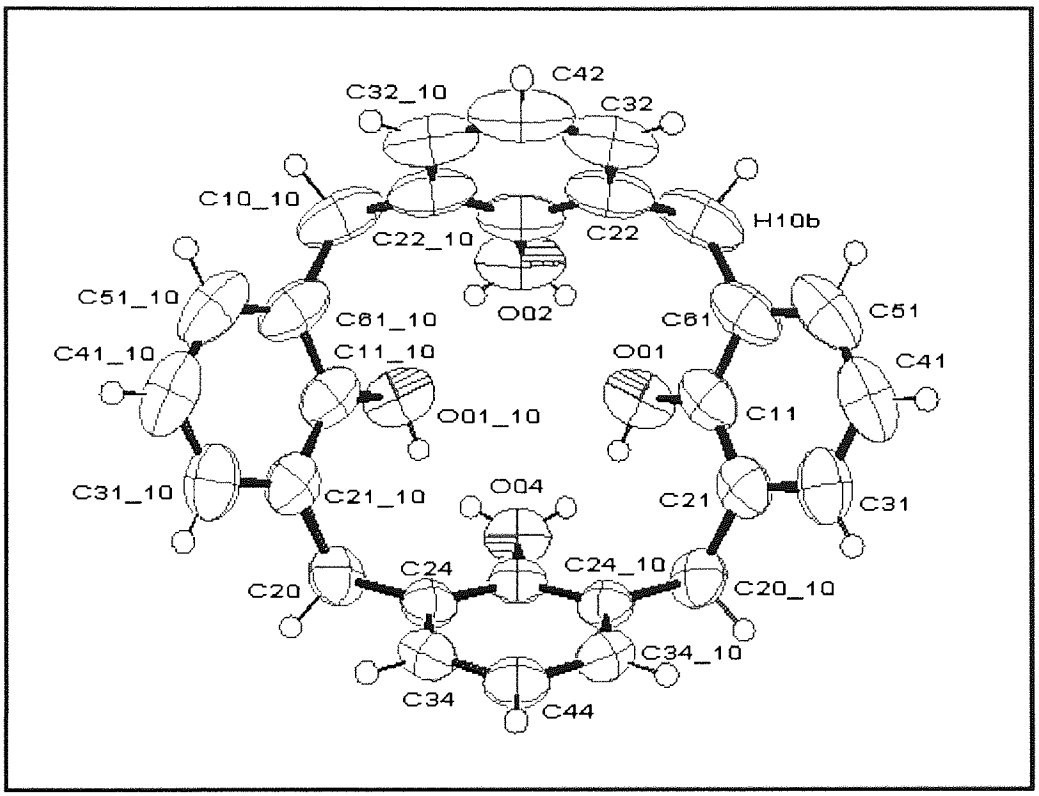


FIGURE 4.16 ORTEP III view of calix-4-arene (PYRXL) showing labelling scheme. Thermal ellipsoids drawn at the 50% probability level and H atoms shown as 0.1Å spheres. Disordered acetonitrile solvent has been excluded.

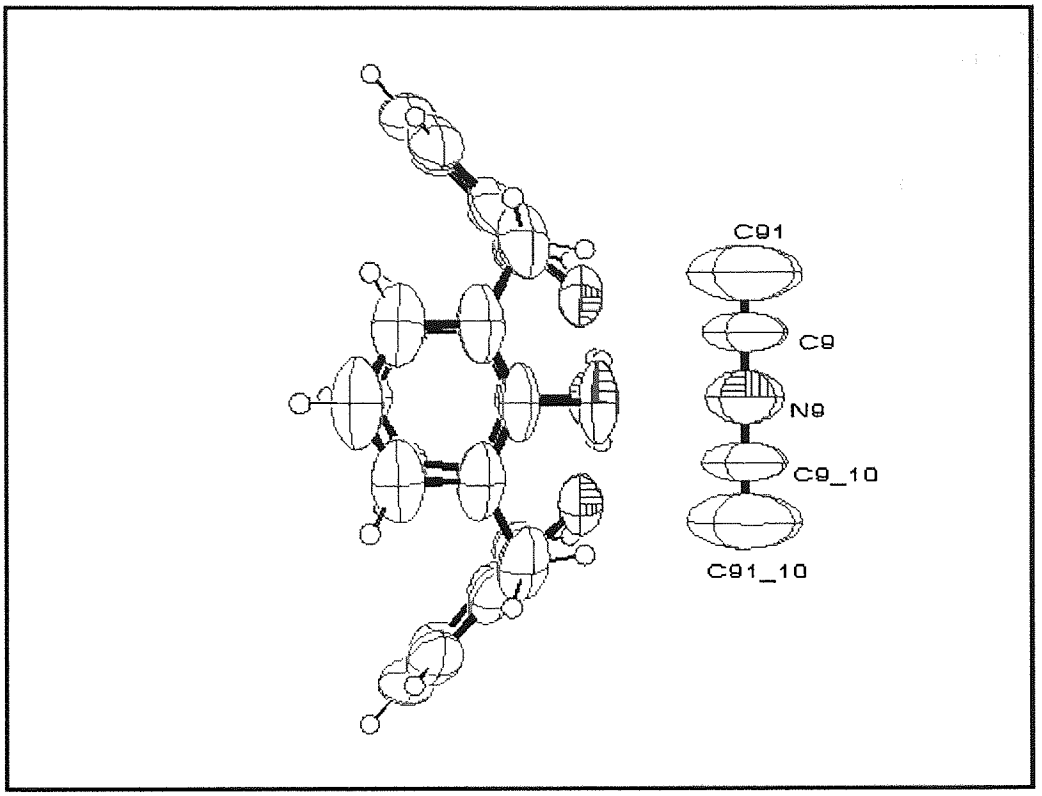


FIGURE 4.17 ORTEP III view of calix-4-arene (PYRXL) showing labelling scheme on the disordered acetonitrile. Thermal ellipsoids drawn at the 50% probability level and H atoms shown as 0.1Å spheres

TABLE 4.8 Selected bond lengths (Å) and bond angles (°) for PYRXL

	Bond length
O(01)-C(11)	1.373(3)
C(11)-C(21)	1.390(4)
C(11)-C(61)	1.393(4)
C(21)-C(31)	1.384(4)
C(21)-C(20)#1	1.510(4)
C(31)-C(41)	1.377(5)
C(41)-C(51)	1.376(5)
C(51)-C(61)	1.374(5)
C(61)-C(10)	1.520(5)
C(10)-C(22)	1.513(5)

	Bond angle
O(01)-C(11)-C(21)	119.5(2)
O(01)-C(11)-C(61)	118.2(3)
C(21)-C(11)-C(61)	122.3(3)
C(31)-C(21)-C(11)	117.3(3)
C(31)-C(21)-C(20)#1	121.5(3)
C(11)-C(21)-C(20)#1	121.2(2)
C(41)-C(31)-C(21)	121.7(3)
C(51)-C(41)-C(31)	119.3(3)
C(41)-C(51)-C(61)	121.6(3)
C(51)-C(61)-C(11)	117.7(3)

TABLE 4.8 continued

	Bond length
O(02)-C(12)	1.382(4)
C(12)-C(22)#1	1.390(4)
C(12)-C(22)	1.391(4)
C(22)-C(32)	1.398(4)
C(32)-C(42)	1.369(4)
C(42)-C(32)#1	1.369(4)
C(20)-C(21)#1	1.508(4)
C(20)-C(24)	1.520(3)
O(04)-C(14)	1.390(3)
C(14)-C(24)#1	1.393(3)
C(14)-C(24)	1.394(3)
C(24)-C(34)	1.385(3)
C(34)-C(44)	1.372(3)
C(44)-C(34)#1	1.373(3)
N(1)-C(12)#1	1.113(10)
N(1)-C(12)	1.113(10)
C(12)-C(4)#2	1.223(12)
C(12)-C(4)#3	1.225(12)
C(12)-C(4)	1.225(12)
C(4)-C(4)#2	1.57(3)
C(4)-C(4)#3	1.57(3)

	Bond angle
C(51)-C(61)-C(10)	120.5(3)
C(11)-C(61)-C(10)	121.7(3)
C(22)-C(10)-C(61)	113.1(2)
O(02)-C(12)-C(22)#1	118.7(2)
O(02)-C(12)-C(22)	118.7(2)
C(22)#1-C(12)-C(22)	122.6(4)
C(12)-C(22)-C(32)	117.2(4)
C(12)-C(22)-C(10)	122.2(3)
C(32)-C(22)-C(10)	120.6(3)
C(42)-C(32)-C(22)	121.7(4)
C(32)-C(42)-C(32)#1	119.5(5)
C(21)#1-C(20)-C(24)	113.6(2)
O(04)-C(14)-C(24)#1	118.92(13)
O(04)-C(14)-C(24)	118.99(13)
C(24)#1-C(14)-C(24)	122.1(3)
C(34)-C(24)-C(14)	117.6(2)
C(34)-C(24)-C(20)	120.2(2)
C(14)-C(24)-C(20)	122.2(2)
C(44)-C(34)-C(24)	121.5(2)
C(34)-C(44)-C(34)#1	119.6(3)
C(12)#1-N(1)-C(12)	179.998(2)
N(1)-C(12)-C(4)#2	132.1(10)
N(1)-C(12)-C(4)#3	132.1(10)
C(4)#2-C(12)-C(4)#3	79.9(15)
N(1)-C(12)-C(4)	132.1(10)
C(4)#2-C(12)-C(4)	79.9(15)
C(4)#3-C(12)-C(4)	79.9(15)
C(12)-C(4)-C(4)#2	50.0(8)
C(12)-C(4)-C(4)#3	50.0(8)
C(4)#2-C(4)-C(4)#3	59.972(10)

Symmetry transformations used to generate equivalent atoms:

#1 x, y, -z + 1/2 #2 –x + y, -x + 1, z #3 –y + 1, x – y +1, z

4.7.3 Discussion

A similar structure has previously been reported by Harrowfield *et al* (1993; PEZWIA), their final *R* value was reported as 4.4%. Again, a disordered acetonitrile group was reported.

Figures 4.16 and 4.17 show the structure of calix-4-arene without and with the disordered acetonitrile group. The thermal displacement values of the acetonitrile group are extremely high also illustrated by figure 4.17. Table 4.8 identifies the *exo* acetonitrile group possessing the C9 and N9 group in special positions (Wyckoff notation *f*). The angle produced by the N9-C9-C91 acetonitrile unique atoms is 132.1°, differing somewhat from the 180° angle that would be expected for this group. Consequently, further refinement attempts were made, placing C91 in the special position also (Wyckoff notation *f*). This resulted in an increase in the final *R* from 5.89 to 6.63, as well as an increase in thermal displacement values of N9-C9-C91. The resultant bond length of C9-C91 reduced from 1.225Å to 1.076Å suggesting that this refinement was incorrect.

4.8 BUTYLCIPROFLOXACIN (BUCIP4) AND NALIDIXIC ACID (NAL3XL)

4.8.1 Introduction

Both nalidixic acid and butylciprofloxacin are based on a quinolone structure and possess negative donor oxygen atoms capable of donating electrons to bind to an electropositive Al. Butylciprofloxacin is a derivative of ciprofloxacin, a potent antibiotic used routinely to treat infections and is contraindicated for use in conjunction with Al containing antacids due to the formation of insoluble complexes (BNF, 1999).

4.8.2 Crystal data for BUCIP4

A single crystal (0.25mm x 0.175mm x 0.125mm) of BUCIP4 [$C_{42}H_{52}O_6F_2N_6$] crystallised in the triclinic space group number 2, $P\bar{1}$, Z = 2. At 293 K, the geometric parameters were a = 4.369(1) Å, b = 9.240(1) Å, c = 24.317(3) Å, α = 80.59(1)°, β = 89.45(2)°, γ = 89.40(1)° and V = 968.39 Å^3. The formula weight was 774.90, the calculated density was 1.329 Mgm^{-3}, agreeing well with the experimentally determined density of 1.331 Mgm^{-3} as determined using the flotation method described in section 2.3.2. The absorption coefficient was μ = 0.10 mm^{-1}, $R(F)$ = 0.0600; $wR(F^2)$ = 0.199.

Unit cell dimensions were obtained from least squares analysis of setting angles of 25 unique reflections with $2.6° \leq \theta \leq 17.2°$. Intensity data were collected by the ω-2θ scan technique with ω scan range of 1.35 + 0.35 tanθ and a ω scan speed of 0.32 to 1.37deg min^{-1} with graphite monochromated Mo-Kα radiation. Three intensity standards were measured every two hours and in every 200 experimental reflections 3 orientation monitor reflections were located. Significant alterations did not occur, but by the end of the data collection the intensity standards had reduced by approximately

4.2%. These were compensated using a linear and isotropic decay estimate. A total of 3989 reflections were collected $-5 \leq h \leq 5$, $-10 \leq k \leq 10$, $-28 \leq l \leq 1$ in the range $2 < \theta < 25°$ and were merged to give 3389 unique reflections (R_{int} = 6.43%) of which 1104 were deemed observed with Fo > 4σ (Fo). Data reduction was performed with DATREDXL. All non-hydrogen atoms were located by direct methods using the SHELXS-86 program. All H atoms were located using SHELXL using the DFIX command.

4.8.3 Crystal data for NAL3XL

A single crystal (0.275mm x 0.225mm x 0.175mm) of NAL3XL crystallised in the monoclinic space group $P2_1/c$, Z = 4. At 293 K, the geometric parameters were a = 8.907(3) Å, b = 13.159(2) Å, c = 9.359(2) Å, $\alpha = \gamma = 90°$, β = 100.02(2)°, and V = 1080.36 Å^3. The formula weight was 928.94, the calculated density was 1.428 Mgm^{-3}, agreeing well with the experimentally determined density of 1.436 Mgm^{-3} as determined using the flotation method described in section 2.3.2. The absorption coefficient was μ = 0.13 mm^{-1}, $R(F)$ = 0.0539; $wR(F^2)$ = 0.1688.

Unit cell dimensions were obtained from least squares analysis of setting angles of 25 unique reflections with $6.6° \leq \theta \leq 17.4°$. Intensity data were collected by the ω-2θ scan technique with ω scan range of 1.35 + 0.35 tanθ and a ω scan speed of 0.59 to 1.83 deg min^{-1} with graphite monochromated Mo-Kα radiation. Three intensity standards were measured every two hours and in every 200 experimental reflections 3 orientation monitor reflections were located. Significant alterations did not occur, but by the end of the data collection the intensity standards had reduced by approximately 2%. These were compensated using a linear and isotropic decay estimate. A total of 3481 reflections were collected $-1 \leq h \leq 10$, $-15 \leq k \leq 15$, $-11 \leq l \leq 11$ in the range $2 < \theta < 25°$ and were merged to give 1893 unique reflections (R_{int} = 5.06%) of which 827 were deemed observed with Fo > 4σ (Fo). Data reduction was performed by DATREDXL. All non-hydrogen atoms were located by direct methods using the SHELXS-86 program.

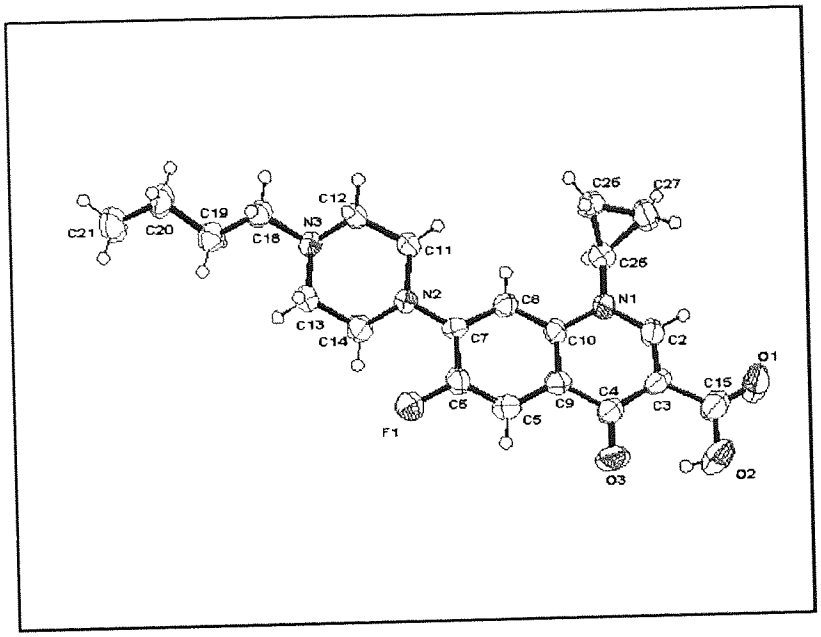


FIGURE 4.18 ORTEP III view of butylciprofloxacin (BUCIP4) showing labelling scheme. Thermal ellipsoids drawn at the 50% probability level and H atoms shown as 0.1Å spheres

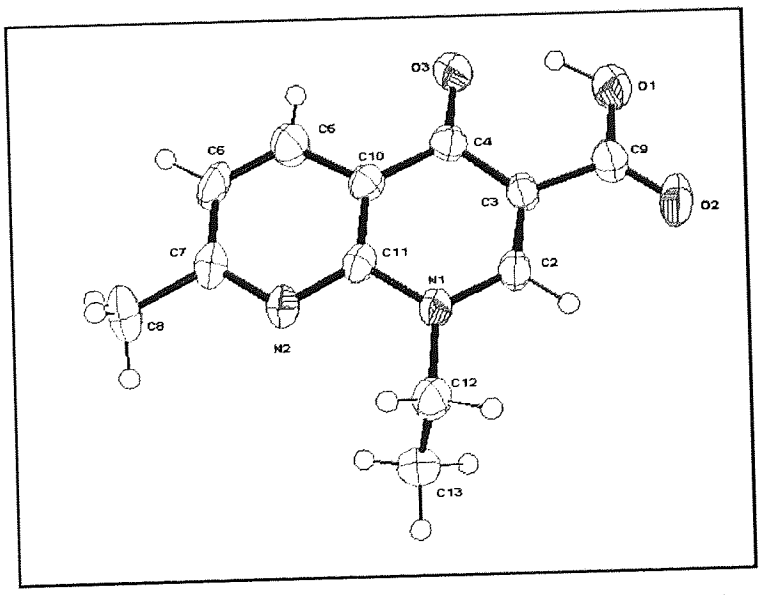


FIGURE 4.19 ORTEP III view of nalidixic acid (NAL3XL) showing labelling scheme. Thermal ellipsoids drawn at the 50% probability level and H atoms shown as 0.1Å spheres

TABLE 4.9 Selected bond lengths (Å), bond and torsion angles (°) for BUCIP4

	Bond length
N(1)-C(2)	1.342(6)
N(1)-C(10)	1.403(6)
N(1)-C(25)	1.451(6)
C(2)-C(3)	1.366(7)
C(3)-C(4)	1.415(8)
C(3)-C(15)	1.478(8)
C(4)-O(3)	1.268(7)
C(4)-C(9)	1.447(7)
C(9)-C(10)	1.389(7)
C(9)-C(5)	1.415(8)
C(5)-C(6)	1.352(7)
C(6)-F(1)	1.363(6)
C(6)-C(7)	1.423(7)
C(7)-N(2)	1.383(6)
C(7)-C(8)	1.393(7)
C(8)-C(10)	1.405(6)
C(15)-O(1)	1.188(8)
C(15)-O(2)	1.345(8)
C(15)-C(16)	1.479(7)
C(15)-C(17)	1.482(7)
C(16)-C(17)	1.478(8)
N(2)-C(14)	1.458(6)
N(2)-C(11)	1.462(6)
C(11)-C(2)	1.504(7)
C(2)-N(3)	1.458(7)

	Bond angle
C(2)-N(1)-C(10)	119.3(5)
C(2)-N(1)-C(15)	121.0(5)
C(10)-N(1)-C(15)	119.7(4)
N(1)-C(2)-C(3)	124.1(6)
C(2)-C(3)-C(4)	120.3(5)
C(2)-C(3)-C(15)	117.1(6)
C(4)-C(3)-C(15)	122.6(6)
O(3)-C(4)-C(3)	123.6(6)
O(3)-C(4)-C(9)	121.2(6)
C(3)-C(4)-C(9)	115.2(6)
C(10)-C(9)-C(5)	117.2(5)
C(10)-C(9)-C(4)	122.4(6)
C(5)-C(9)-C(4)	120.4(6)
C(6)-C(5)-C(9)	120.5(6)
C(5)-C(6)-F(1)	117.5(6)
C(5)-C(6)-C(7)	124.0(6)
F(1)-C(6)-C(7)	118.5(5)
N(2)-C(7)-C(8)	123.1(5)
N(2)-C(7)-C(6)	121.7(5)
C(8)-C(7)-C(6)	115.0(5)
C(7)-C(8)-C(10)	121.9(5)
C(9)-C(10)-N(1)	118.6(5)
C(9)-C(10)-C(8)	121.5(5)
N(1)-C(10)-C(8)	119.9(5)
O(1)-C(15)-O(2)	120.8(6)

TABLE 4.9 continued

N(3)-C(13)	1.462(7)
N(3)-C(18)	1.470(6)
C(13)-C(14)	1.512(7)
C(18)-C(19)	1.508(7)
C(19)-C(20)	1.506(7)
C(20)-C(21)	1.505(8)

O(1)-C(15)-C(3)	125.5(7)
O(2)-C(15)-C(3)	113.7(7)
N(1)-C(15)-C(16)	120.6(5)
N(1)-C(15)-C(17)	120.0(5)
C(16)-C(15)-C(17)	59.9(4)
C(17)-C(16)-C(15)	60.2(4)
C(16)-C(17)-C(15)	59.9(4)
C(7)-N(2)-C(14)	120.9(5)
C(7)-N(2)-C(11)	117.3(5)
C(14)-N(2)-C(11)	110.5(4)
N(2)-C(11)-C(2)	110.6(5)
N(3)-C(2)-C(11)	112.6(5)
C(2)-N(3)-C(13)	107.9(4)
C(2)-N(3)-C(18)	109.5(5)
C(13)-N(3)-C(18)	111.4(4)
N(3)-C(13)-C(14)	110.2(5)
N(2)-C(14)-C(13)	110.8(5)
N(3)-C(18)-C(19)	115.3(5)
C(20)-C(19)-C(18)	112.8(5)
C(21)-C(20)-C(19)	113.9(6)
C(25)-N(1)-C(2)-C(3)	-179.3(5)
N(1)-C(2)-C(3)-C(15)	179.5(5)
C(2)-C(3)-C(4)-O(3)	-177.9(6)
C(15)-C(3)-C(4)-O(3)	3.3(8)
O(3)-C(4)-C(9)-C(5)	-1.6(8)
C(9)-C(5)-C(6)-F(1)	-177.8(5)
C(5)-C(6)-C(7)-N(2)	-174.1(5)
F(1)-C(6)-C(7)-N(2)	3.2(8)
N(2)-C(11)-C(12)-N(3)	-56.5(6)
N(1)-C(25)-C(26)-C(27)	109.1(5)
C(18)-C(19)-C(20)-C(21)	-176.9(6)

TABLE 4.10 Selected bond lengths (Å) bond and torsion angles (°) for NAL3XL

C(13)-C(12)	1.491(7)
C(12)-N(1)	1.490(6)
N(1)-C(2)	1.349(5)
N(1)-C(11)	1.392(5)
C(2)-C(3)	1.363(6)
C(3)-C(4)	1.431(6)
C(3)-C(9)	1.478(6)
C(4)-O(3)	1.260(5)
C(4)-C(10)	1.445(6)
C(10)-C(11)	1.386(6)
C(10)-C(5)	1.401(6)
C(5)-C(6)	1.354(7)
C(6)-C(7)	1.392(6)
C(7)-N(2)	1.337(5)
C(7)-C(8)	1.506(6)
N(2)-C(11)	1.352(5)
C(9)-O(2)	1.208(5)
C(9)-O(1)	1.325(6)

N(1)-C(12)-C(13)	112.2(4)
C(2)-N(1)-C(11)	119.4(4)
C(2)-N(1)-C(12)	119.4(4)
C(11)-N(1)-C(12)	121.2(4)
N(1)-C(2)-C(3)	123.6(4)
C(2)-C(3)-C(4)	120.2(4)
C(2)-C(3)-C(9)	118.4(4)
C(4)-C(3)-C(9)	121.3(4)
O(3)-C(4)-C(3)	122.9(4)
O(3)-C(4)-C(10)	121.9(4)
C(3)-C(4)-C(10)	115.3(4)
C(11)-C(10)-C(5)	116.2(4)
C(11)-C(10)-C(4)	121.8(4)
C(5)-C(10)-C(4)	122.0(4)
C(6)-C(5)-C(10)	119.8(5)
C(5)-C(6)-C(7)	119.7(5)
N(2)-C(7)-C(6)	122.8(4)
N(2)-C(7)-C(8)	116.3(5)
C(6)-C(7)-C(8)	120.8(5)
C(7)-N(2)-C(11)	116.1(4)
N(2)-C(11)-C(10)	125.2(4)
N(2)-C(11)-N(1)	115.2(4)
C(10)-C(11)-N(1)	119.5(4)
O(2)-C(9)-O(1)	121.1(4)
O(2)-C(9)-C(3)	123.5(5)
O(1)-C(9)-C(3)	115.4(4)

TABLE 4.10 continued

	Torsion angles
C(13)-C(12)-N(1)-C(2)	-98.5(5)
C(13)-C(12)-N(1)-C(11)	81.2(6)
C(11)-N(1)-C(2)-C(3)	1.3(6)
C(12)-N(1)-C(2)-C(3)	-179.1(4)
N(1)-C(2)-C(3)-C(4)	2.6(6)
N(1)-C(2)-C(3)-C(9)	-179.1(4)
C(2)-C(3)-C(4)-O(3)	175.3(4)
C(9)-C(3)-C(4)-O(3)	-2.9(6)
C(2)-C(3)-C(4)-C10	-4.3(6)
C(9)-C(3)-C(4)-C(10)	-4.3(6)
O(3)-C(4)-C(10)-C(11)	-177.2(4)
C(3)-C(4)-C(10)-C(11)	2.4(6)
O(3)-C(4)-C(10)-C(5)	3.7(7)
C(3)-C(4)-C(10)-C(5)	-176.6(4)
C(4)-C(10)-C(5)-C(6)	179.1(4)
C(12)-N(1)-C(11)-N(2)	-1.7(6)
C(12)-N(1)-C(11)-C(10)	177.2(4)

4.9.4 Discussion

Structures for nalidixic acid have previously been reported, (NALIDX, Achari, 1976; NALIDX01, Huber, 1980; NALIDX02, Yong, 1986) with that reported by Huber (1980) producing the best *R* of 3.9%. As expected, the pyridine rings are planar in both structures.

The cyclohexyl ring in BUCIP4 is in the chair conformation producing a torsion angle N(2)-C(11)-C(12)-N(3) of 56.6°. An intramolecular hydrogen bond also exists between atoms O2-H2A...O3 producing a distance of 1.763Å and an angle of 173.8°. No apparent intermolecular hydrogen bonds exist. The C4-O3 bond distance is 1.27Å, a distance larger than a typical carbonyl bond (1.21Å as shown in the previous structure of tartaric acid). The C3-C15 (1.48Å) in BUCIP4 is significantly shorter than the corresponding C1-C2 (1.58Å) and C3-C4 (1.52Å) bond lengths in ALTAR. This may in part, be attributed to sp^2-sp^2 rather than sp^2-sp^3 hybrids on the bonded carbon atoms, but may also be attributed to resonance effects as depicted in figure 4.17 below.

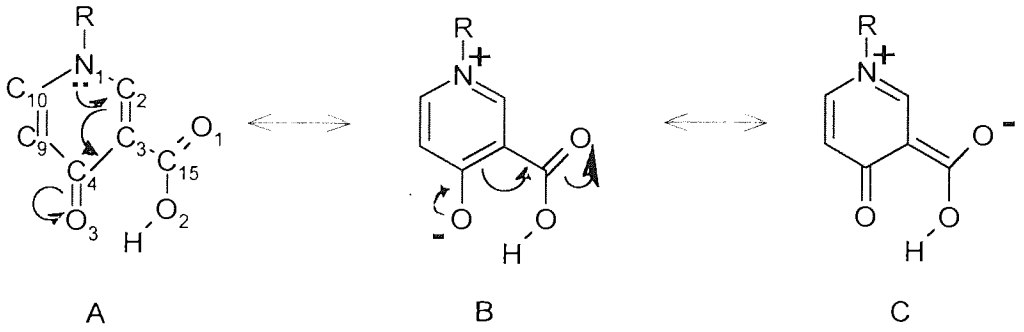


FIGURE 4.17 Resonance structures of part of the BUCIP4 molecule

C15-O1 is clearly a double bond indicating resonance structure C (figure 4.17) is of limited importance. Thus, structures A and B seem to be the likely resonance forms applicable.

CHAPTER FIVE

MOLECULAR ORBITAL STUDIES

5.1 INTRODUCTION

The database searching within chapter three has provided the foundations for these studies. They have shown that Al prefers to bind as a six co-ordinate octahedral complex with bidentate ligands possessing oxygen donor atoms. Al-O distances obtained from this work are depicted in Figure 5.1 below.

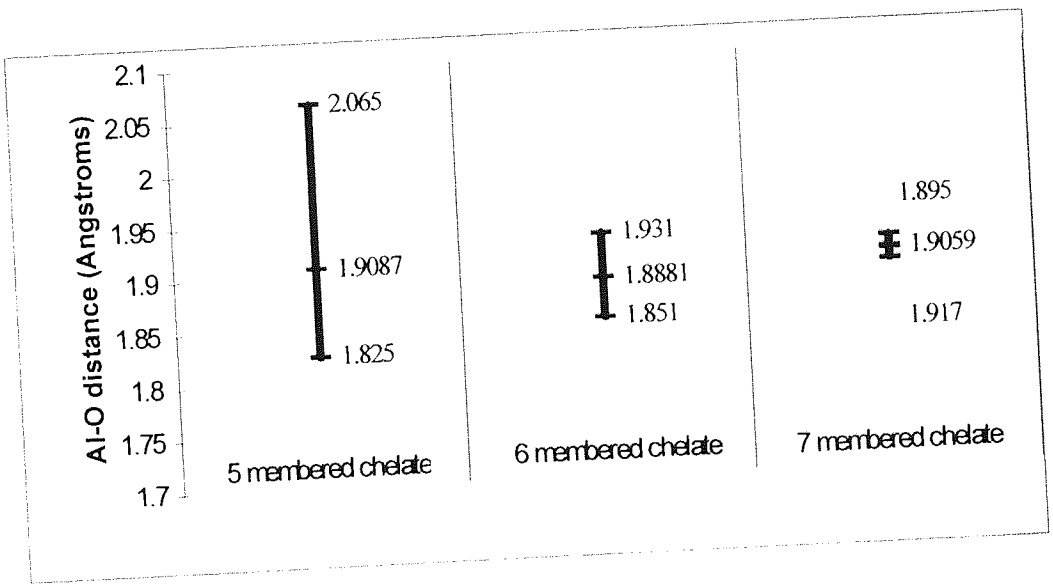


FIGURE 5.1 Mean Al-O distances of six co-ordinate Al complexes within the CSD showing upper and lower limits

Of the semi-empirical MO methods discussed in chapter one, only MNDO, AM1 and PM3 have been parameterised for Al. However, to date no comparison has been made as to which basis set, if indeed any, produces the correct geometry for an energy minimised octahedral six co-ordinated Al structure with both aliphatic and aromatic ligands.

5.2 AIM

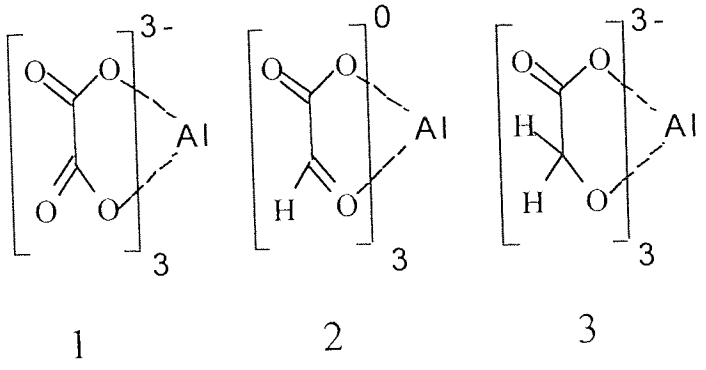
To date, very little work has been done on Al compounds involving complexation with organic ligands and MO calculations. Consequently, this study is a path finding exercise.

The structures modelled within these studies range from approximately twenty to fifty atoms. The lower range, consisting of Al complexes with oxalate (1), glycolate (2) and glyoxalate (3), were used to conduct the most powerful *ab initio* calculations, namely the 6-31G basis set. The studies review the semi-empirical methods available for geometric optimisation and energy minimisations of Al complexes. The resultant optimal geometry from the 6-31G calculations was used as the bench mark and compared to the other less powerful methods. Ultimately the most favourable semi-empirical method identified from the study was used for further calculations giving a balance between speed and accuracy of the model being tested.

Nitrogen as a functional atom in contact with a metal ion reduces the specificity of a ligand towards Al. Using this method, the effect of changing a carbonyl moiety to a hydroxamate functional group, the group responsible for DFO chelation to Al, can be studied.

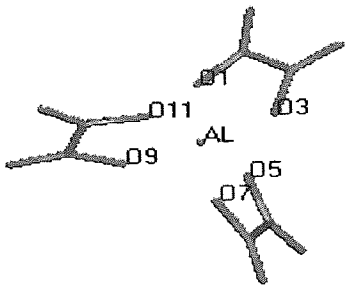
5.3 EVALUATION OF BASIS SETS

As already mentioned, the three simplest ligands were used in this study, namely oxalate, glyoxalate and glycolate. The 3:1 complexes of oxalate (1) and glycolate (3) with Al were extracted from the CSD and edited in CHEM-X prior to being subjected MO calculations [COKFOX (Bulc, 1984) and SERNAE (Venema, 1990), respectively]. The 3:1 complex of Al glyoxalate was made using (1) as a template. These co-ordinates were used as the starting points for GAMESS calculations using the semi-empirical Hamiltonians MNDO, AM1 and PM3, as well as using the more complex and computationally expensive *ab initio* basis sets 6-31G, 3-21G and STO-3G. The most powerful of these, 6-31G was used as the bench mark.

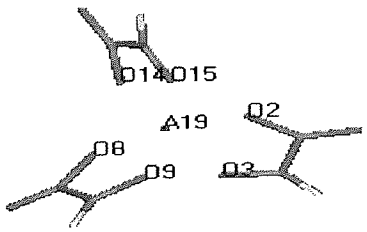


1 2 3

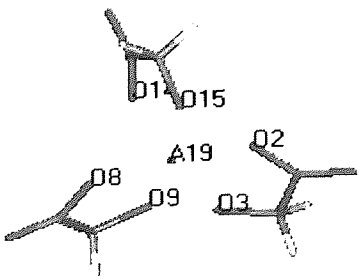
FIGURE 5.2 3:1 structures of Al complexes with oxalate (1), glyoxalate (2), and glycolate (3)



(1)



(2)



(3)

FIGURE 5.3 Stick diagrams of the octahedral 3:1 complexes of Al with (1) oxalate, (2) glyoxalate and (3) glycolate, showing numbering scheme of oxygen donor atoms (Weblab viewlite)

5.3.1 Comparison of computational time for MO optimisations.

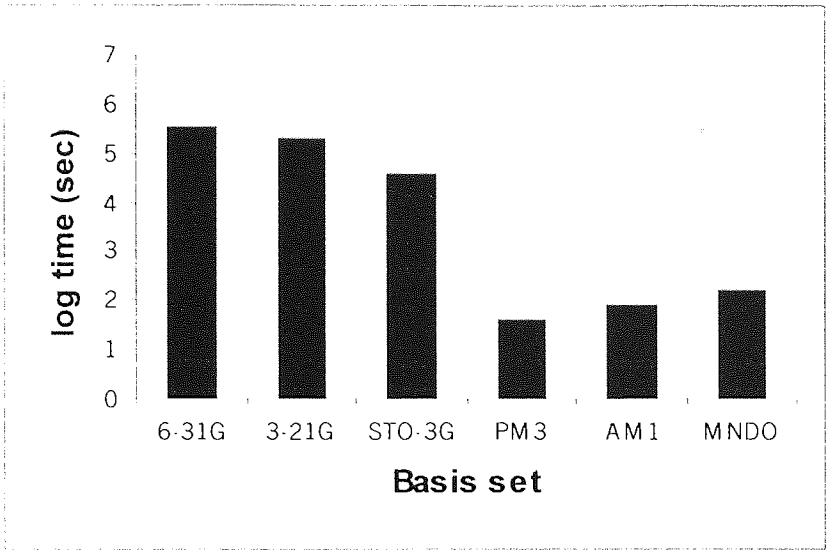


FIGURE 5.4 Computational time taken for each basis set to optimise (1) using crystallographic co-ordinates as starting points (COKFOX)

The use of semi-empirical methods has the primary advantage of reducing computational time to reach an energy minimised structure by several fold. As shown by figure 5.2, these methods take minutes to minimise Al structures containing about 20 atoms, whereas the *ab initio* methods employed take hours in the case of the STO-3G basis set to days in the case of the 3-21G and 6-31G sets.

TABLE 5.1 Comparison of Al-O bond lengths obtained from MO optimisations of 3:1 Al complexes of 1, 2, and 3

Structure	Al-O bond	MNDO	AM1	PM3	STO-3G	3-21G	6-31G
oxalate	O1	1.948	1.843	1.903	1.881	1.897	1.850
	O3	1.812	1.843	1.904	1.881	1.897	1.841
	O5	1.816	1.843	1.904	1.881	1.897	1.850
	O7	1.958	1.843	1.903	1.881	1.897	1.850
	O9	1.821	1.843	1.903	1.881	1.897	1.836
	O11	4.783*	1.843	1.903	1.881	1.897	1.850
glyoxalate	O2	1.948	1.761	1.776	1.795	1.815	1.830
	O3	1.812	2.538*	2.417*	2.035	2.040	2.147
	O8	1.816	1.789	1.785	1.799	1.828	1.850
	O9	1.959	1.867	2.406*	1.968	1.977	2.044
	O14	1.822	1.790	1.822	1.799	1.813	1.838
	O15	4.784*	1.878	1.933	1.965	1.977	2.042
glycolate	O2	1.955	1.804	1.855	1.919	1.950	2.022
	O3	1.884	1.820	2.004	1.871	1.870	1.900
	O8	1.960	1.771	1.892	1.918	1.951	2.024
	O9	1.884	2.438*	1.829	1.873	1.872	1.899
	O14	1.971	1.768	1.808	1.929	1.963	2.046
	O15	1.882	4.661*	2.019	1.870	1.870	1.896

* indicates bond length outside range outlined in Figure 5.1

The optimisation of (1) has resulted in all distances within the expected range, with the exception of the Al-O_{11} distance (4.783Å) obtained from the MNDO optimisation. Otherwise, each method gives nearly the same Al-O distance for the six chemically identical carboxylate oxygen atoms. Optimisations of structure three, the glycolate complex resulted in the AM1 Hamiltonian producing the poorest results with two Al-O out of the range discussed in Figure 5.1. All three semi-empirical methods produced poorer results for the glyoxalate complex (2) relative to the *ab initio* methods employed. The Al-O distances to the negatively charged carboxyl oxygen atoms are shorter than those to the aldehyde oxygen atoms, which are formally neutral and only gain negative charge through polarisation.

5.3.2 Comparison of Al oxalate optimised structures using different starting geometries

All optimisations involving Al started from the same crystallographic co-ordinates as COKFOX for the oxalate, and SERNAE for the glycolate complexes of Al. The manually constructed co-ordinates were used in all optimisations of the 3:1 Al complex with glyoxalate. To establish if the final geometry is dependent on the initial starting geometry, the 3-21G final co-ordinates were used as starting co-ordinates for a subsequent PM3 optimisation. The results were compared to the original PM3 optimisation discussed previously.

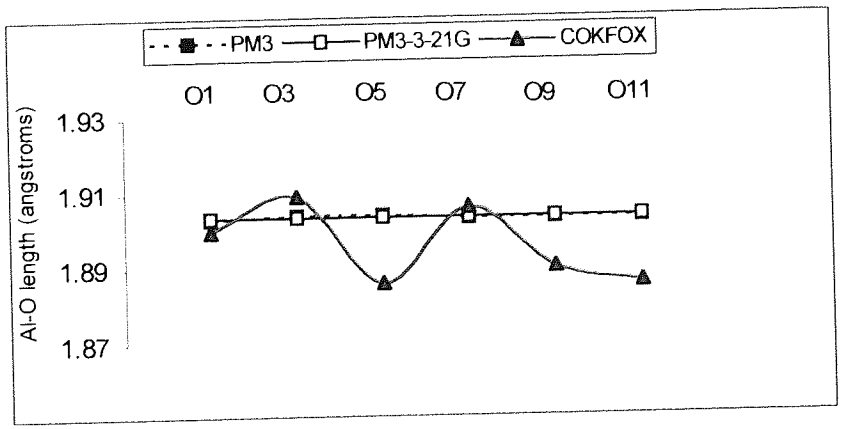


FIGURE 5.5 Effect on Al-O bond lengths after using different starting co-ordinates for MO calculations

The Al-O bond lengths values tend to be similar for both starting geometries and ΔH_f for both are the same (-624.27 Kcal mol^{-1}) suggesting that both optimise to produce a global minimum as opposed to a local minimum.

5.3.3 Tsar analysis of geometric results

Analysis of Al-O bond lengths in table 5.1 show AM1 and PM3 tend to produce a better optimal geometry relative to MNDO, however it is difficult to differentiate between AM1 and PM3 based on these bond lengths. Consequently the optimised co-ordinates were used for Tsar analysis as outlined in 2.4.3.

Prior to input of the cssr files into Tsar, the structures were using the 'rigid fit' command within Chem-X. Where existing crystal structures were available these were also compared to the optimised structures.

Each optimisation is coded, the first six letters indicating complex type, and final three digits denoting type of basis set used for optimisation. For instance, ALOXAL631 signifies an Al oxalate 3:1 complex optimised via the 6-31G basis set, while ALOXALPM3 signifies a structure optimised via the PM3 Hamiltonian.

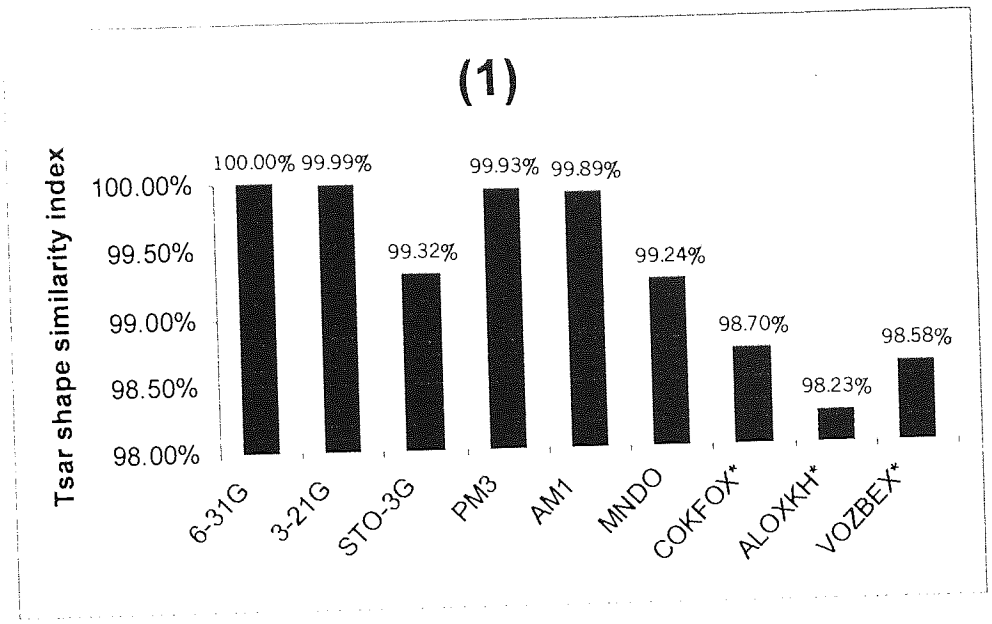


FIGURE 5.6 Tsar analysis of ALOXAL structures (1).* indicate CSD refcodes

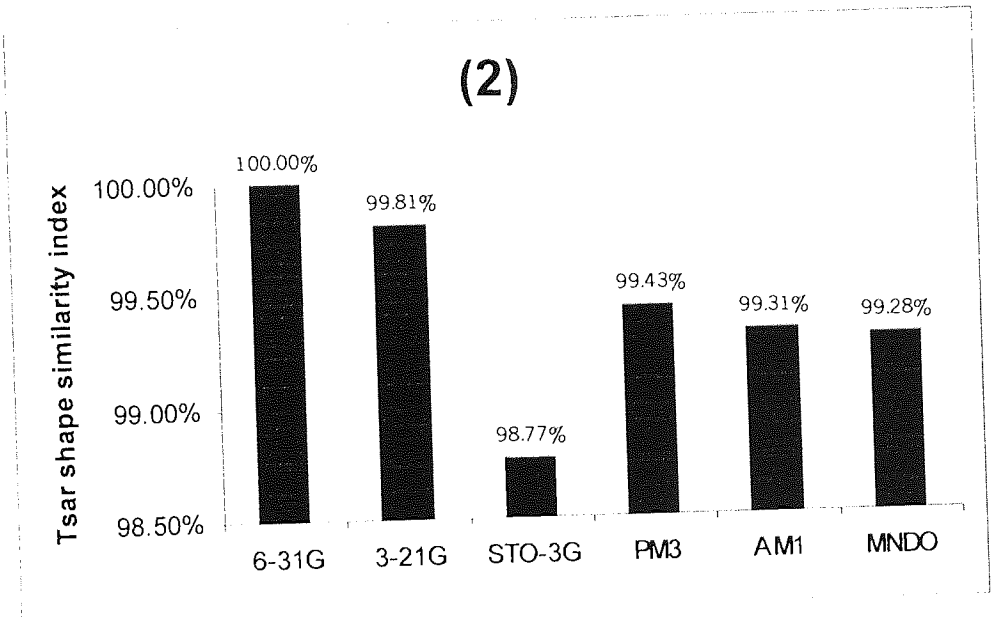


FIGURE 5.7 Tsar analysis of ALGLYO structures (2)

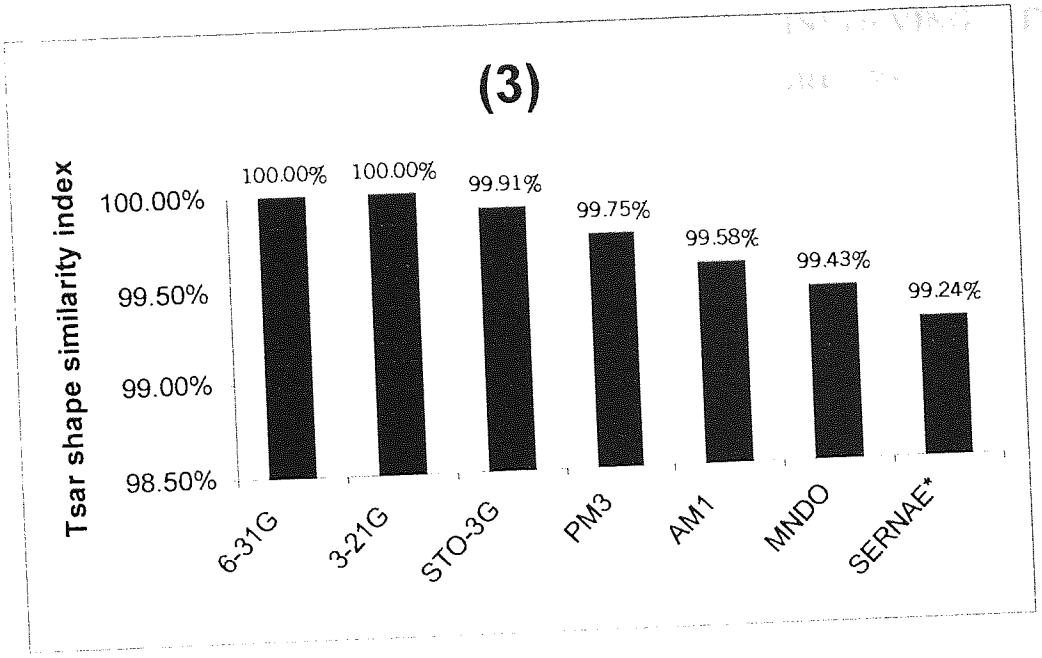


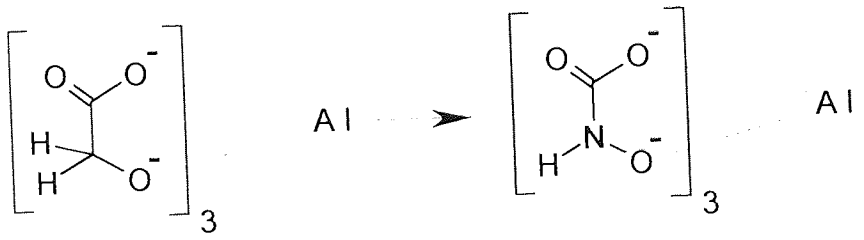
FIGURE 5.8 Tsar analysis of ALGLYC structures (3). * indicate CSD refcodes

Among the computationally rapid methods, in all cases the optimised structures using PM3 most closely resemble the optimal geometry resulting from 6-31G calculations. PM3 calculations prove to produce a better fit geometry than its semi-empirical predecessors, AM1 and MNDO, and more importantly than the more computationally expensive *ab initio* method STO-3G. Consequently, the PM3 Hamiltonian was selected as the semi-empirical method of choice and was used for further MO calculations on larger ligands within these studies.

5.4 MO COMPARISONS ON CALCULATIONS INVOLVING THE ALKOXIDE AND HYDROXAMATE FUNCTIONAL GROUPS

The hydroxamate moiety is a chelating function which has been widely adopted by bacteria and fungi for siderophore construction (Hider, 1994). The log K_1 values of hydroxamates with Group III metals are much lower than values for corresponding catechol chelates, as only one oxygen is protonated under physiological conditions ($pK_a = 9.35$) and therefore competition is much less marked. Hydroxamates also have the ability to form uncharged 3:1 complexes as discussed in the introductory chapter, a characteristic that would be greatly desirable to allow the complex to pass between cell membranes in the clinical situation. Hider *et al.*, (1991) showed there is a clear relationship between the pK_a values of the ligands and the K_1 value for Fe, indicating a dominant influence of electrostatic interaction between the metal and ligating atoms.

Using MO calculations, an electrostatic potential map of (3) and (4) can be compared to identify differences that may explain the differences in stability between the two types of complexes.



(3) (4)

FIGURE 5.9 Changing a carbon to a nitrogen and deprotonation results in the glycolate (3) being transformed to a hydroxamate (4) whereby both complexes retain an overall 3- charge

The 6-31G optimised glycolate complex (3) was manually edited using Chem-X to form the hydroxamate (4) (Figure 5.9). This complex was then subjected to PM3 optimisations to obtain ΔH_f for each of the complexes and to 3-21G optimisations to generate an electrostatic potential map.

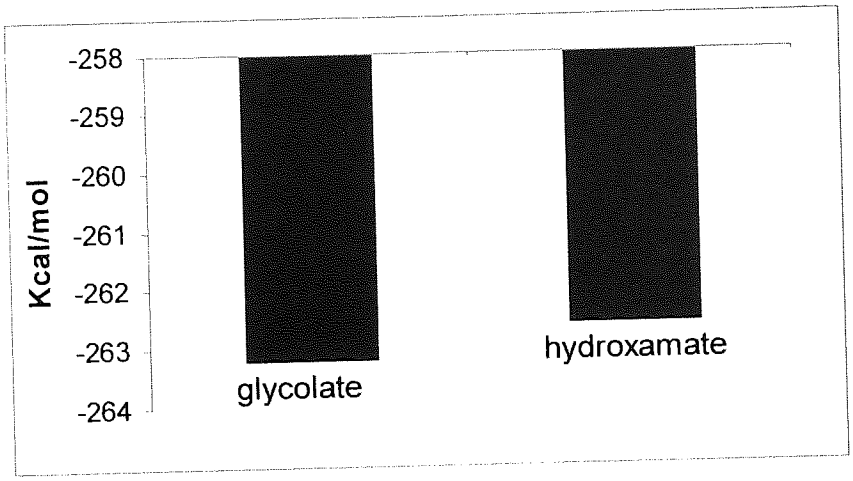


FIGURE 5.10 PM3 calculated ΔH_{eff} for structures (3) and (4)

The ΔH_{eff} produces similar results for PM3 optimisation of the alkoxide and the hydroxamate counterpart showing negligible difference in affinity for Al (-263.2 and –262.6 Kcal mol^{-1}, respectively). This is also outlined in similar potential maps of these structures produced via the *ab initio* 3-21G optimisations.

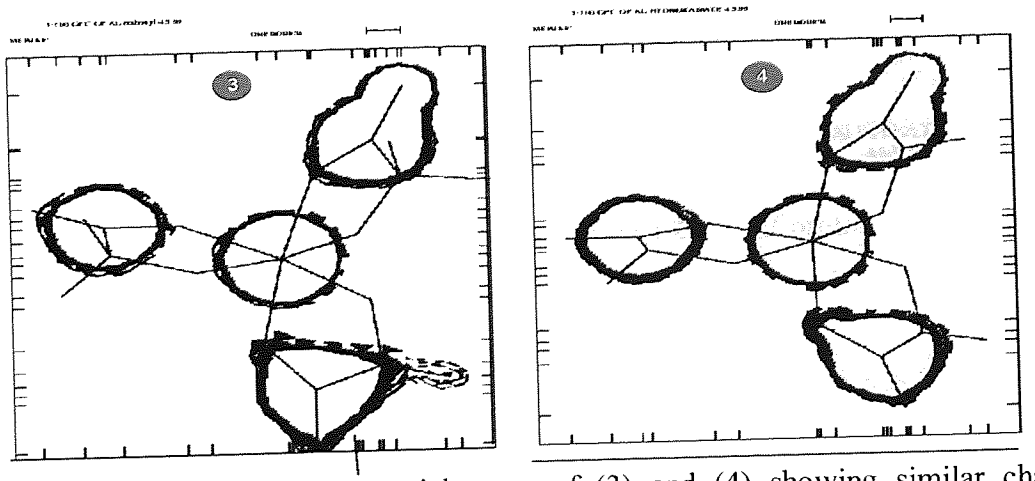


FIGURE 5.11 Electrostatic potential maps of (3) and (4) showing similar charge distribution throughout both complexes

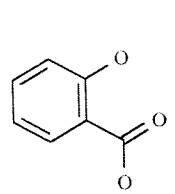
Thus, figures 5.10 and 5.11 conclude the alkoxide and the hydroxamate moieties have similar affinities for the trivalent Al ion.

5.5 PM3 OPTIMISATIONS ON 3:1 COMPLEXES OF AL

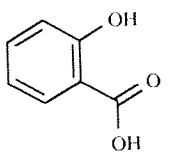
5.5.1 Influence of protonated and deprotonated donor atoms upon complexation to Al

In all cases it is assumed that a ligand protonated at its oxygen donating site will be deprotonated upon complexation with Al. The CSD studies in section 3.8 show deprotonation occurs in the majority of Al complexes observed. Al complexes based on salicylic acid were constructed to identify the expense of deprotonation on complexation.

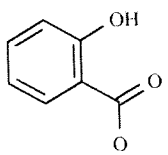
No crystal structures of the 3:1 complex of the Al salicylate complex were available, consequently the starting co-ordinates were manually constructed in CHEM-X using the 3:1 complex of the 1,2-dimethyl-3-hydroxy-4-pyridonate complex with Al (FIMLOC10) (Nelson, 1988) as a template. Once constructed all structures were subjected to GAMESS PM3 optimisations as outlined in section 2.4.2.1.



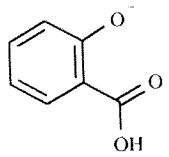
SALICYLATE DIANION (SAL1)



SALICYLIC ACID (SAL2)



SALICYLATE CARBOXYLIC ANION (SAL3)



SALICYLATE (PHENOLIC) ANION (SAL4)

FIGURE 5.12 Structures of ligands used to investigate effect of proton at ligation site to form 3:1 Al complexes

The Al:salicylic acid complex (SAL2) has an overall charge of 3, the salicylate dianion (SAL1) complex of -3, whereas those of the anions, SAL3 and SAL4 would have an overall neutral charge as deprotonation is only at one site per salicylate ion. As explained in the introductory chapter, the ideal chelator would form an overall

neutral charge to allow transport through biological lipid membranes, so clearly these complexes would be desirable.

TABLE 5.2 Al-O bond lengths of salicylate structures falling outside range identified from the CSD work

Oxygen donor site	Complex	Bond length (Å)
Carboxylic	SAL2	2.481
	SAL3	1.749, 1.749, 1.748
	SAL4	2.453, 2.454, 2.453
Phenolic	SAL3	2.458, 2.458, 2.459
	SAL4	1.760, 1.760, 1.760

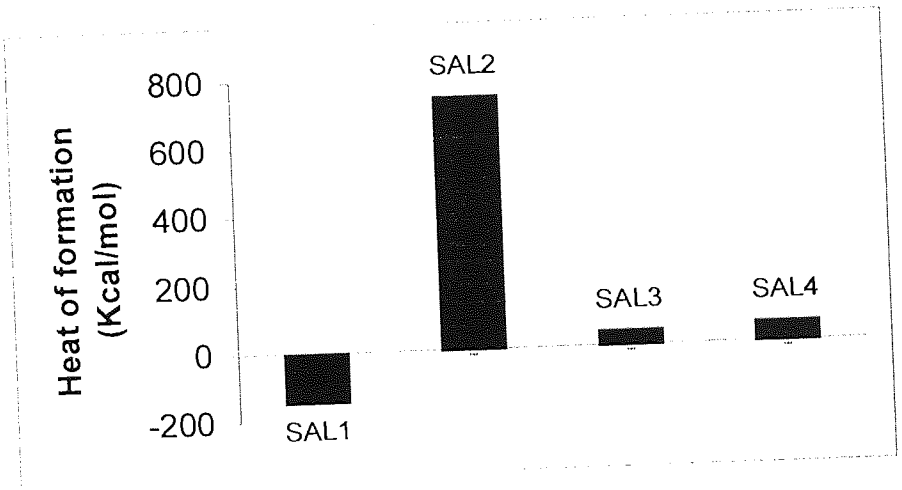


FIGURE 5.13 ΔH_{eff} for 3:1 complexes of SAL1, SAL2, SAL3, and SAL4

SAL1, the deprotonated species produces Al-O bond lengths within the limits set out in Figure 5.1. All the protonated species however resulted in at least one abnormally large Al-O bond length (Table 5.2) suggesting that the protons attached to the donor atoms involved were affecting its binding ability.

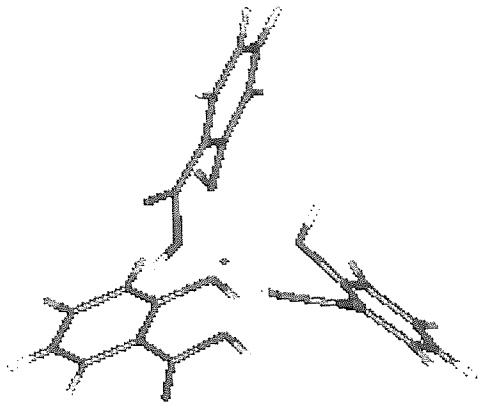


FIGURE 5.14 Structure of SAL2 showing position of hydrogens

Figure 5.13 indicates only the dianion complex is likely to be formed agreeing well with earlier CSD work which shows deprotonation occurs in 76% of all six co-ordinate Al complexes possessing oxygen donor atoms (section 3.8). The carboxylic hydrogen (pKa = 4.06) would dissociate before the phenolic hydrogen (pKa = 9.92). (CRC Handbook of Chemistry and Physics, 1988-1989). The ΔH_{eff} being less positive for SAL3 compared to SAL4 reflects this. Al has a charge of +3 with a small ionic radius (0.54Å), consequently has a high charge/radius ratio. Due to this high charge to mass ratio any other atom possessing a positive charge such as a proton will be repelled as shown by the hydrogen positions in Figure 5.14. It would be expected that a complex of this nature would produce a tri-planar structure as that resulting from optimisation of SAL1, however the monoprotonated and diprotonated species resulted in a 'kink' suggesting that that repulsion between the proton and the Al ion affected the ring system also. Perhaps this explains why ligands tend to be deprotonated at the donor sites when complexing with Al.

5.5.2 Correlations of published stability constants with output data produced from MO PM3 calculations

Previous sections concentrated on MO calculations of complexes containing approximately 20 atoms, identifying the PM3 Hamiltonian as that which most closely resembles the geometry produced by 6-31G optimisation. This study concentrates on optimisation of larger complexes using this semi-empirical method, and comparing the ΔH_{eff} with published stability constants in view of an existing correlation that will identify a method for predicting ligand affinity for the Al ion. A random selection of ligands with published stability data for the 3:1 Al complex were manually constructed as set out in section 2.4.2 and put through GAMESS PM3 optimisations as previously discussed.

TABLE 5.3 Ligands used to construct 3:1 Al complexes for PM3 optimisations with published stability constants

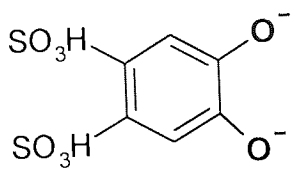
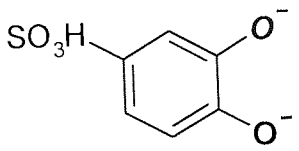
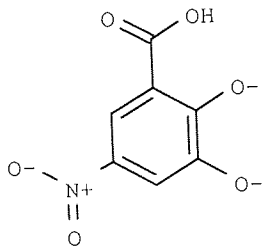
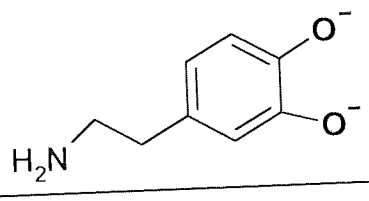
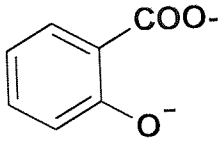
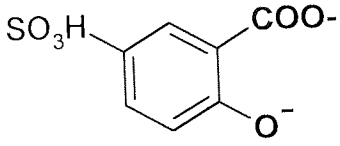
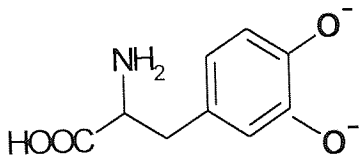
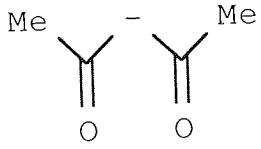
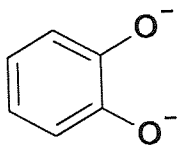
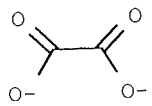
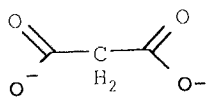
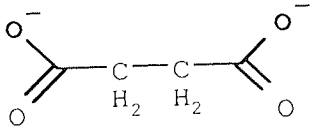
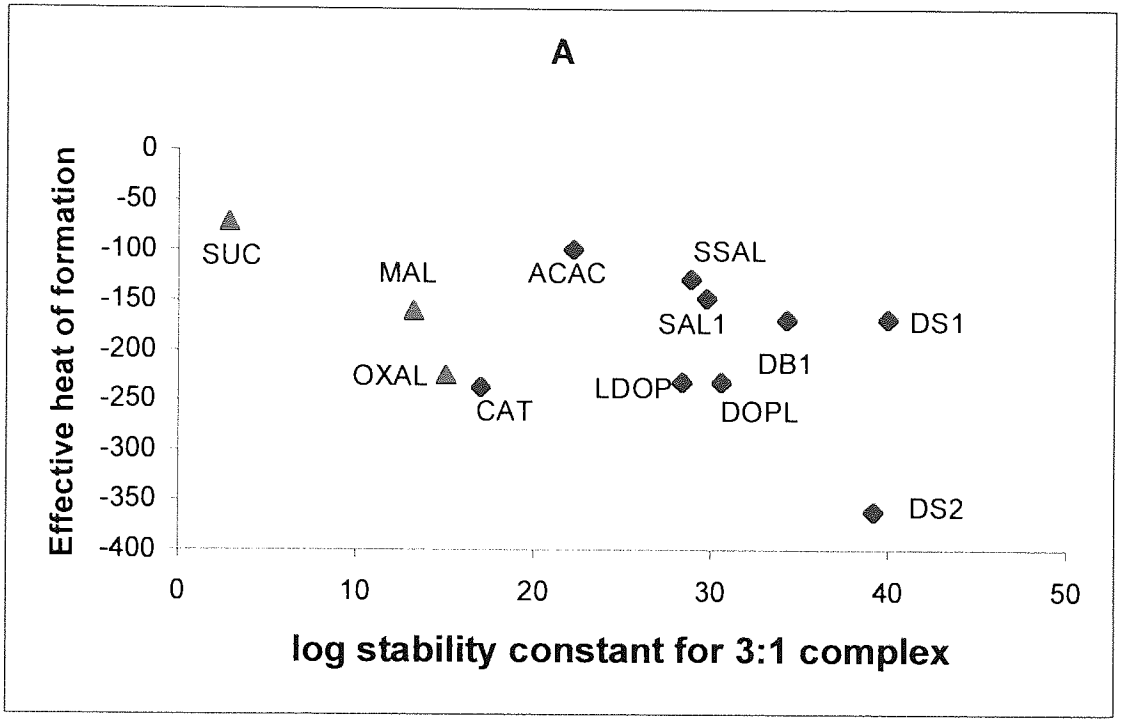
Name	Code	Structure	Log stability constant for Al 3:1 complex
1,2-Dihydroxy-3,5-disulphonic acid*	DS1		40.0 (Perrin, 1979)
1,2 Dihydroxy-4-sulphonic acid*	DS2		39.2 (Perrin, 1979)
4-nitro-1,2-dihydroxybenzoic acid**	DB1		34.3 (Smith, 1989)
Dopamine	dop1		30.6 (Martell, 1990)
Salicylate	SAL1		29.8 (Perrin, 1979)
5 sulphosalicylate*	SSAL		28.9 (Sillen, 1964)

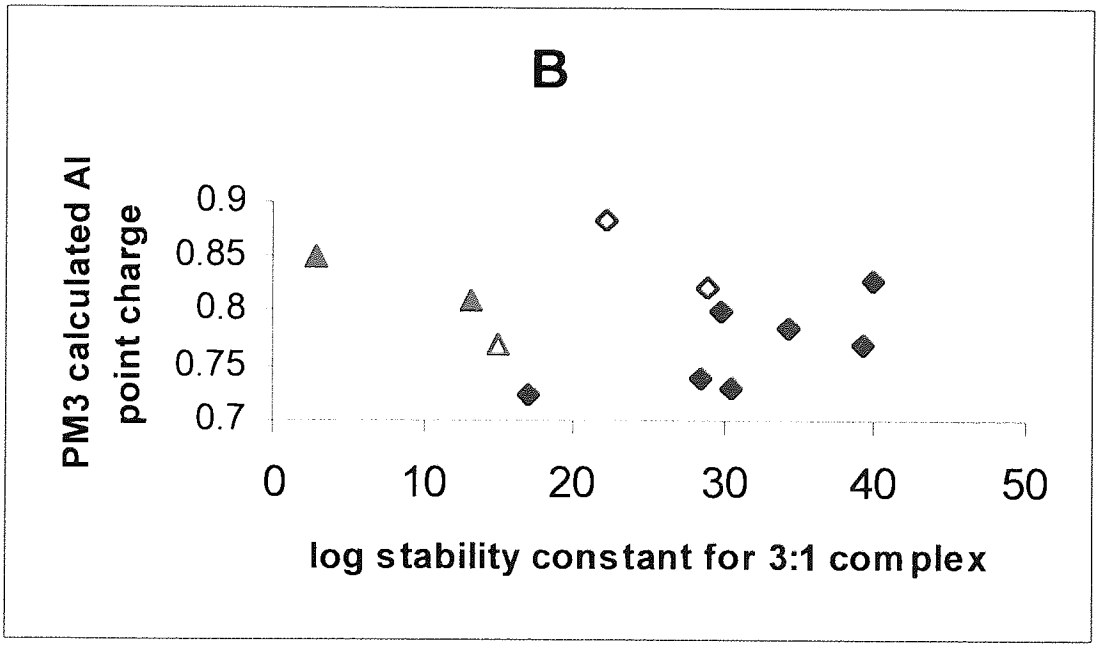
TABLE 5.3 continued

Name	Code	Structure	Log stability constant for Al 3:1 complex
L-Dopa**	Ldop		28.4 (Martell , 1990)
Acetylacetonate	Acac		22.3 (Sillen, 1964)
Catecholate	Cat		17.1 (Rajan 1978)
Oxalate	Oxal		15.1 (Perrin, 1979)
Malonate	Mal		13.3 (Jackson, 1989)
Succinate	Suc		2.9 (Smith, 1989)

* since the SO_3H group is strongly acidic, it will deprotonate long before any COOH or OH group. However, deprotonation will distribute a net charge of –1 over three oxygens, rendering it less likely to bind to Al. Also, deprotonation at this site would result in the Al complex possessing an overall charge of –6, which is likely to affect the MO calculations, hence is ignored.

** For reasons described above deprotonation on COOH groups not involved in binding to Al are also ignored


A
Effective heat of formation
0
-50
-100
-150
-200
-250
-300
-350
-400
SUC
MAL
ACAC
SSAL
SAL1
DS1
DB1
OXAL
LDOP
CAT
DOPL
DS2
0
10
20
30
40
50
log stability constant for 3:1 complex


B
PM3 calculated Al point charge
0.9
0.85
0.8
0.75
0.7
0
10
20
30
40
50
log stability constant for 3:1 complex

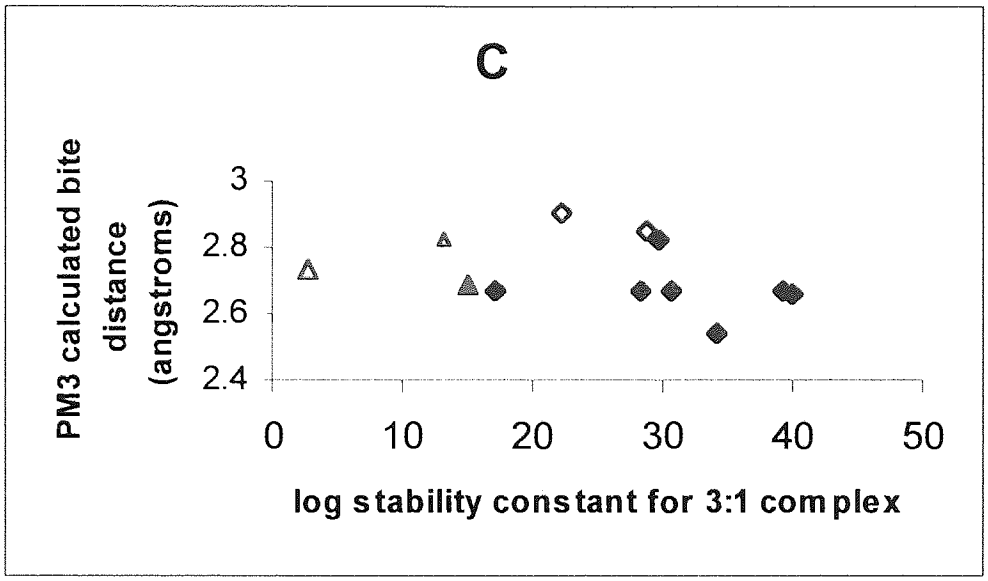


FIGURE 5.15 Relationship of published stability constants for 3:1 complexes and PM3 calculated

a: ΔH_{eff} - Red triangles show complexes of Al oxalate, succinate and malonate producing a correlation of 0.96 with respect to ΔH_{eff}.

b: Al point charge

c: bite distance: Filled shapes indicate 5 chelate systems, and hollow systems indicate 6 membered systems.

All structures with the exception of the 3:1 complexes with malonate and succinate produced Al-O distances within the range discussed earlier. Both these complexes resulted in one of the six Al-O distances being larger than that accepted for bonding, producing lengths of 2.508Å and 2.574Å respectively.

The correlations for all parameters were poor (correlation coefficients of 0.24017, 0.04394, and 0.04951, when compared to ΔH_{eff}, Al point charge and O-O bite distance respectively) (Figures 5.11A, B and C, respectively) showing no linear relationship. Further analysis using a multiple regression statistical programme, MREG (Irwin W, Aston University, Dept. of Pharm. and Biol. Sciences, 1982), also showed no correlation between stability constant data and any of the parameters investigated.

However, the structures investigated vary considerably. Further analysis of ΔH_{eff} for the related ligands, namely the three dicarboxylates, oxalate, malonate and succinate results in a correlation of 0.96, showing promise for affinity prediction. Further investigation was needed to establish a definite positive or negative correlation for two reasons. Firstly this trend can only realistically have three points that ultimately employ complexes consisting of five, six and seven membered chelate systems. Further extensions of the aliphatic carbon chain would result in unfeasible complexes consisting of eight membered chelate systems or more. Secondly, two of these structures produce large Al-O bonds which will ultimately affect the final PM3 calculated ΔH_{eff}.

PM3 minimisation of an existing Al acetylacetonate crystal structure (Rahman *et al.*, 1990) resulted in Al-O bond lengths decreasing, however the bond lengths produced are still within the range shown in figure 5.1, therefore validating the thermodynamic PM3 data generated. The observed difference may be attributed to the presence of external influences, such as the influence of solvents surrounding the chelate, which the PM3 Hamiltonian fails to consider, as it assumes gas phase.

5.5.3 PM3 optimisations of oxygen ligands suspected to bind to Al

5.5.3.1 Monocarboxylate ligands

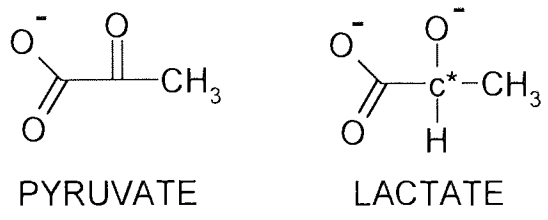


FIGURE 5.16 Structures of pyruvate and lactate ions

The lactate ion has an asymmetric carbon, therefore can exist as R and S isomers as well as the racemate. Consequently optimisations were carried out on manually

constructed 3:1 complexes of both with the aim of identifying the most stable. The pyruvate was constructed using the tris Al oxalate, COKFOX as the template.

TABLE 5.4 PM3 calculated Al-O bond lengths (Å) for R and S isomers of 3:1 complexes of Al lactate

R	S
1.903	1.905
1.835	1.856
2.366*	2.409*
1.812	1.798
2.379*	2.392*
1.825	1.803

* indicates bond length outside range outlined in Figure 5.1

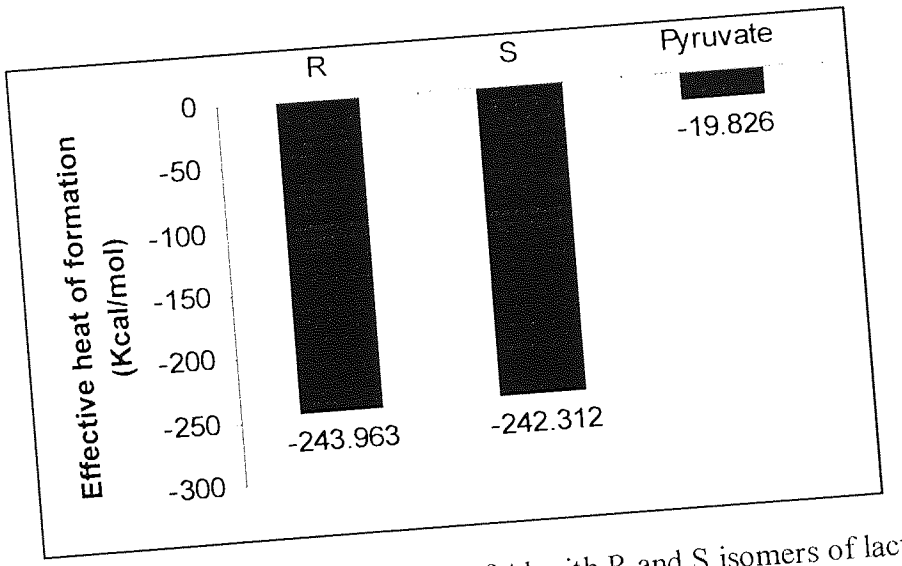
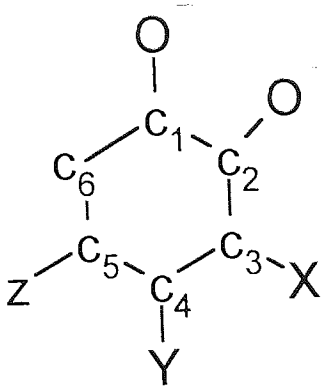


FIGURE 5.17 ΔH_{eff} for the 3:1 complexes of Al with R and S isomers of lactic acid and with pyruvate

The Al-O bond lengths of the tris Al pyruvate, calculated via PM3 optimisations all fell within the limits established in figure 5.1, however as observed in table 5.4, both isomers of lactate produced two abnormally large bond lengths.

5.5.3.2 Catechol ligands



Structure	Code	X	Y	Z
catecholate	CAT	H	H	H
4-methylcatecholate	CAT1	H	Me	H
3-methylcatecholate	CAT2	Me	H	H
4-ethylcatecholate	CAT3	H	Eth	H
4,5-dimethylcatecholate	CAT4	H	Me	Me

FIGURE 5.18 Structures of various catechols used in PM3 calculations

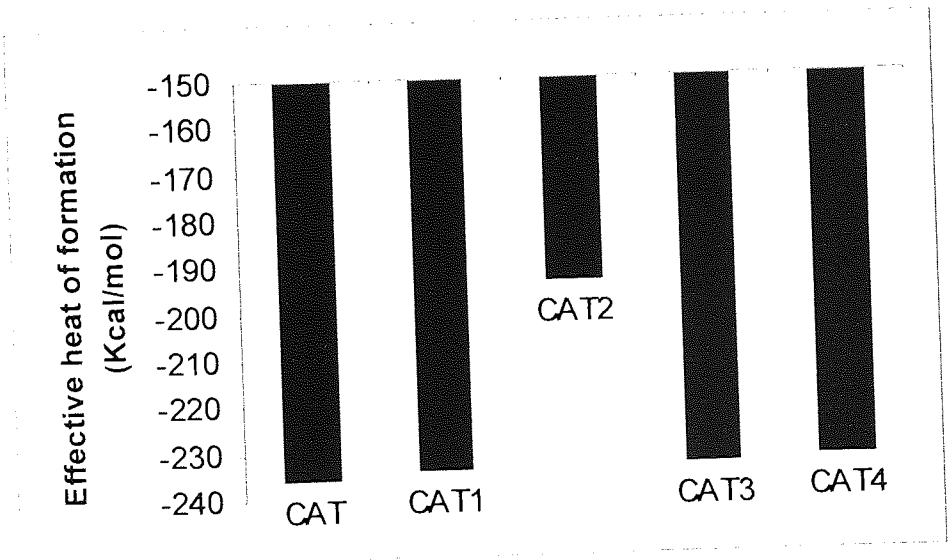
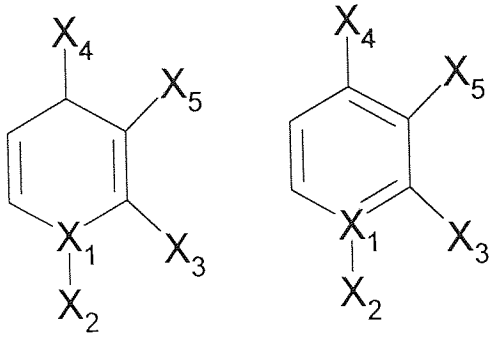


FIGURE 5.19 PM3 calculated ΔH_{eff} for various catechols

Geometric optimisation of the catechols falls well within the range shown in figure 5.1. Analysis of the ΔH_{eff} suggests that addition of an alkyl group to catechol at the 3 position as in CAT2 significantly decreases the affinity of the ligand for Al, while at more remote positions an alkyl substituent, either a methyl (CAT1) or an ethyl (CAT3) shows little effect. All the catechol based structures produced acceptable Al-O bond lengths.

5.5.3.3 Hydroxypyridinones (HPs)

The previous section outlined a possible correlation between PM3 calculated ΔH_{eff} and published log stability constants for the related dicarboxylates oxalate, malonate and succinate to produce five, six and seven-membered chelate ring systems respectively. Using these molecules the study was limited to a maximum four carbon aliphatic chain producing an unlikely seven membered system. This study concentrates on PM3 MO calculations on related ligands based on the hydroxypyridinone structure, ensuring that the chelate ring system of the final 3:1 complex remains constant at five. Thus the chelate effect will not influence differences in results.



Structure Code	X1	X2	X3	X4	X5
HP1	N	H	H	O	OH
HP1ME	N	H	Me	O	OH
HP1NME	N	Me	H	O	OH
L1	N	Me	Me	O	OH
L2*	N^+	Me	O	H	OH
CP21	N	Eth	Me	O	OH
JASMIZ	N	Me	Eth	O	OH
CP94	N	Eth	Eth	O	OH
L3*	N^+	O^-	OH	OH	H
L4*	N^+	O^-	OH	H	H
L5	O	-	Me	O	OH
HPPP*	N	Me	Benz	O	OH

* structures adopt structure B bonding scheme.

FIGURE 5.20 Structures of HPs investigated via PM3 MO optimisations

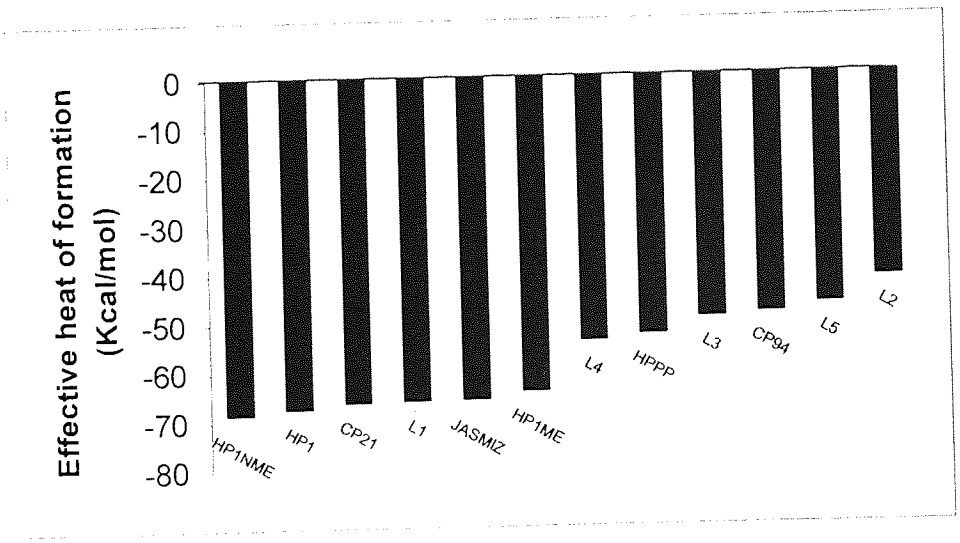


FIGURE 5.21 ΔH_{eff} for HPs calculated using the PM3 Hamiltonian

All HPs investigated produced Al-O lengths within the geometry limits specified in chapter two, thus fulfilling the requirements set out to accept the thermodynamic data. Binding affinity as measured by ΔH_{eff} appears to be influenced by electronic and steric factors. The pyridinone nitrogen atom can supply electron density to the 4-oxo group thus enhancing its ability as a ligand:

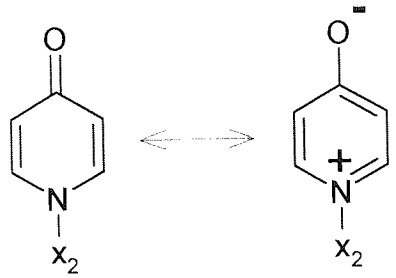


FIGURE 5.22 Charge distribution in HPs

Compared to the parent compound HP1, an electron donating X_2 makes ΔH_{eff} somewhat more negative (HP1NME), while replacement of N with O weakens the affinity (L5). As with the catechols though not to the same degree, introduction of an alkyl substituent at X_3 adjacent to the hydroxyl group is harmful (HP1ME vs. HP1, and L1 vs. HP1NME), and an ethyl group is worse than methyl (JASMIZ vs. L1). As seen with the catechols, an alkyl group at X_2 is remote enough from X_4 and X_5 that steric effects are small and electronic effects can dominate. However, two adjacent ethyl groups apparently cause enough congestion to depress affinity (CP94 vs. JASMIZ). If the 4 –oxo group is shifted to the 2-position adjacent to X_2=Me, affinity is impaired (L2 vs. HP1NME).

5.6 CONCLUDING REMARKS

These studies have shown that PM3 is the most suitable Hamiltonian for organo-aluminium complex optimisations. In general many of the final geometries produce Al-O distances within the range outlined by previous database work in chapter three, however for some complexes such as the lactates some of the Al-O lengths tend to be larger than anticipated. Consequently the output data from these optimisations which produce these suspect geometries must be treated with caution as it is likely that a false final geometry will also affect final thermodynamic data. Examination of the charge distribution on the donating oxygen atoms shows no obvious reasons for such large lengths suggesting that it may be attributed to a discrepancy within the parameterisation of the PM3 Hamiltonian for Al. It is important to note that data used for parameterisation of Al within PM3 is limited to more simple molecules than those used in the investigation namely HAl, AlO, AlF, AlF_3, AlF_4^-, AlCl, $AlCl_3$, AlBr, $AlBr_3$, AlI_2, Al_2 and Al_2O. (Stewart, 1989) as described in the introductory chapter.

The study has shown that ligands tend to deprotonate upon complexation with Al, as well as the fact that like for like alkoxides and hydroxamates have similar affinities for the Al ion.

Dopamine and L-Dopa are of interest as both possess a high overall stability constant for Al (log stability constants for 3:1 complexes of 30.6 and 28.4, respectively) (Martell, 1990). L-Dopa is of particular interest as this is one of a few ligands which have a higher log K_1 for Al over Fe (logK, AlL=19.6; FeL=18.4) (Rajan, 1978). L-Dopa differs structurally from dopamine by possessing a carboxylic group on the carbon atom adjacent to the amine nitrogen, which results in a reduction in the value of the experimentally determined stability constant. PM3 optimisation has little effect on the geometric or thermodynamic data calculated.

No relationship, as shown by the correlation coefficients, exists between known stability constants and individual parameters calculated by the semi-empirical method. Further analysis using a multiple regression statististical programme, MREG (Irwin W, Aston University, Dept. of Pharm. and Biol. Sciences, 1982), also showed no

correlation between stability constant data and any of the parameters investigated. However, analysis of the three aliphatic dicarboxylic acids, oxalate, malonate, and succinate produced a correlation of 0.9162 with stability constant data, showing promise for affinity prediction with related ligands. On the basis of this hypothesis, the HPs, a class of compounds renowned for their chelating potential, were evaluated, the results showing the ligand HP1NME, 1-methyl-3-hydroxypyridin-4-one produces the most stable 3:1 complex.

CHAPTER SIX

MOLECULAR ORBITAL STUDIES ON TARTARIC ACID

6.1 INTRODUCTION

Tartaric acid is common not only in the metabolic pathways of plants and animals but it is also used as an antioxidant and flavouring agent (E334) in food preparations, which is the probable source in humans. Naturally occurring tartaric acid can be found in wine and grape juice.

This dicarboxylic acid has been studied crystallographically for the past 150 years (Pasteur, 1848). Numerous structure determinations have been carried out on optically active tartaric acid (Albertsson, 1979; Okaya, 1966; Stern, 1950), although all of them seem to apply to the same unit cell in space group $P2_1$. Having the lowest *R* factor, the data of Hope and de la Camp (1972, TARTAC23) will be used for comparisons of this structure. Crystal structures have been determined (Bootsma & Schoone, 1967) for *meso* tartaric acid in an anhydrous triclinic form (TARTAM), a triclinic monohydrate (TARTMM), and a monoclinic monohydrate (TARTMM01). Racemic tartaric acid (TARTDL) has been studied as a monohydrate (Parry, 1951).

Deprotonated forms of aliphatic alpha-hydroxy acids have high affinities for Al(III), (Martell, 1996). Consequently, tartaric acid, a renowned chelator, would be expected to be a good ligand for chelation with Al as it possesses two aliphatic hydroxyl groups and two terminal carboxyl groups. Indeed crystal structures of tartaric acid with a number of metal ions K^+ (KMTART), Rb^+ (RMTART), Co^{3+} (BELSUG), and Fe^{3+} (SFTART) have been made and solved (Ivanov, 1975). The pKa's for tartaric acid have been reported as 2.98 and 4.34 (CRC Handbook of Physics and Chemistry, 1988), thus at physiological pH, both acidic groups would be ionised (O_2H, and O_6H) (Figure 4.8), hence more likely to complex with a cationic species such as Al. The log

stability constants for Al tartrate have been reported to be 5.6 and 10.0 for the 1:1 and the 2:1 complexes, respectively (Martell, 1977). To date, no complex with tartaric acid and Al has been crystallised and solved.

6.2 AIMS AND OBJECTIVES

The structure of tartaric acid is shown in figure 4.8. This molecule is relatively small and possesses four possible oxygen donor sites that have the potential to bind to Al. Hence, this molecule was chosen for further MO studies.

The previous chapter concludes the PM3 Hamiltonian to be the best for optimisations of simple 3:1 Al complexes; this may not be the case for simple organic molecules. MO calculations of the various forms of tartaric acid would allow a review of basis sets from semi-empirical sets such as PM3 and AM1 to the most powerful *ab initio* basis set used in this study, namely 6-31G*. Thus, a well informed choice of basis set could be made for further studies balancing speed of computation against accuracy. In these studies, the anhydrous DL tartaric acid numbering scheme will be used (Figure 4.10).

Only potentiometric data gives an idea of the complexation sites involved between the tartaric acid ligand and the metal ion. MO calculations of these complexes would perhaps give a better understanding as to the stoichiometry of the complex and which oxygen atoms preferentially bind to an Al ion.

6.3. COMPARISON OF ANHYDROUS TARTARIC ACID WITH OTHER CRYSTAL FORMS WITHIN THE CSD

For comparison purposes the crystallographic co-ordinates of all tartaric acid crystal structures were extracted from the CSD and superimposed onto anhydrous DL tartaric acid (ALTAR) before similarity calculations were carried out in Tsar as described in section 2.4.

TABLE 6.1 Crystallographic and Tsar data for tartaric acid structures

Crystal	R_{factor}	Density (g cm^{-3})	molecular surface area $Å^2$	molecular surface volume $Å^3$	Hodgkin Index Gaussian Combined	Hodgkin Index shape	Hodgkin Index Lipophilicity
Anhydrous DL-tartaric acid (ALTAR)	0.0434	1.802	135.37	97.798	1.0	1.0	1.0
DL-tartaric acid monohydrate (TARTDL) with hydrogen atoms added using CHEMX	0.22	1.708	132.84	97.683	0.980	0.962	0.997
D-tartaric acid (TARTAC, Okaya *et al*, 1966)	0.04	1.756	134.86	96.195	0.996	0.993	1.0
D-tartaric acid (TARTAC02, Stern, 1950)	0.26	1.762	144.89	99.66	0.995	0.990	1.0
D-(+)-tartaric acid (TARTAC04, Albertsson,1979)	0.03	1.757	134.9	95.112	0.935	0.873	0.996
D-(+)-tartaric acid (TARTAC06, Albertsson, 1979) 105°C	0.029	1.707	134.5	95.628	0.937	0.877	0.997
D-(+)-tartaric acid (TARTAC07, Albertsson,1979) 35°C	0.034	1.795	137.96	94.607	0.936	0.876	0.996
(+)-(2R,3R)-tartaric acid (TARTAC23, Hope,1972)	0.023	1.755	137.45	95.035	0.938	0.879	0.997
meso-tartaric acid (TARTAM, Bootsma,1964)	0.076	1.691	148.4	103.92	0.969	0.949	0.988
meso tartaric acid monohydrate (TARTMM, Bootsma, 1964)	0.048	1.665	134.74	96.764	0.963	0.933	0.994
meso tartaric acid monohydrate (TARTMM01, Bootsma, 1964)	0.078	1.669	134.36	98.244	0.883	0.780	0.987
3-hydroxyquinuclidinium tartrate tartaric acid solvate (POCFUI, Erman, 1994)	0.043	1.558	137.36	94.99	0.937	0.879	0.995
bis-4-(4-chlorophenyl)pyrrol-2-one) (2R,3R)-(+)-tartaric acid (ZUWKUX, Caira 1996)	0.045	1.74	134.71	98.493	0.928	0.888	0.968

All crystal structures retrieved from QUEST3D were analysed using VISTA v2.1 (CSSD) to identify any anomalies in torsion angles of the 4 carbon backbone, the carboxylic hydroxyls and the interior hydroxyl groups, or hydroxyl oxygen intramolecular distances.

SFTART (Ivanov, 1975), although a 2:1 complex of ferric tartrate, has been included in Table 6.2 to show the influence of metal complexation on the parameters measured.

TABLE 6.2 Various torsion angles indicative of backbone geometry and functional group arrangement, and hydroxyl O3-O4 distances of tartaric acid structures from the CSD

Refcode	Carbon backbone torsion angle C_1-C_2-C_3-C_4 (°)	Carboxylic OH improper torsion angles O_1-C_1-C_4-O_6 (°)	hydroxyl torsion angle O_3-C2-C3-O4 (°)	hydroxyl oxygen intramolecular distance O3-O4 (Å)
ALTAR	-177.7	66.6	65.3	2.962
TARTDL	-179.3	70.9	62.3	2.810
TARTAC	175.4	63.1	58.2	2.857
TARTAC02	179.1	132.2	51.3	2.873
TARTAC04	175.3	-62.8	-58.5	2.859
TARTAC06	175.6	-63.2	-58.2	2.864
TARTAC07	175.5	-63.7	-59.5	2.869
TARTAC23	-175.4	-63.1	-58.1	2.864
TARTAM	75.0	-88.0	-71.1	2.899
TARTMM	-73.4	-91.9	-71.3	2.992
TARTMM01	75.4	-141.4	73.4	2.986
POCFUI	171.0	54.9	59.5	2.825
ZUWKUX	170.7	-61.4	-72.7	2.871
SFTART	-174.1	159.2	-52.5	2.647

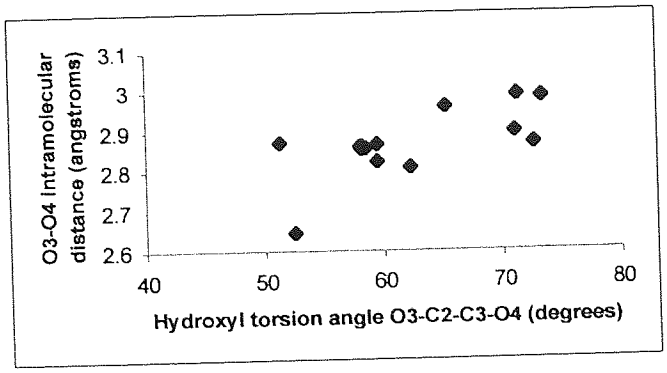


FIGURE 6.1 A comparison of O3-C2-C3-O4 torsion angles and O3-O4 contact distance

Torsion angles of ALTAR are similar to those of existing tartaric acid structures, however table 6.2 shows the intramolecular hydroxyl oxygen distance to be significantly higher in ALTAR. This may be attributed to the spreading effect of intramolecular (between O_3-O_4) and intermolecular hydrogen bonding involving O_3-O_4 of adjacent tartaric acid molecules. The absence of solvent interactions for our anhydrous structure perhaps allows a closer overall packing, although no apparent correlation exists between published densities and calculated distances between centroids of neighbouring tartaric acid molecules for those extracted from the CSD (Figure 6.2).

In the tartaric acid molecules studied, the O_3-C_2-C_3-O_4 torsion angle and O_3-O_4 contact distance would be strictly related if bond distances and bond angles remained constant. As shown in Figure 6.1, this is not the case.

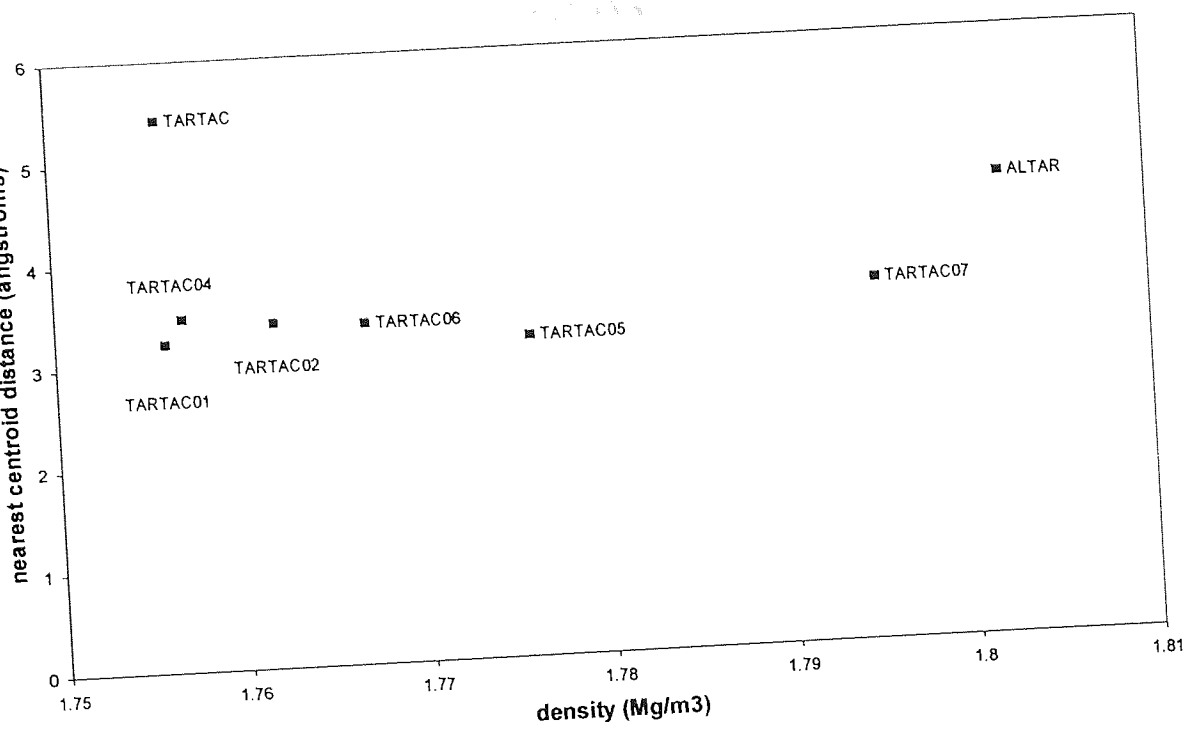


FIGURE 6.2 Analysis of centroid distances and published densities of tartaric acid structures within the CSD

6.4 MOLECULAR ORBITAL CALCULATIONS

6.4.1 Optimisation of solvated molecules

Computational chemistry is becoming an increasingly powerful tool to the chemist in that minimisations allow prediction of compound stability using thermodynamic data obtained from quantum mechanical calculations. However, one of the main disadvantages of this theoretical work is that calculations are usually done *in vacuo*. MOPAC allows optimisations to be carried out in solvents (using the keyword EF EPS=78.4 for water), so to test the validity of these results they were compared with optimisations *in vacuo* as well as the original crystal structure.

The DL tartaric acid crystal structure was subjected to PM3 and AM1 minimisations, both with and without solvent using MOPAC and compared to the original using ASP.

TABLE 6.3 Comparison of influence of solvent on semi-empirical optimisations using MOPAC

Filename/Basis set	Carbo Index combined	Carbo Index Electrostatic	Carbo Index Shape	Carbo Index Lipophilic
ALTAR	1.0	1.0	1.0	1.0
ALTARMOP (PM3 using solvent)	0.97	0.942	0.969	1.0
ALTARPM3(without solvent)	0.929	0.850	0.938	0.998
ALTARMOP1 (AM1 using solvent)	0.881	0.738	0.914	0.993
ALTARAM1	0.901	0.760	0.948	0.995

Optimisation of solvated molecules show mixed results; while it has shown a significantly greater similarity to the original crystal structure using the PM3 Hamiltonian it has reduced the similarity in the AM1 Hamiltonian.

6.4.2 Single point semi-empirical calculations

To ascertain which crystal structure contained the molecule in its most stable form they were subjected to single point PM3 calculations using MOPAC.

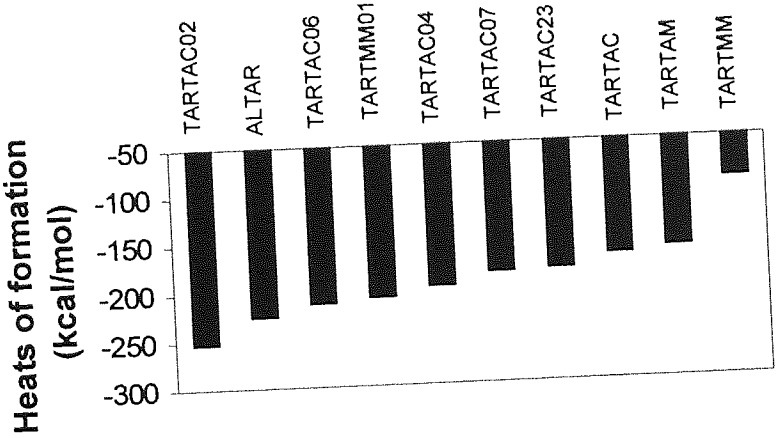


FIGURE 6.3 PM3 calculated ΔH_f of various D conformations extracted from the CSD

In general all the structures subjected to the single point PM3 calculations tend to have less negative ΔH_f when compared to ALTAR, with the exception of TARTAC02, suggesting that the atomic orientations of the D-enantiomorphs when packed into a crystal with only their own kind, are less stable.

Only TARTAC02 (D-tartaric acid) has similar or greater magnitude of the PM3 calculated ΔH_f. Table 6.2 illustrates that both these structures have a carbon backbone torsion of almost 180°.

TARTMM has a considerably smaller heat of formation in comparison to the other enantiomorphs. Perhaps this is attributable to the C chain torsion angle, which is only 73.4°. This twisting may create steric hindrance that could contribute to its apparent lack of stability, and the carboxyl groups are less well separated.

A complicating factor is that X-ray crystallography can locate hydrogen positions only with limited accuracy. Errors in hydrogen positions in particular structures can raise the energy, quite apart from any general trend. This problem is addressed in section 6.5.3.

6.5 *AB-INITIO* MOLECULAR ORBITAL CALCULATIONS

6.5.1 Overview of *ab initio* basis sets used

STO-3G, the simplest of the *ab initio* basis sets used, is effective in predicting geometry (Pople, 1976), which is attributed to the large basis set superposition error which cancels out other defects producing reasonable bond lengths. Energetics on the other hand are not predicted with the same accuracy. Both σ and π p functions are restricted to a single factor, resulting in π bonds which are weak relative to the σ bonds.

3-21G is a 'split valence' basis set with a compromise between the speed obtainable using STO-3G and the accuracy of larger, slower sets. Skewing of the σ bond energies is significantly reduced compared with the STO-3G basis (Gordon, 1982; Binkley, 1980).

By increasing the number of primitives devoted to the core and 1st valence function, 6-31G basis improves at the expense of increased computer time. Adding all 6 components of a Cartesian d function for 1st row atoms gives the 6-31G* basis set. This is further explained in section 1.4.2.1.1.

6.5.2 Methodology

The fractional co-ordinates of each crystal were extracted from the CSD and converted into internal co-ordinates (using Babel v1.1) (Walters P). The internal co-ordinates were then subjected to the simplest of the *ab initio* calculations, namely STO-3G ensuring that both the C backbone and hydroxyl oxygen torsion angles were constrained to their original crystallographic values.

The aim was to maintain the D isomer conformations, hence the torsion constraints, while allowing the bond lengths and angles to relax to more favourable energies. Hydrogen atoms in several of the structures were located inexactly or not at all, so missing ones were added and all were allowed to relax freely.

The procedure used for MO calculations with GAMESS is outlined in section 2.4.2. Upon fulfilling the default GAMESS convergence criteria, the final cartesian co-ordinates were extracted and again converted into internal co-ordinates before being subjected to the next basis set, namely 3-21G. This was repeated using 6-31G and finally 6-31G*. The thermodynamic and geometrical data were analysed.

6.5.3 Comparisons of basis sets on MO calculations of tartaric acid

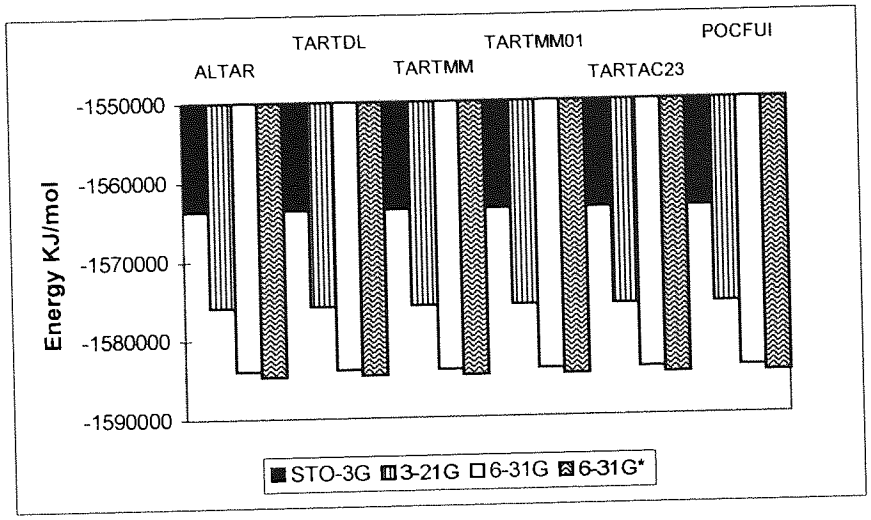


FIGURE 6.4 Comparison of energy values obtained by different MO calculations with the carbon backbone (C_1-C_2-C_3-C_4) and hydroxyl torsion angles (O_2-C_2-C_3-O_4) constrained to their original crystallographic values

As expected, the more powerful basis sets produce a more stable geometry. This can be partly attributed to the fact that the larger basis sets have a better fit of Gaussians to the true orbitals and the more powerful basis sets better represent intramolecular hydrogen bonding. It would be reasonable to assume that 6-31G is comparable to the more powerful 6-31G* basis set for a fraction of the computational time.

Finally, the 6-31G* optimised co-ordinates of the torsion constrained ALTAR crystal were extracted and subjected to free optimisation within the same basis set until the GAMESS default criteria were met.

6.5.4 6-31G* optimisations of tartaric acid structures

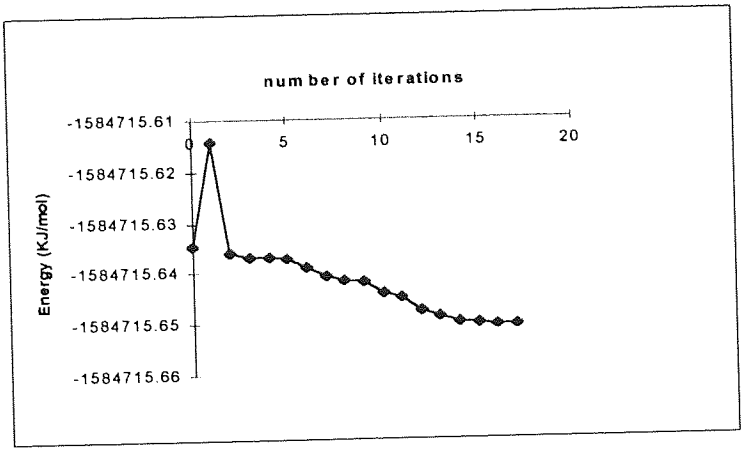


FIGURE 6.5 Fluctuations in energy upon free optimisation of ALTAR using 6-31G*

The energy became increasingly more negative illustrating the change in geometry was producing a more stable structure. The anomaly on the second iteration is commonly observed.

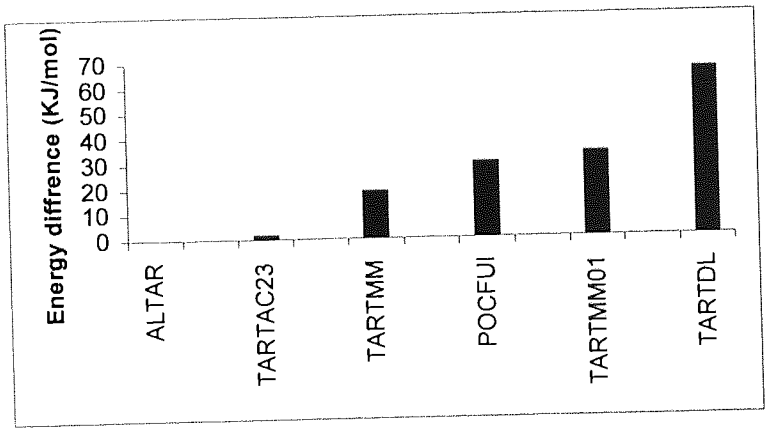


FIGURE 6.6 Energy difference of torsion constrained optimisations against freely optimised ALTAR using 6-31G*

The geometry of the 6-31G* optimised structures was analysed using Tsar. All structures were superimposed onto the ALTAR structure at the terminal carbons and carboxylic hydroxyls (i.e. C_1, C_4, O_1 and O_6) using the rigid fit command in Chem-X,

with the exception of TARTMM and TARTMM01 which were superimposed at C_1, C_3 and O_1.

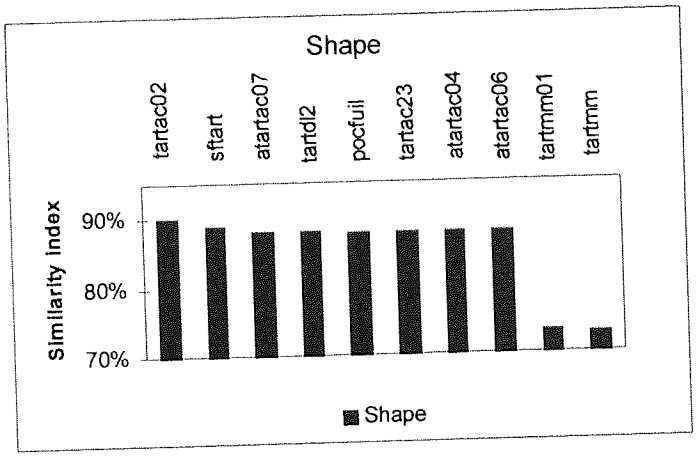


FIGURE 6.7 Tsar shape comparison of torsion constrained 6-31G* optimised tartaric acid structures with ALTAR

6.5.5 Influence of *ab initio* basis sets on intramolecular distances between O_3-H_2 and O_5-H_5

The different basis sets give a variety of energy data. As the complexity of the basis set is increased, the energy is also reduced to give a more stable geometry and a better fit to the actual electron distribution as described previously (section 6.5.3). An important factor may be the more accurate representation of intramolecular hydrogen bonds in the higher basis sets as shown in the example for TARTAC23, which has the lowest *R* value of the tartaric acid crystal structures studied (Figure 6.8). This is also depicted in figure 6.9, which illustrates the movement of hydroxyl protons.

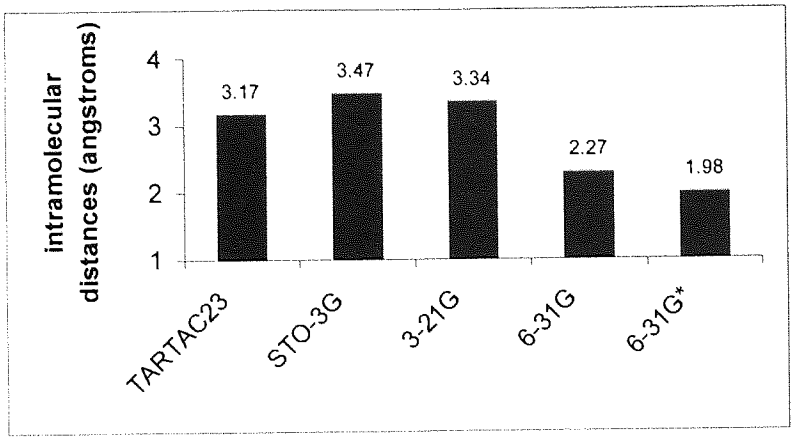


FIGURE 6.8 Mean intramolecular hydrogen bond distance (O_2-H_3 and O_5-H_5) produced by optimisation of TARTAC23 by 4 different *ab initio* basis sets

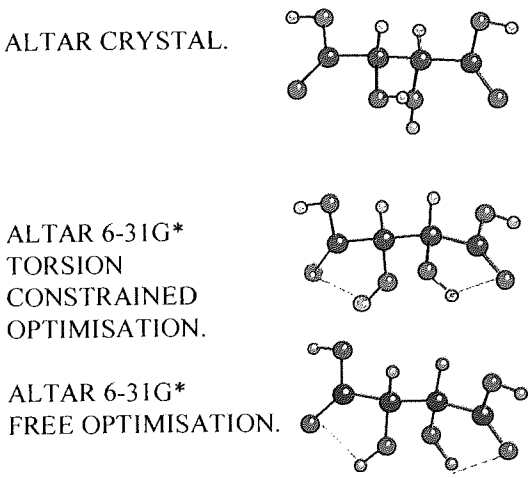


FIGURE 6.9 Movement of hydroxyl hydrogens to form intramolecular hydrogen bonds in ALTAR crystal

Optimisation of ALTAR leads to the hydrogens of the hydroxyl groups (H_3 and H_5) being pulled out towards the carboxylic oxygens, forming intramolecular hydrogen bonding. This forms a more stable conformation of the isolated molecule that ultimately makes the ΔH_f more negative as shown by the energy data.

All the molecules that were optimised via *ab initio* experienced this phenomenon. Below shows the change in intramolecular hydroxyl hydrogen and carboxylic oxygen distances as the basis set being used for optimisation was progressively increased.

6.5.6 Molecular electrostatic potential maps (MEPmaps)

A MEPmap of each of the optimised tartaric structures was generated as described in section 2.4.2.3. No noticeable difference was observed between the basis sets investigated, hence only that produced by 6-31G* is depicted (figure 6.10).

As expected, the MEPmap shows net negative potential on the carboxylic oxygens O_2 and O_5, as well as the hydroxyl oxygens O_3 and O_4, both potential sites of binding with Al.

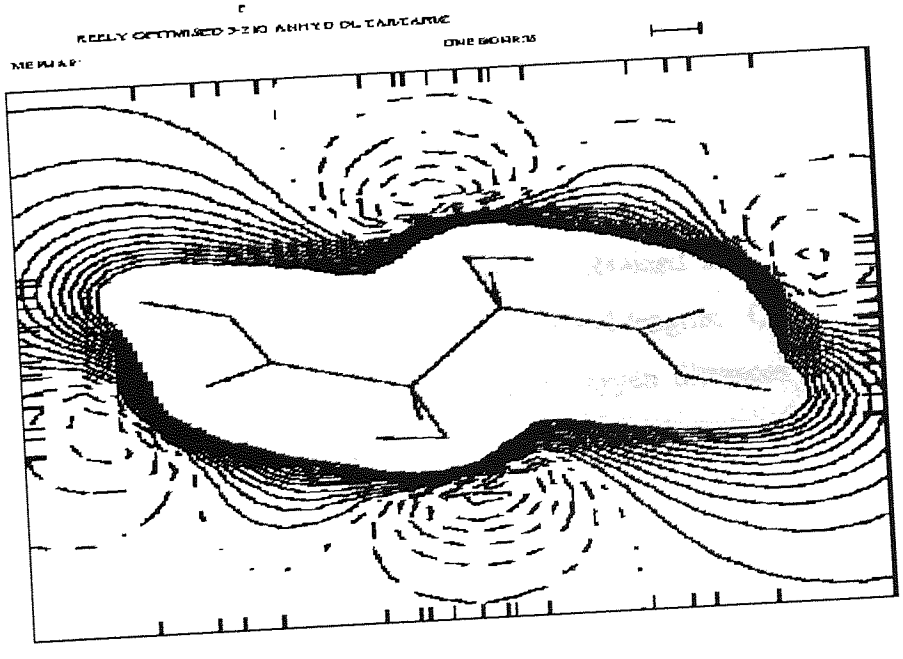


FIGURE 6.10 MEPmap produced for the free optimisation of anhydrous DL tartaric acid using 6-31G*

6.6 ALUMINIUM TARTRATE COMPLEXES

In experiments in which rabbits were exposed to repeated subcutaneous injections of Al tartrate, elevated brain levels of Al were recorded. At higher doses the treatment resulted in neurological disorders (DeBoni, 1976).

As mentioned, a variety of foods contain tartrates, and there is a ubiquitous distribution of Al within the environment giving rise to potential complexation which may be hazardous to the mammalian brain. While a thorough search of the CSD failed to find a complex of Al with tartaric acid, a 2:1 complex of Fe (III) with tartaric acid was found (SFTART).

6.6.1 Al tartrate 2:1 complexes

The introduction has shown Al exhibits the same chemistry as Fe, and indeed all known Al chelators are also effective Fe chelators. Consequently it would be reasonable to assume that there is a high probability that Al would bind to tartaric acid in a similar fashion to Fe. On this assumption, the co-ordinates of SFTART were extracted, and after changing the central ion from Fe to Al and attaching a proton to the carboxylate ion not involved in Fe binding, were subjected to MO calculations as outlined in section 2.4.2. However, a stationary point was not obtained and presumably this failure is attributable to the higher than normal Al-O bond lengths. Consequently the structure was modified so as to decrease the metal oxygen distances to 1.85 Å, a distance more realistic for Al-O bond lengths.

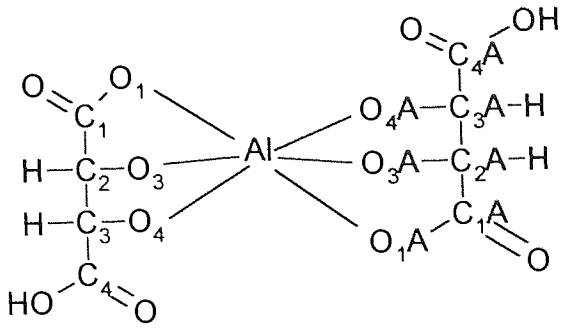


FIGURE 6.11 Numbering scheme for Al tartrate 2:1 complex using SFTART as template

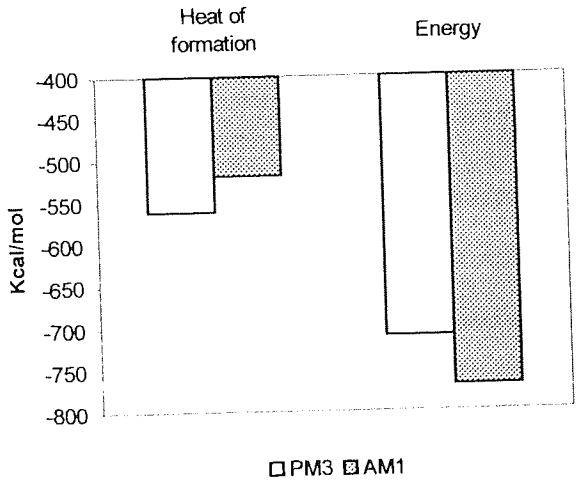


FIGURE 6.12 Thermodynamic data obtained from semi-empirical optimisations of Al tartrate 2:1 complex

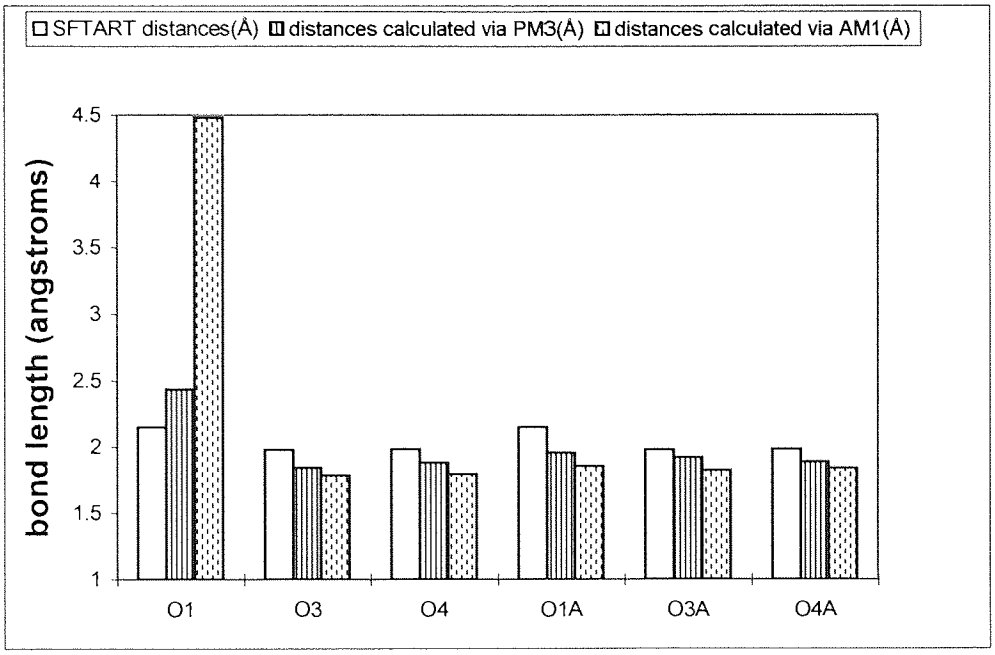


FIGURE 6.13 Comparison of Al-O distances between SFTART and optimised structures via PM3 and AM1

Both PM3 and AM1 basis sets converge to give the Al-O bond lengths acceptable crystallographic values with the exception of the Al-O1 bond length. Thus in the optimized complexes the Al is assumed to be 5 coordinate which is known to exist, although less frequently than its 6 coordinate counterpart. This may be at least partly due to the smaller Al (0.54Å) ionic radius relative to Fe (0.64Å). A search in the CSD via QUEST revealed a total of 215 crystal structures possessing at least one 5-coordinated Al atom. (c.f. 1539 crystal structures possessing at least one 6 coordinate Al atom within the CSD) (chapter 3). The abnormally large Al-O1 bond length may be due to the smaller Al ionic radius relative to Fe resulting in ineffective packing of donor oxygen atoms (Hider and Hall, 1994) or it may possibly be due to lack of suitable parameterisation for Al in the AM1 and PM3 Hamiltonians. In general both are parameterised using Al halide complexes as described in section 1.4.2.

Marklund *et al.*, (1990) have suggested, via equilibrium studies in aqueous solution, the tartaric acid forms a binuclear complex with Al being bridged by two quadridentate tartaric acid molecules $[Al_2(H_{-2}L)_2]^{2+}$, hence from each of the tartaric acid molecules

two of the four OH groups donate a proton (Marklund, 1990). As no crystallographic co-ordinates were available as starting points for optimisation of this structure, it was manually constructed by converting the Fe of SFTART to Al and bringing in the Al-O distances to 1.8Å (a length shown in chapter three to be well within the limits of known crystallographic Al-O distances). Attempts to minimise this manually constructed structure failed to find a self consistent field (SCF).

6.6.2 Al tartrate 3:1 complexes

Previous studies (chapter three) shows Al prefers binding in a six co-ordinate manner, ideally leading to octahedral complexes, which are most likely to be achieved via complexation with bidentate ligands. Tartaric acid possesses many oxygen atoms capable of donating electrons and binding to Al, thus it theoretically has the capability of being mono, bi, tri and even quadridentate. On this assumption, 3:1 complexes of Al tartrate were constructed in Chem-X and energy minimised using the PM3 basis Hamiltonian. Several variations are possible, therefore three were constructed, based on 5, 6, and 7 membered chelate systems (Chapter two) and energy minimised

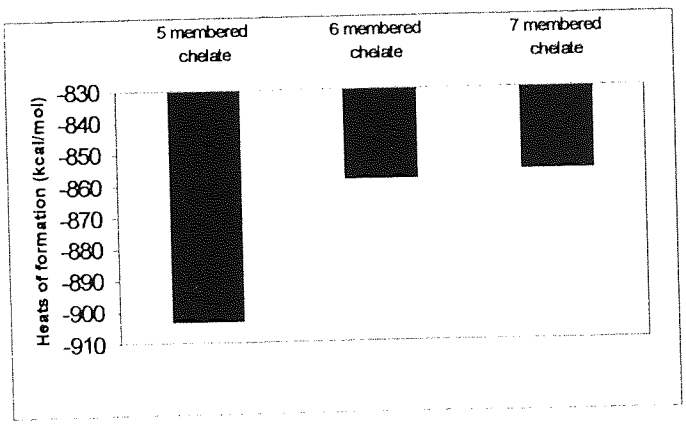


FIGURE 6.14 ΔH_f calculated by PM3 for 5, 6 and 7 membered chelate ring complexes of Al tartrate

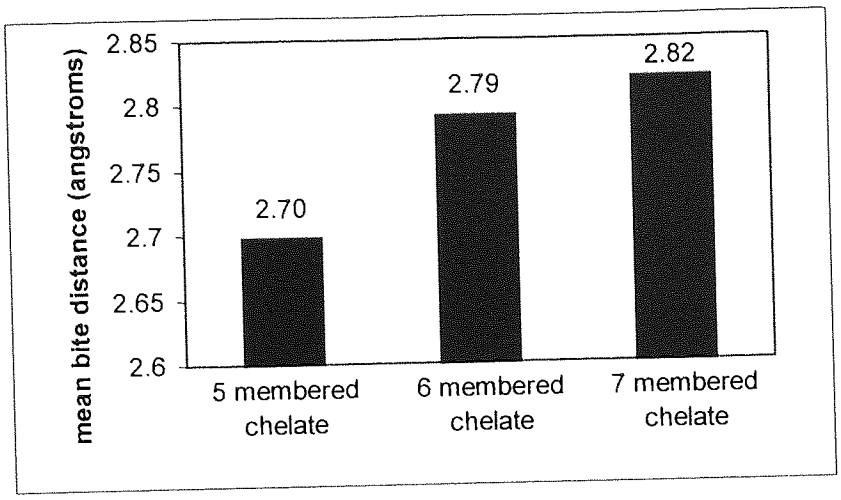


FIGURE 6.15 Bite distances for PM3 calculated 5, 6, and 7 chelate ring complexes of Al tartrate

TABLE 6.4 Al-O bond distances (Å) in PM3 minimised Al tartrate complexes

5 membered chelate		6 membered chelate		7 membered chelate	
O1	O3	O1	O4	O1	O6
1.9509	1.8705	1.8301	1.8167	1.8546	1.8866
1.9082	1.9257	1.8317	1.8167	1.8292	1.8276
1.9176	1.8649	2.4883*	2.4753*	1.8707	2.5087*

* -bond lengths above accepted crytallographical values for Al-O bond distances.

Chapter 3 also shows that Al prefers to complex as a 6 membered chelate ring system when oxygen exists as the donating atom. The results of the PM3 minimisations (figure 6.16) suggest the 5 ring system to be the most stable followed by the 6 and then finally the 7 chelate system.

All Al-O bond lengths are of acceptable crystallographical values in the 5 chelate system. Optimisation of the 6 membered chelate ring complex resulted in coordination

to one of the tartrate molecules being lost and ultimately forming a 2:1 complex with a four coordinated Al. The 7 membered chelate complex possesses a 5 coordinated Al similar to that found with the modified SFTART complex.

6.7 CONCLUDING REMARKS

These studies have shown the merits of the basis sets studied. The most primitive of the *ab initio* basis sets, STO-3G is comparable to the semi-empirical methods employed in this study. The MEPmap shows the hydroxyl groups possess the greatest negative potential within the tartaric acid molecule, consequently in terms of electrostatic potential would be the most favourable binding site the tripositive Al ion. MO point calculations of the conformations found in crystal structures show ALTAR and TARTAC02 to be the most stable possessing a carbon backbone torsion of almost 180°. The *meso* structures tend to be the least unstable, where the main chain is forced to be gauche. A major drawback of MO calculations is that, in general, they are performed *in vacuo*. To overcome this, parameters have been developed in the MOPAC program to allow solvent optimisations, with results tending to favour solvent optimisations using the PM3 Hamiltonian.

A review of the *ab initio* sets shows 6-31G* to produce the lowest conformational energy of optimised tartaric acid structures. However, little justification warranted the large increase in computational time for the apparently small energy difference to that of the 6-31G basis method.

Chapter five concludes no apparent correlation between the log of published stability constants and differences in heats of formation described in that chapter. However, for similar systems described in this chapter, MO calculations prove to be a valuable tool in predicting the most favourable formation of complex from the endless number that may be possible.

CHAPTER SEVEN

EVALUATION OF POTENTIAL AL CHELATORS

7.1 INTRODUCTION AND OBJECTIVES

Thus far, all work has been based on theoretical studies. This work, a path-finding exercise, aims to evaluate the ability of a chelator to bind to Al and enter cells using both *E. coli* and U87-MG glioblastoma cells as models.

Little is known about Al in biological systems relative to other trivalent metal ions such as Fe^{3+}. In part this is attributable to the fact that the ^{26}Al is extremely expensive making its use limited. Hence the aim of this study was to develop, optimise and validate the Al-morin assay, a spectrofluorimetric assay for the detection of Al. Using the two models above, the association (adsorption and absorption) of Al into cells can be evaluated. The hypothesis being that complexes entering cells will also pass out of cells. As no work of this nature has previously been reported, studies from first principles were undertaken.

Many organisms including bacteria such as *E. coli* produce highly specific iron chelators known as siderophores in response to iron limitation. These siderophores chelate and transport iron via specific transport systems to promote cell growth. It has been shown that under iron depleted conditions, these bacteria can take up Al by the use of these siderophores. Hu and Boyer (1996) used *Bacillus megaterium* to produce two hydroxamate siderophores, schizokinen and N-deoxyschizokinen under iron limited conditions. In addition to their high affinity for ferric ions (log stability constant of approximately 30), these siderophores also chelate Al ions (log stability constant of approximately 20). At low concentrations of Al, siderophore mediated uptake was the dominant process for Al accumulation. At high concentrations of Al, passive transport dominated and siderophore production slowed the passive transport of Al into the cell. Siderophore uptake was affected by the Al content within the

media. Al in high concentrations stimulated siderophore production in iron limited cultures which continued into the stationary phase, however no effect was seen with iron replete conditions.

It has also been reported that Al when complexed with a potent siderophore, namely enterochelin, has bacteriostatic effect (Rogers, 1978). On this basis, *E. coli* was used as the initial model to test the influence of Al on a range of antibiotics that are likely to bind to Al based on their structure.

The second model employed was a U87-MG glioblastoma cell line. This cell line was used as it resembles a typical human brain cell more closely than the *E. coli*. The most obvious difference lying in that this cell line only has a cell membrane consisting of a phospholipid bilayer, while that of *E. coli* consists of a cell wall also.

7.2 DEVELOPMENT AND OPTIMISATION OF THE MORIN FLUORESCENCE ASSAY.

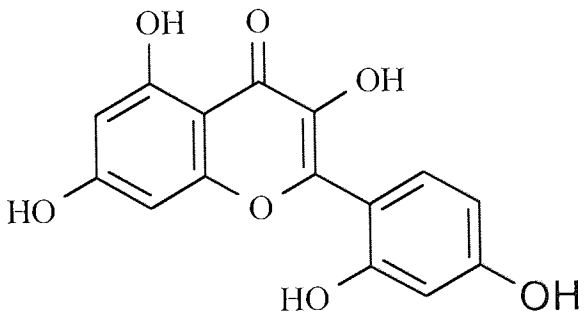


FIGURE 7.1 Morin molecule (2', 3, 4', 5, 7-pentahydroxyflavone)

Morin has many potential binding sites; it is thought that the Al complex with morin exists as a 3:2 morin:Al complex (Ahmed, 1995), although a more recent study identifies a 2:1 morin:Al complex (Liu, 1999). Complexation of Al to morin leads to a deep yellow chelate that has an absorption maximum at 421nm and a fluorescence maximum between 510 and 525nm, allowing detection via spectrophotometric (Ahmed, 1995) and spectrofluorescence methods (Sabbioni, 1999). There are several

methods that now can be employed for the spectrophotometric and/or spectrofluorimetric detection of Al. Some of these are summarised in the table 7.1 below.

TABLE 7.1 Comparison of reagents used for the detection of Al

REAGENT	$\lambda_{ex}/\lambda_{em}$ (nm)	SENSITIVITY (ppb)	MAJOR INTERFERENCES	REFERENCE
Morin	440/525	50	Cu^{2+}, Cr^{3+}, Fe^{3+}, F^-, PO_4^{3-}	Will, 1961
8-hydroxyquinoline	350/415	20	Ga^{3+}, In^{3+}, Cu^{2+}, Fe^{3+}, Co^{2+}, Ni^{2+}, Bi^{III}	Rees, 1962
SASH	375/450	1.2	In^{3+}, Ga^{3+}, Be^{2+}, F^-, $H_2PO_4^{3-}$, Fe^{3+}, Ga^{3+}	Jiang, 1996
SABH	375/450	1.4	Sn^{IV}, V^V, Mo^{VI}, $C_2O_4^{2-}$, EDTA, Ga^{3+}	Cui, 1992
Lumogallion	365/548	0.5	-	Ishibashi, 1972
OSH	387/474	5	In^{3+}, Ga^{3+}, Be^{2+}, F^-, $P_2O_7^{2-}$, As^V, Zr^{IV}	De Pablos, 1986
OBSH	390/475	5	In^{3+}, Ga^{3+}, Bi^{III}, F^-, Pd^{2-}, Be^{2+}, $C_2O_4^{2-}$, Zr^{IV}	Gòmez Ariza, 1984
SHPA	382/440	4	In^{3+}, Zn^{2+}, Be^{2+}, F^-, As^V, EDTA	Gallego, 1983

Morin was used in these studies, as this reagent is inexpensive and readily available (Aldrich). The main disadvantage of this reagent is apparent from the table, in that its sensitivity is relatively poor compared with the other methods.

7.2.1 Calibration graph for morin assay

An initial preliminary scan of the Al:morin complex against a morin blank identified an optimal excitation and emission wavelength of 440nm and 510nm respectively, values similar to those reported by Vitorello *et al* (1996) (440nm and 515nm).

The initial aim was to identify a correlation between the fluorescence emitted by the Al:morin complex relative to Al content. The method for preparing the morin solution is outlined in section 2.5.1. 100µL of $AlCl_3.6(H_2O)$ of concentrations ranging from 1mM to 1.6µM were added to 3mL of 10% morin solution. The fluorescence was measured as outlined in section 2.5.2

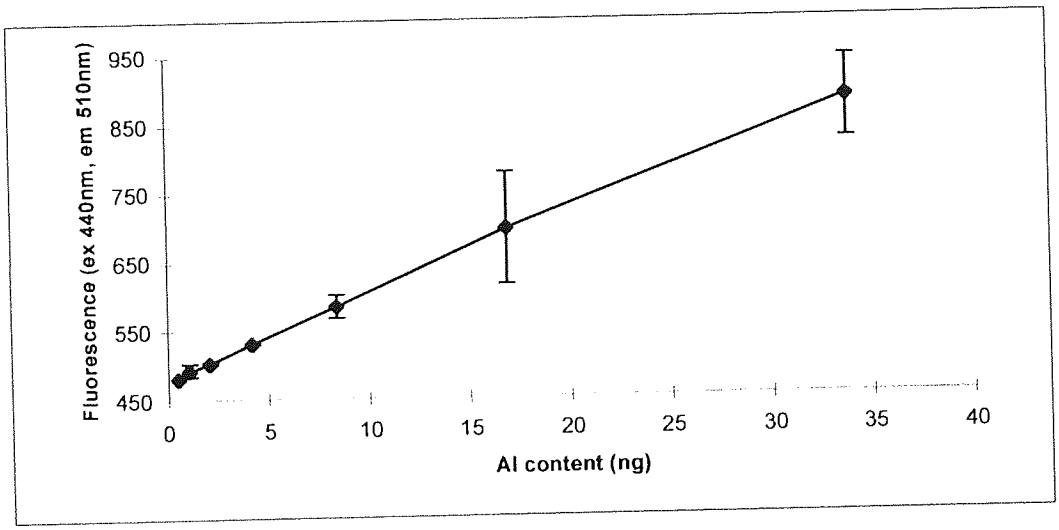


FIGURE 7.2 Calibration plot of morin assay using $AlCl_3.6(H_2O)$ as the Al source (n = 4, mean ±SD)

Changing the Al salt to Al lactate resulted in a similar calibration plot, indicating that the nature of the anion has little or no influence on the morin assay.

Figure 7.2 reveals a straight line with a correlation coefficient (R^2) of 0.9984, an improvement on a previously discussed method by Vitorello and Haug (1997) producing an R^2 value of 0.94. The following equation can be used to determine Al content.

$$y = 12.134x + 480.76$$

Equation 7.1

Equation 7.1 can be rearranged using the calibration graph (figure 7.2) to give:

$$\text{Al content (ng)} = \frac{\text{fluorescence} - 480.76}{12.134}$$

Equation 7.2

Using this spectrofluorimetric method, Al levels between 1- 33ng within a sample can be measured (5-165ng/mL), a wider range than that reported by Sabbioni (1999) of between 1-80ng/mL. These differences may result from the use of different excitation and emission wavelengths used in their studies (475nm and 555nm, respectively). Thus, all future samples containing Al were diluted as necessary to these Al levels to obtain fluorescence reading within the range detectable by the spectrofluorometer.

7.2.2 Influence of sample volume

As demonstrated in section 7.2.1, different quantities of Al sources are required for the calibration and for subsequent studies. This exercise aims to show that differences in Al sample volumes have negligible influence on the final fluorescence reading. Consequently, doubling the amount of Al in a calibration sample can be achieved by doubling the volume of the same concentration of $AlCl_3.6(H_2O)$.

TABLE 7.2 Influence of sample volume on morin:Al fluorescence. Figures in parentheses show standard deviation SD, n = 4

Al lactate (12.5μM) (mL)	d/d water (mL)	10% morin solution (mL)	final volume (mL)	Fluorescence (arbitrary units, a.u)
0	0.1	3	3.1	3 (±2)
0.1	0	3	3.1	884(±59)
0.1	0.1	2.9	3.1	880 (±54)
0.1	0.2	2.8	3.1	879 (±56)
0.1	0.3	2.7	3.1	879 (±58)
0.1	0.4	2.6	3.1	877 (±64)

Table 7.2 shows that over the range of volumes shown, changes in volume have negligible influence on the fluorescence and consequently analysis of Al. Another point to note is that double distilled (d/d) water has undetectable amounts of Al within it consequently is suitable for dilutions where necessary.

7.2.3 Stability of Al:morin complex

The previous section shows a linear correlation between Al content and fluorescence produced (Figure 7.2), however to use the morin assay in further association studies using the models discussed in section 7.1, this method must first be optimised. As a trivalent ion, Al is known for its slow reaction kinetics (Jones, 1984), consequently to establish a protocol, a study was undertaken investigating the fluorescence of the Al:morin complex with respect to time.

For this study 100 μL of Al lactate (12.5μM) was added to 3mL of 10% morin stock solution. The fluorescence was measured at various intervals to identify the most suitable time for equilibration of the complex and fluorescence measurement.

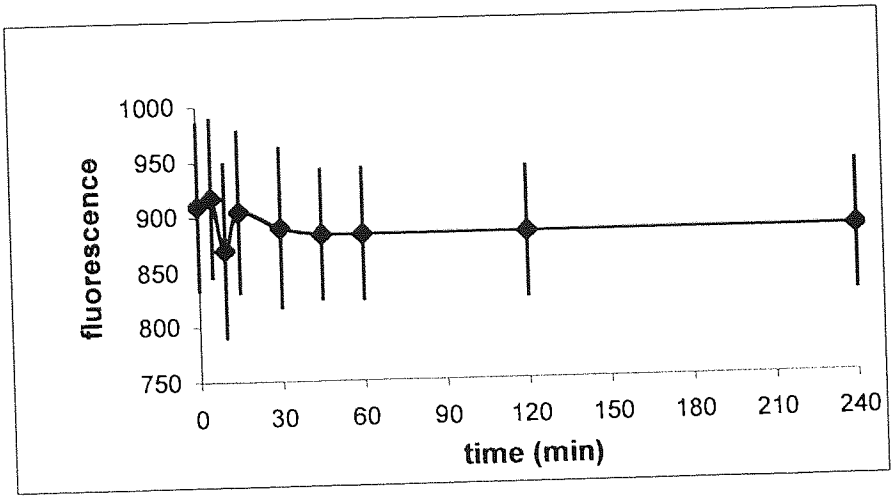


FIGURE 7.3 Stability of Al:morin complex (n = 4, mean ±SD)

This study shows that equilibrium is achieved approximately 40 minutes after Al is added to the morin solution. All subsequent studies involving Al detection were allowed to stand for an hour to allow the Al:morin complex to equilibrate prior to fluorescence measurement. The complex remained stable over the course of this study being 48 hours.

7.2.4 Influence of other ions and recovery of Al

Table 7.1 shows that the morin assay is affected by various ions. Those of particular interest in biological systems are Fe^{3+} and PO_4^{3-}. However, if this assay is to be used in the models discussed later (sections 7.3 and 7.4), then the extent of interference by these ions needs to be identified. Thus, those ions thought likely to be abundant within biological systems, consequently in the models studied, were investigated.

An Al sample containing 337.5ng of Al (100μL of 12.5μM $AlCl_3.6H_2O$) was used as the control. Both free and Al doped samples of equivalent amounts of Fe^{3+}, as ferric chloride, PO_4^{3-}, as Al phosphate, Ca^{2+}, as calcium chloride, Mg^{2+}, as magnesium chloride and EDTA, as the tetrasodium salt were studied. The fluorescence detected was expressed in terms of % interference relative to Al (Figure 7.4) and was converted to amount of Al per sample (in ng) using equation 7.2, as the ultimate objective of these studies was to determine Al content (Figure 7.5).

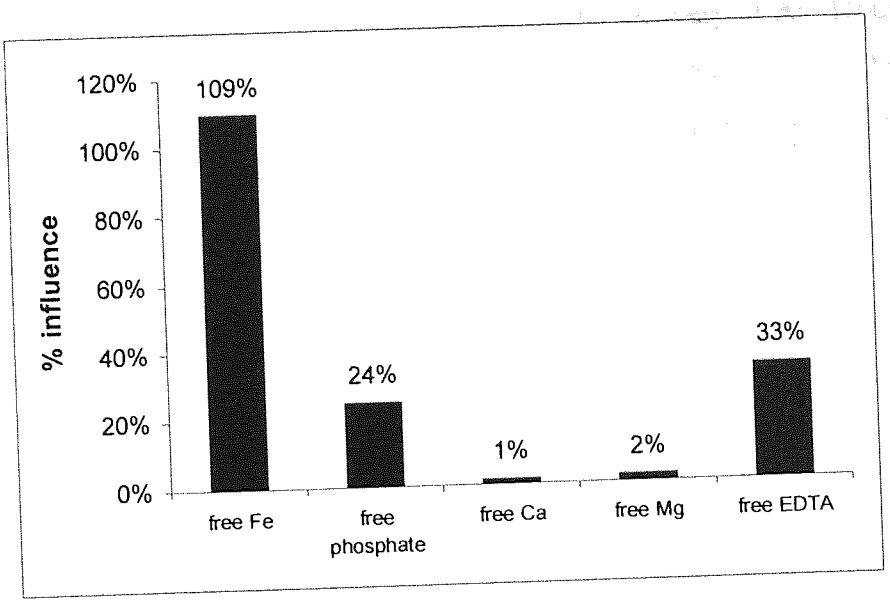


FIGURE 7.4 Interference of Al analysis using the morin assay expressed in terms of % control

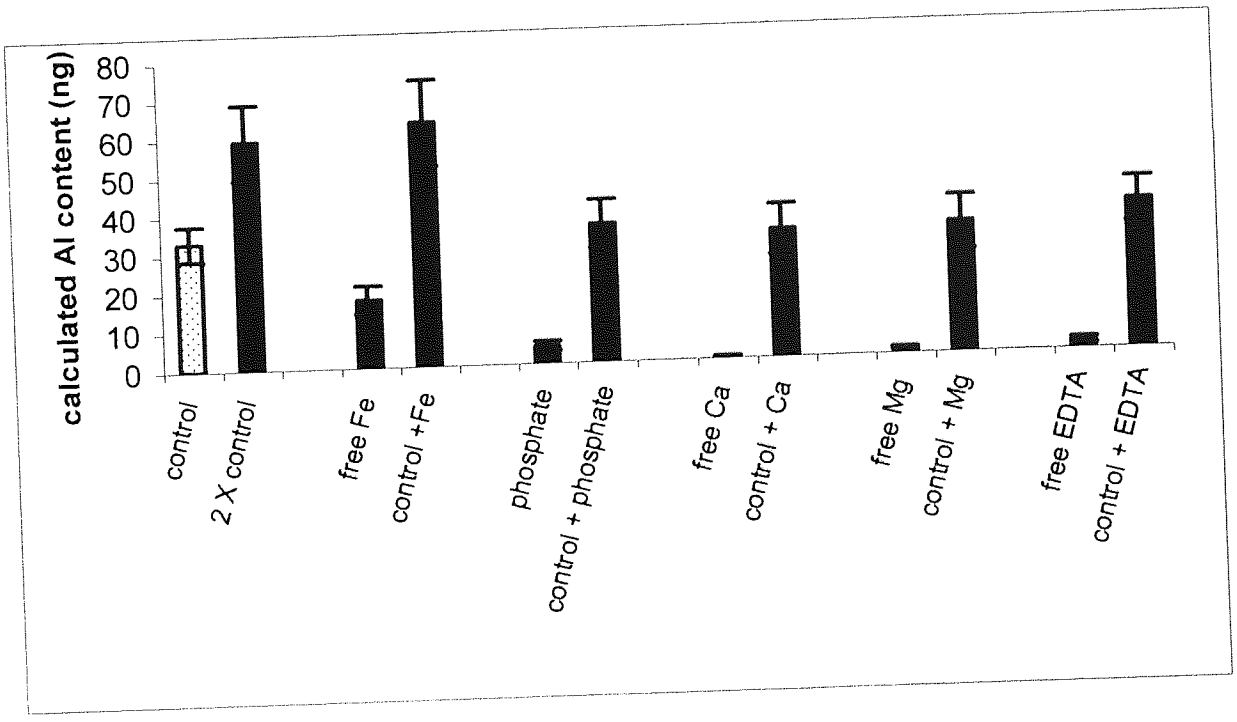


FIGURE 7.5 Interference of ions on Al analysis using the morin assay. Control containing 33.75ng $AlCl_3.6(H_2O)$ (n = 4, mean ±SD)

Figure 7.4 illustrates the effect of various ions on the morin assay. Ca^{2+} and Mg^{2+} had little influence on the morin assay, although Fe^{3+}, PO_4^{3-} and EDTA had marked

effects. Fe^{3+} had the greatest influence with equivalent quantities of Fe producing more than 100% interference. Figure 7.5 also shows the recovery of Al. Doubling the quantity of Al (shown as 2 x control) resulted in a 91% recovery. Free EDTA had a 33% influence on Al fluorescence, which is most likely attributable to the presence of the ferric and aluminium cations. To investigate this, an aqueous solution of 12.5μM EDTA (sodium salt) was passed through a pre-acidified Chelex 100 column, an ion exchange column designed to bind to metal cations, and analysed using the morin assay.

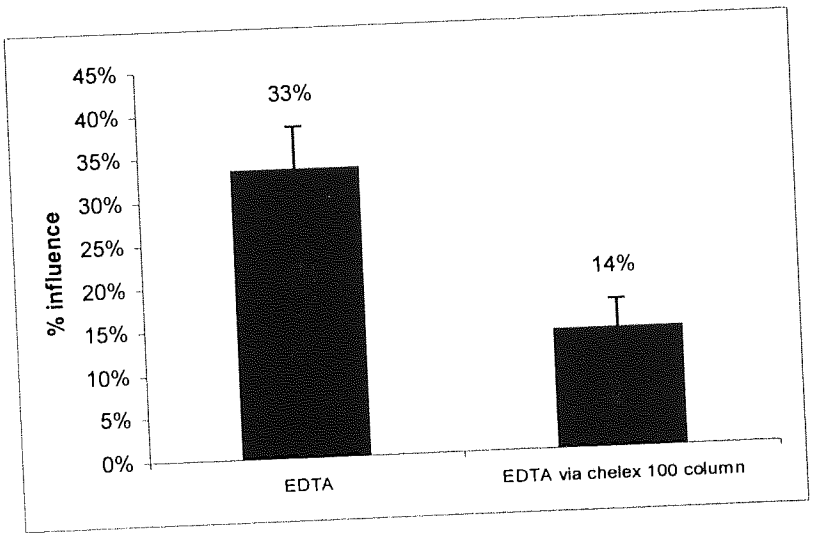


FIGURE 7.6 Influence of passing reagents through an ion exchange Chelex 100 column (n = 4, mean ±SD)

Passing the chelator through an ion exchange column markedly reduced the influence of EDTA on the fluorescence produced in the morin assay suggesting that the interference was most likely attributable to cations already present within the EDTA solution.

A comparative study of the morin assay with the AAS method to assess Al analysis is discussed in section 7.4.4.

7.2.5 Discussion

These studies have shown an inexpensive and simple method of detecting Al producing a correlation of 0.994 and low SDs. The recovery of Al was shown to be significant at 91%. The main disadvantage of this method of analysis is the influence of interfering ions, in particular $Fe^{3+}$and PO_4^{3-}, both ions of importance and in abundance in biological systems. However, using suitable controls, these assays can be used to determine Al association into the model cells as it would be assumed that these interfering ions would remain constant in the experiments undertaken.

7.3 MICROBIAL INVESTIGATION OF TOXIC EFFECTS OF AL

Bacteria synthesise siderophores to solubilise external ferric ions to enable uptake as explained in section 7.1. Under certain conditions these siderophores can be used to transport Al (Haug, 1994). As these studies were to be used to investigate the influence of chelators on the internalisation of Al, the presence of siderophores would complicate the study. Consequently, an *E. coli* W3110 strain was used, which does not produce the potent Fe chelators enterobactin and aerobactin, known to also bind strongly to Al (Cohen, 1998).

7.3.1 Correlation of OD with *E. coli* in a 96 well plate

All studies were undertaken in 96 well plates, consequently the cell number needed to be established using an OD. A preliminary investigation was carried out to identify a correlation of OD_{470nm} with *E. coli* cell number.

A calibration study was undertaken as outlined in section 2.6.3.

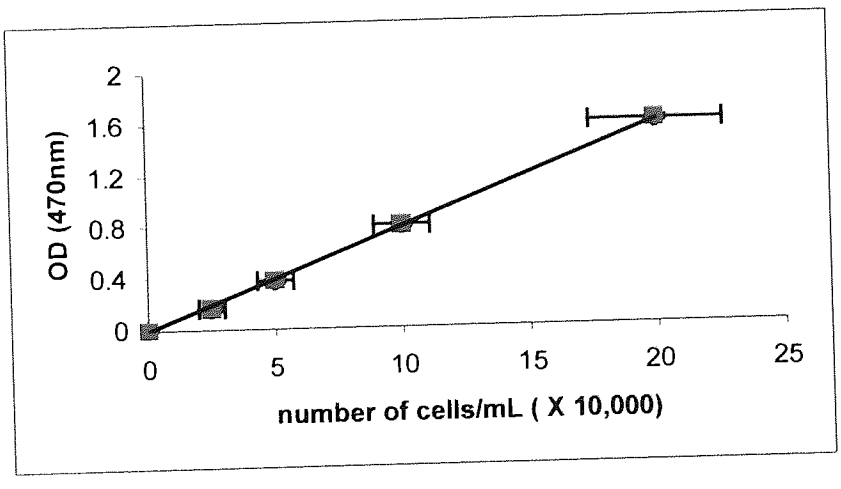


FIGURE 7.7 Correlation of OD_{470nm} with *E. coli* using a 96 well plate (n = 4, mean ±SD)

A linear correlation of 0.9993, with a linear equation of:

$$\text{number of } E.coli \text{ cells/mL } (\text{x } 10{,}000) = \frac{\text{OD }_{470nm}}{0.0793}$$

Equation 7.3

7.3.2 Influence of Al on antimicrobial activity of a variety of commercially available antibiotics

Many antibiotics possess oxygen and nitrogen donor atoms, which as shown within the CSD studies (chapter three) are likely candidates for complexing with Al. Consequently a variety of antibiotics chosen for their potential to bind to Al based on their structure were used in this study.

The method used is outlined in section 2.6.3

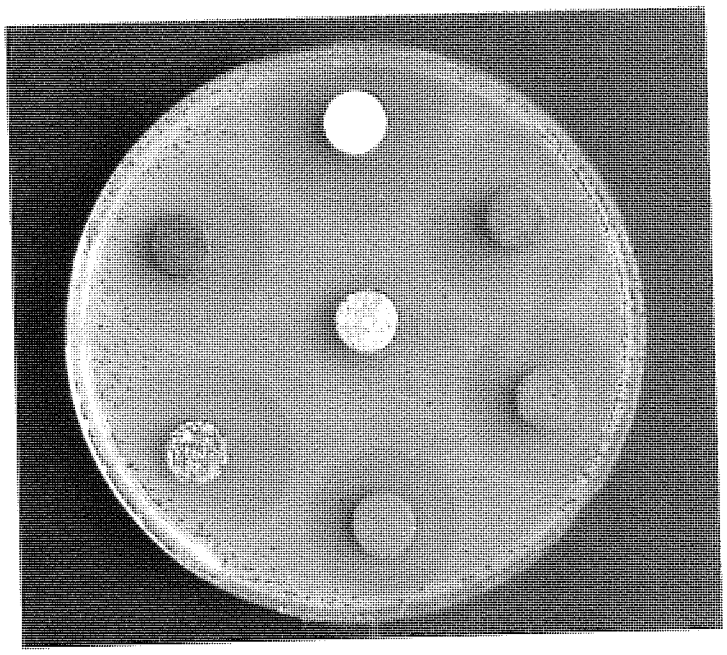


FIGURE 7.8 Photograph of antibiotic doped neo sensitabs illustrating zones of inhibition produced on growth of *E. coli* on NA

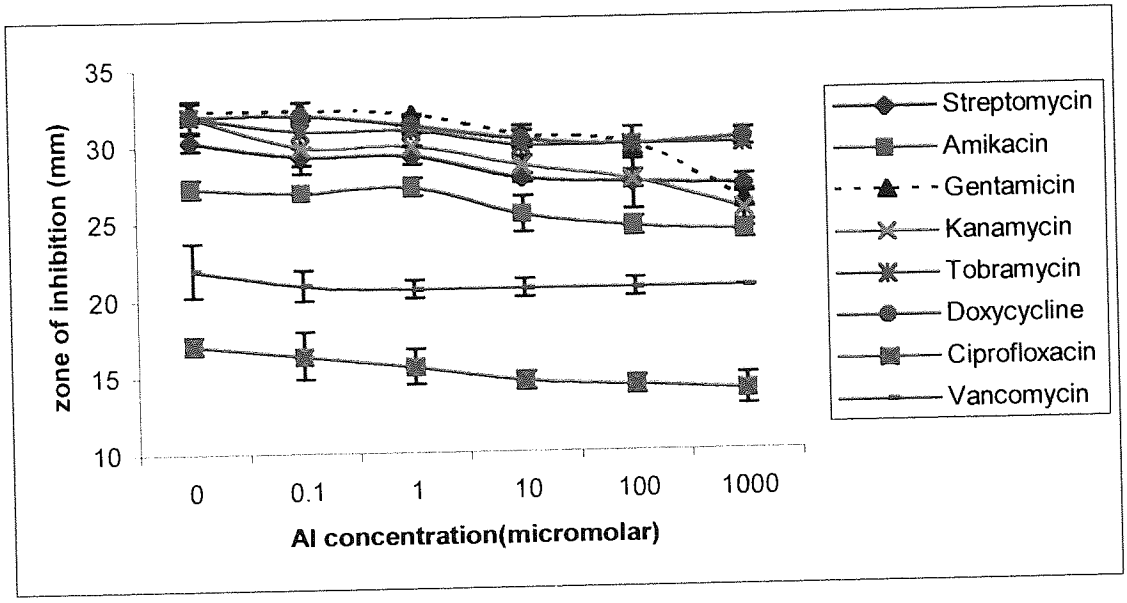


FIGURE 7.9 Influence of Al on zones of inhibition produced by antibiotic containing neo-sensitabs on *E. coli* (n = 4, mean ±SD)

The eight antibiotics tested (figure 7.8) were influenced by Al content within the media. In all cases the inhibitory actions of the antibiotics were reduced.

It has been reported that second generation quinolone antibiotics such as ciprofloxacin have reduced efficacy when given with other medication such as antacids which are high in Al salts (Brouwers, 1992). Those studies have shown that Al complexes with the ciprofloxacin forming a complex which is unable to cross the gastric mucosa (Helena, 1995), consequently decreasing the bioavailability and therefore the efficacy of the antibiotic. However, no work to date has been reported as to whether the Al complex possesses antimicrobial activity. Thus, primary investigations were to evaluate the influence of Al on the antimicrobial activity of ciprofloxacin on *E. coli*.

7.3.3 MIC of ciprofloxacin on *E. coli*

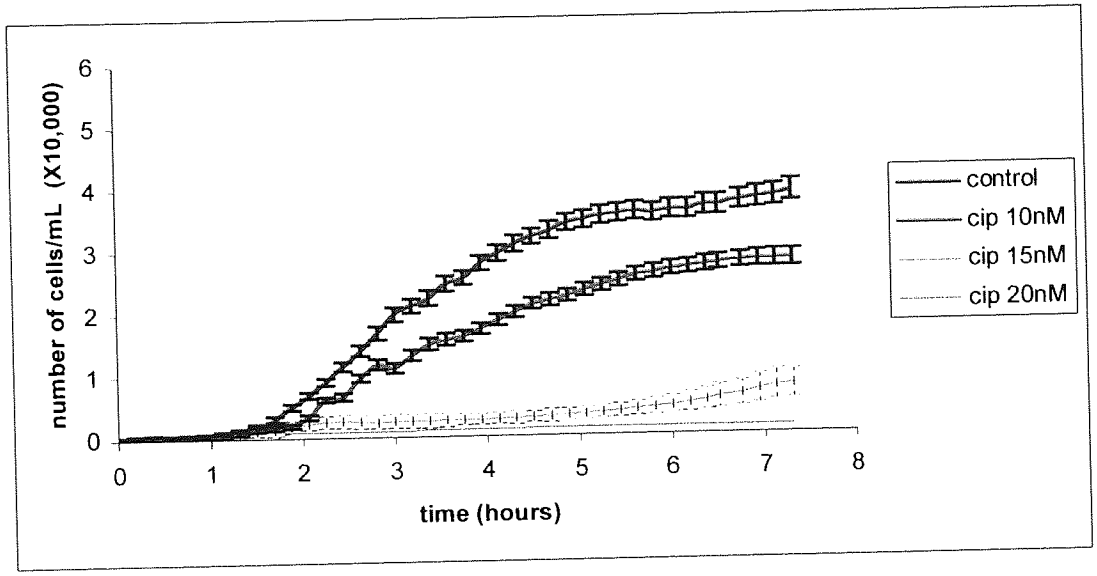


FIGURE 7.10 MIC of ciprofloxacin on *E. coli* (n = 8, ±SD)

The control shows an initial lag period of approximately 90 minutes prior to the exponential phase which continues for approximately three hours, with a doubling time of about 30 minutes during this period. The exponential phase reaches a plateau after approximately 5 hours post inoculation. Thus, studies of uptake were undertaken over a four hour period ensuring the *E. coli* had established exponential growth during the period of study.

The MIC for ciprofloxacin on *E. coli* is 20nM; a final concentration of 15nM resulting in approximately 10% growth relative to the control, was therefore chosen for further investigations.

7.3.4 Influence of Al on growth of *E. coli*

Ultimately, this study aimed to show the delivery of Al into microbial cells. A toxicity test was undertaken to identify the maximum concentration of Al within the media that can be tolerated by *E. coli*.

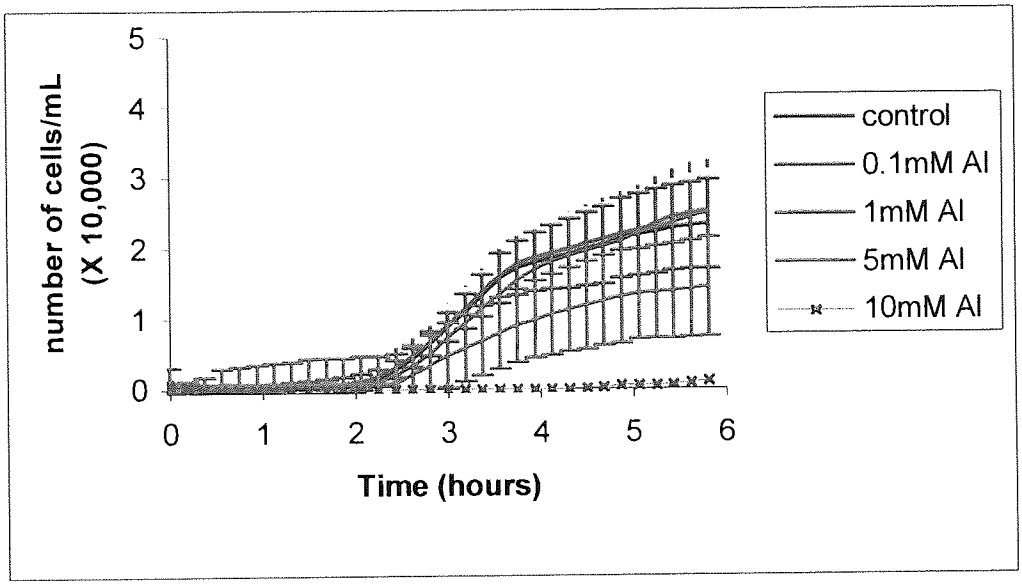


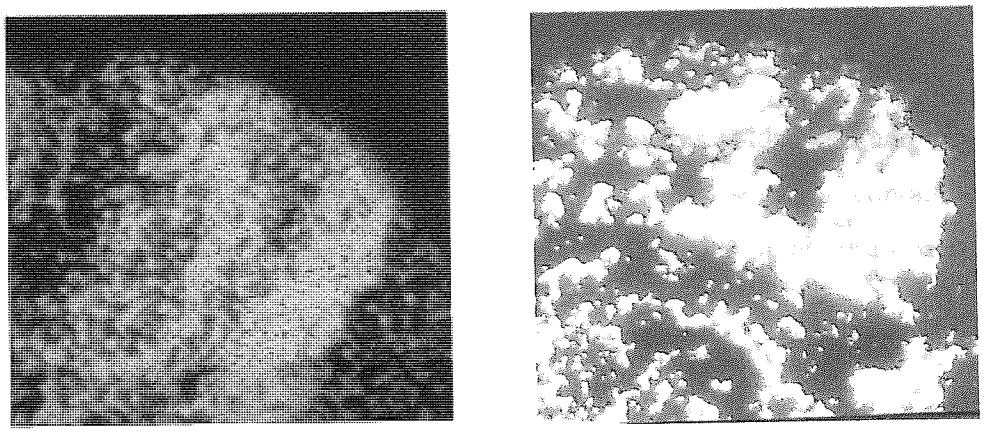
FIGURE 7.11 Influence of Al on growth of *E. coli* (n = 8, mean ±SD)

The above figure shows the effects of Al (0.1-10mM) on the growth of *E. coli*. The MIC, taken as the minimum concentration of Al (as the chloride) required for inhibiting growth is shown to be 10mM. A final concentration of 100μM of Al within the NB is the maximum Al concentration that can be tolerated by the *E. coli* without any observable effect on growth. The graph uses the OD_{470nm} to calculate the total number of cells. It would be expected that all initial OD_{470nm} would be similar, as the same quantity of *E. coli* inoculum was added to each concentration of Al used. However the initial OD's have varied considerably upon increasing concentrations of Al to 5mM, suggesting that some precipitation of an Al salt had occurred. OD adjustments were made by subtracting OD_{470nm} values of sterile duplicates and have been accounted for in figure 7.11.

Al is amphoteric in nature, perhaps explaining the slight decrease in precipitation upon increasing Al content to 10mM (data not shown). NB has minimal buffering

capacity, consequently it would be unable to control the pH influence of 10mM Al, which was found to decrease pH from 6.7 (control) to 5.1.

Incubation of *E. coli* in 100μM Al lactate over a two hour period, as described in section 2.6.7 shows the influx of Al into the cells, as shown in the fluorescence photograph below.



(a) (b)

FIGURE 7.12 Fluorescence photographs of morin stained *E. coli* as a: control and b: doped with 100μM Al lactate over a 2 hour period (magnification x 400)

Fluorescence is observed in the control, possibly due to the presence of ferric ions inherently present in microbial cells for normal function. However, fluorescence is markedly increased by the presence of Al within the media indicating transport into the cells.

7.3.5 Influence of Al on antibacterial activity of ciprofloxacin

It has been reported that complexes of Al with the potent siderophore Al chelator, enterochelin (Rogers, 1978) have antimicrobial activity. Consequently, growth curves of *E. coli* with inhibitory concentrations of ciprofloxacin (15nM) and Al were investigated. Using the morin assay the effect of Al complexation with ciprofloxacin upon delivery of Al through the microbial cell wall into the cells could be studied.

A concentration of 15nM ciprofloxacin was used in this study with and without the 100nM $AlCl_3.6(H_2O)$. When used with Al a stock solution containing equal concentrations of $AlCl_3.6(H_2O)$ and ciprofloxacin was made up at least one hour prior to the study to ensure equilibration of complexation.

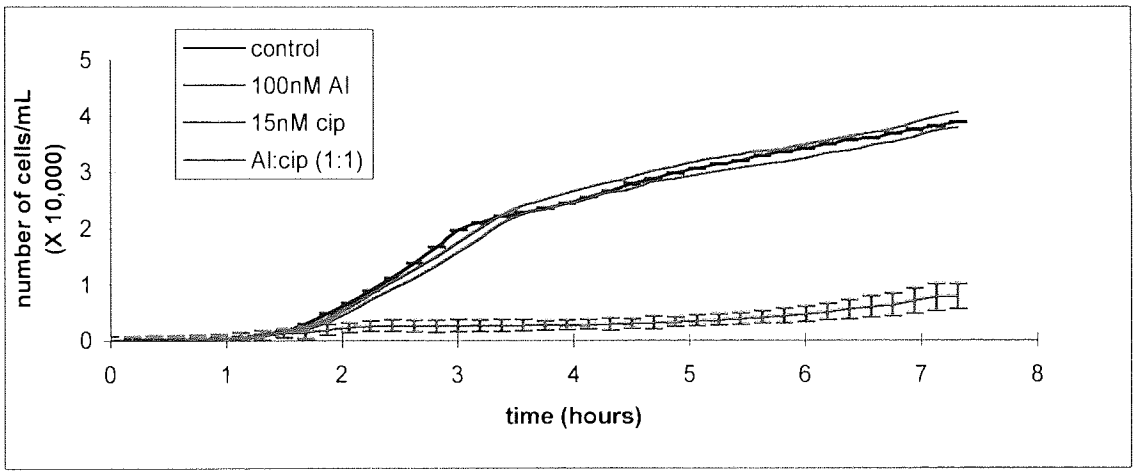


FIGURE 7.13 Influence of Al on the antimicrobial activity of ciprofloxacin using *E. coli* (n = 8, maximum SD = ±3,000 cells)

Al completely eliminated the antimicrobial action of ciprofloxacin as shown in figure 7.13. Further studies were conducted to establish if this is simply due to the complex not being able to pass the cell wall, hence enter the microbial cell, or whether complexation interferes with the active sites of ciprofloxacin. The morin assay was used to quantify the effect of ciprofloxacin on Al entering the *E. coli* microbial cell as described in section 2.5.

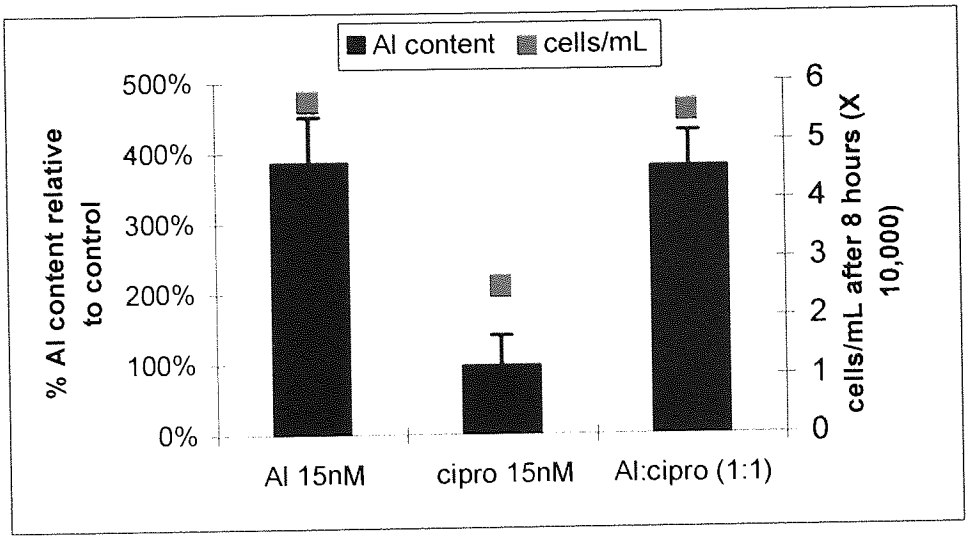


FIGURE 7.14 Influence of ciprofloxacin on Al delivery into *E. coli* cells (n = 4, mean ±SD)

The results show negligible differences in Al entering the cells when complexed with ciprofloxacin or as free Al, suggesting that the Al:ciprofloxacin complex also enters the cell.

Ciprofloxacin selectively inhibits bacterial DNA synthesis by acting on the enzyme DNA gyrase, a topoisomerase that inserts negative supercoils into a DNA helix (Wilson, 1997). The bacterial chromosome comprises a molecule of DNA, which is 1300μm in length, which is compressed into a cell 1 x 2 μm in size. DNA gyrase has four subunits, two A subunits and two B subunits (derived from the *gyrA* and *gyrB* genes, respectively). Supercoiling reduces the size of DNA by introducing 65 domains with a length of 20μm, and achieves further compaction by twisting (around 400 times) (Smith, 1986). During supercoiling of the domains, the two A subunits produce a staggered cut in the DNA, resulting in DNA termini with free 3' hydroxyl groups and a 5' extension. (Morrison, 1989). The 5' termini are covalently bound to the enzyme, the cut being made at a thymidine-guanine dinucleotide on one strand, but at a random position on the other.

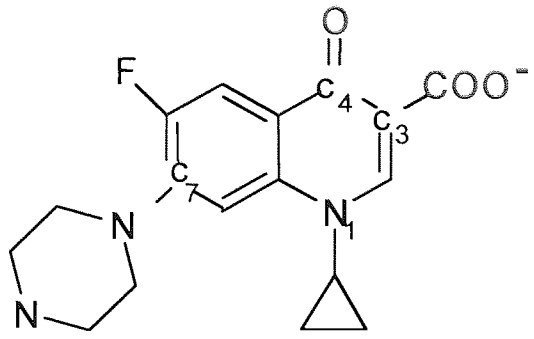


FIGURE 7.15 Structure of ciprofloxacin illustrating the 3-carboxylate and 4-carbonyl moieties which are responsible for binding to DNA gyrase

Figure 7.15 shows the 3-carboxylate and 4-carbonyl moieties of ciprofloxacin, the groups that are responsible for binding to DNA gyrase and essential for antibiotic activity. Both groups possessing donor oxygen atoms with high potential to bind to Al. The C_7 substituent ensures the correct orientation of the quinolone molecule (Mitscher, 1990).

For antibacterial action, ciprofloxacin must bind to DNA. This study has shown that the Al:ciprofloxacin complex enters the cell, suggesting that the complex itself has little or no bactericidal properties. Perhaps the active sites on the ciprofloxacin molecule may be affected by the binding with Al, ultimately inhibiting its antimicrobial action.

7.3.6 Discussion

These studies have shown that Al affects the antibacterial properties of ciprofloxacin, a potent quinolone antibiotic. The Al:ciprofloxacin complex itself can still enter microbial cells but has little or no bactericidal activity, most probably attributed to Al binding at the active sites of the ciprofloxacin molecule.

1. The study involving the use of excess Al (100nM) relative to ciprofloxacin (15nM) assumes 100% complexation of the ciprofloxacin with the excess Al.
2. It is assumed that the excess morin solution has a greater affinity for Al relative to ciprofloxacin, consequently resulting in 100% displacement of Al from the Al:ciprofloxacin complex to form an Al:morin complex leading to fluorescence.

The main drawback of this study is that excess Al was used and the cell wall of *E. coli* differ somewhat from that of a human brain cell, the area likely to be affected. Thus using the same techniques and potential chelators of Al, the studies were adopted using the U87-MG glioblastoma cell line.

7.4 U87-MG CELL LINE

7.4.1 Introduction

These studies were aimed at showing the association, either as an influx of Al into cells or as adsorption of Al on the cell membrane. Consequently they will be highly dependent on the histology of the cells used within the models. As a result the U87-MG glioblastoma cell line was chosen as this probably best mimicked cells within the human brain which were subject to Al intoxication.

7.4.2 Differences in growth between serum free and 10% FCS media using U87-MG cells

The U87-MG cell line was characterised to determine cell growth rates, to identify any variability in cell association using cells incubated for different time periods prior to use and to establish a protocol for removal of loosely associated material by PBS washing.

As with the studies with *E. coli*, ideally the simplest medium for growth was to be used to minimise possible interactions between Al and substituents within the media. Consequently, while normal maintenance of the cells was undertaken in media containing 10% FCS, the aim was to undertake studies involving Al in serum free media. Thus, growth curves of cells seeded at 5 x 10^5 cells/mL in 24 well plates were monitored and evaluated using the trypan blue and MTT assay as described in sections 2.7.1.3 and 2.7.1.4, respectively.

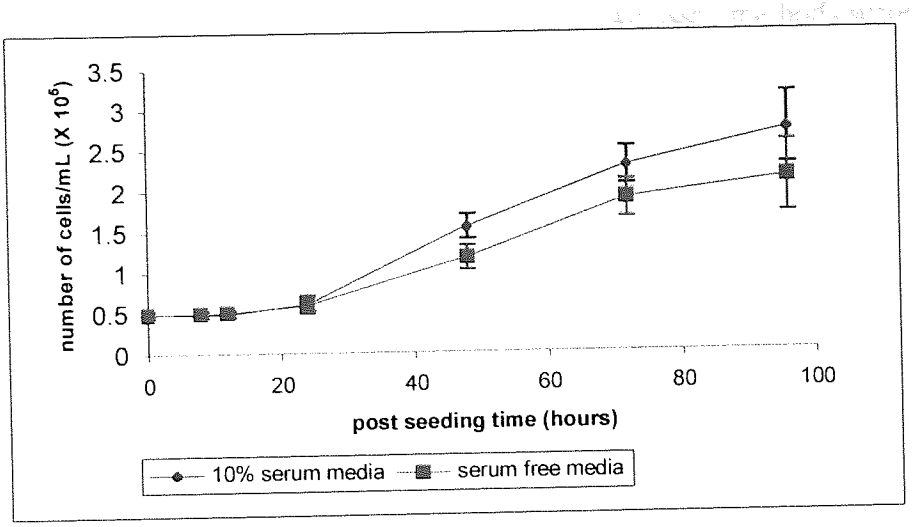


FIGURE 7.16 Growth curves of U87-MG cells in both serum and serum free media calculated from a seeding density of 5 x 10^5 cells/mL using 24 well plates (n = 4, mean ± SD)

The growth curve (Figure 7.16) indicates that following seeding, U87-MG cells enter a lag period of at least 18 hours, followed by a period of exponential growth. Cell number increased by a mean of 20% after 24 hours in both serum free or 10% serum containing media. The cell doubling time during the exponential growth phase was approximately 24 hours in serum free media. If Al delivery studies in U87-MG cells were performed 24 hours post seeding, then cells would probably have entered an exponential period of growth.

The results show minimal and negligible difference in growth over the first 24 hours between serum free and serum containing media. In both cases maximal growth occurs between 24 and 48 hours. In this instance, the trypan blue exclusion assay was used to count the number of cells. However, further studies were to be undertaken in 96 well plates, rendering the methodology used for the trypan blue exclusion assay impractical. As described in section 2.7.1.3, the trypan blue exclusion assay involved the trypsinisation of cells. This procedure is likely to have large errors as undoubtedly some cells adhere to the well chamber or clump together, consequently the MTT assay was employed. To illustrate this, varying concentrations of U87-MG cells were made up by serial dilution in serum free/phenol free media. 200μL aliquots were added to each of the wells in two 96 well plates using a multi-channel pipette. Assuming that

both plates were identical in terms of cell number, the two assay methods were used to identify viable cells.

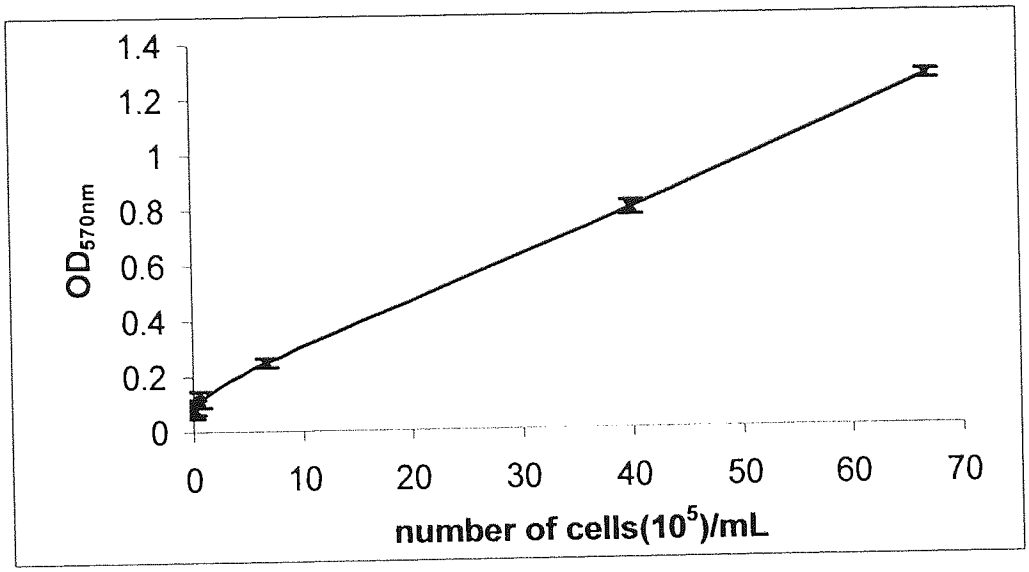


FIGURE 7.17 Calibration plots of OD_{570nm} against cell number using MTT assay (n = 8 ± SD)

The MTT assay produced a correlation of 0.9985. The main advantage of this assay is that it involves fewer steps to obtain a viable count, ultimately producing smaller SD's with respect to the trypan blue assay. Consequently the MTT assay was the method of choice for further studies involving cell viability counts.

The equation for the correlation being

$$y = 0.0175x + 0.0984$$

Equation 7.4

which can be rearranged to calculate cell number as:

$$\text{cells/mL}\,(x10^5) = \frac{OD_{570nm} - 0.0984}{0.0175}$$

Equation 7.5

7.4.3 Toxicity testing

To assess the cellular toxicity of Al on this cell line, studies were initiated as described in section 2.7.2 using a range of concentrations of Al lactate (final concentrations between 1μM-1000μM). Cells were incubated in Al lactate with/without a chelator for four hours in serum free/phenol red free media. The medium was removed and the cells washed with PBS as described in section 2.7.2. The cell count was determined by the MTT assay as described in section 2.7.1.4. Control samples were incubated for the same time period in serum free/phenol red free media alone.

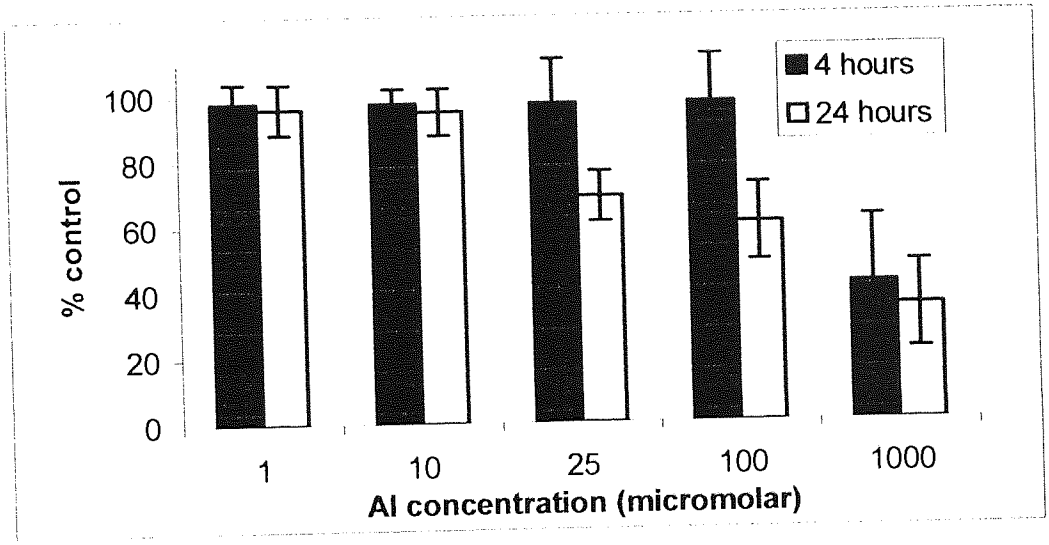


FIGURE 7.18 Graph of percentage of viable U87-MG cells remaining after treatment with various concentrations of Al lactate for 4 and 24 hours at 37°C relative to a control (n = 8, mean ± SD)

The total viable count of cells incubated in serum free/phenol red free media for 4 or 24 hours, in the presence of added Al lactate, was not significantly different to that of the control sample when using Al concentrations in the range of 1-10μM. At these concentrations greater than 96% of this cell population remained viable over a 24 hour period. Incubation over a 4 hour period in an Al concentration of 100μM produced 97.5% of the control cell population. With reference to the growth curve (figure 7.16), the cell doubling time was in excess of 4 hours. Therefore a cytotoxic rather than an anti-proliferative effect would appear to offer the most likely explanation of the reduction in cell number following exposure to high Al concentrations (i.e. high

concentrations of Al did not inhibit cell division but were directly toxic to the U87-MG cells). However the aim at this stage was to establish the maximum non-toxic concentration of Al which could be administered during delivery studies, rather than to establish the mechanism of toxicity. The results indicate that Al lactate concentrations of up to 100μM did not have significant effect on viable U87-MG population over a 4 hour period, and could therefore be used to assess the influence of chelators on the delivery of Al into cells for that period.

7.4.4 Optimising Al delivery into U87-MG cells

An Al cell delivery study was conducted as described in section 2.7.2 to assess the number of PBS washes necessary to ensure that all loosely bound Al was removed from U87-MG cell surfaces was removed. Al lactate was diluted to the required concentration of 100μM in serum free/phenol red free media. After 4 hours, the apical media was removed and 6 x 200μL washes were performed. Each wash was collected separately in separate eppendorf tubes and analysed for Al content using the morin assay described previously.

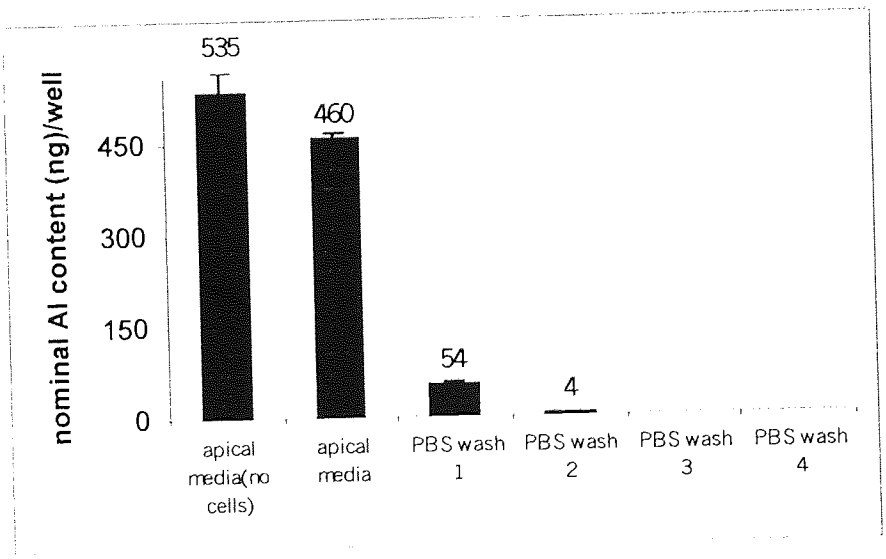


FIGURE 7.19 Graph illustrating number of PBS washes required to remove loosely bound Al (n = 3, mean ±SD)

Shi and Haug (1990) undertook a similar study on neuroblastoma cells, using both citrate and EDTA as washing agents. Both removed detectable amounts of Al in three washes as does this study. Both citrate and EDTA are relatively strong chelators of Al consequently are more likely to remove more tightly adsorbed Al from the cell surface which is probably bound to glycoprotein. Attempts at using washes consisting of these chelators proved unsuccessful as inconsistent results were achieved, probably due to the excessive quantities of Al and ferric ions present in these wash solutions as contaminants even after passing the solutions through a chelex 100 column. Consequently this study concentrated on removing only loosely bound Al using PBS.

This study concluded that approximately 90% of loosely bound Al was collected in the first PBS wash and all detectable amounts of Al were collected within three washes. Hence all further studies involving the washing of the U87-MG cell line and the analysis of Al were washed thrice.

To ensure a maximum surface area of the U87-MG monolayer available for association experiments, a preliminary study was carried out to identify the seeding density required to give maximal confluency 24 hours post seeding. Thus, serial dilutions of media with a cell density ranging from 1×10^6 to 1×10^4 cells/mL were made and seeded into a 96 well plate. Each well was observed using the microscope as described in section 2.6.7.

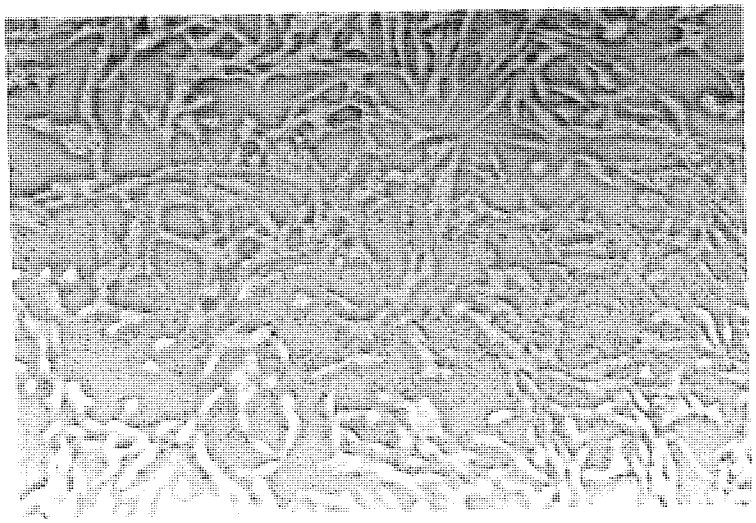


FIGURE 7.20 Photograph of U87-MG monolayer 24 hour post seeding at a density of 5 x 10^5 cells/mL showing approximately 80% confluency (magnification x 100)

7.4.5 Influx of Al lactate into U87-MG cells

A growth curve was first constructed in similar fashion to that undertaken in section 7.4.1 (figure 7.16), to display the influence of Al on growth over a 96 hour period.

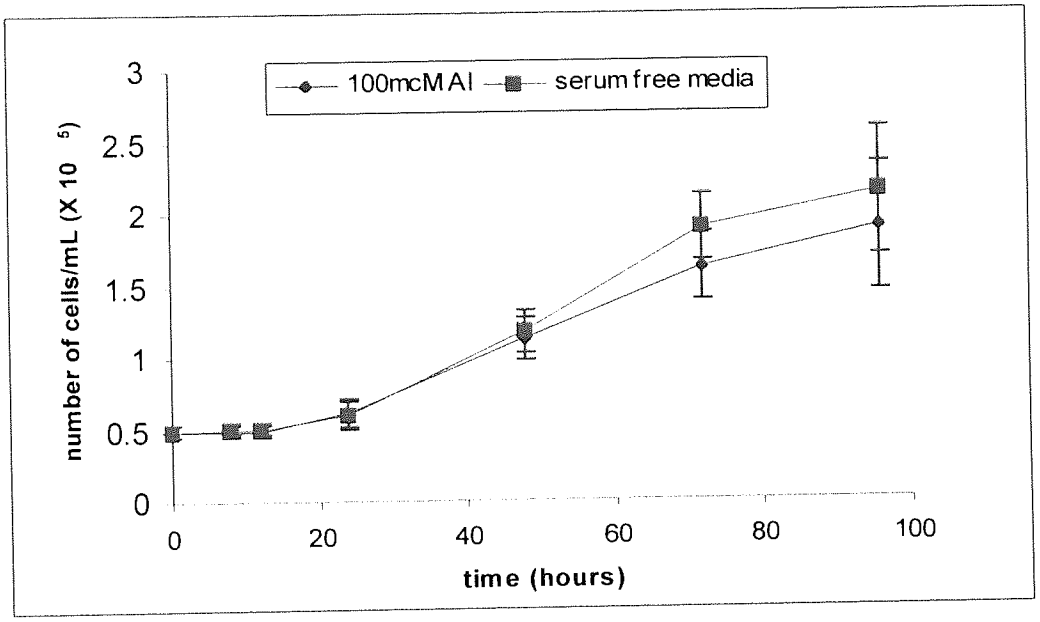


FIGURE 7.21 Influence of 100μM Al lactate on growth of U87-MG cells (n = 4, mean ± SD)

Pre-seeded 96 well plates were loaded with 100μM Al lactate doped media. The cells were then incubated for a period of time ranging from 30 minutes to 4 hours and treated as described in figure 2.4 before determining the Al content via the morin assay (section 2.5.2). The same samples were also analysed using AAS (section 2.5.3), thereby allowing a comparison between the two methods of Al analysis.

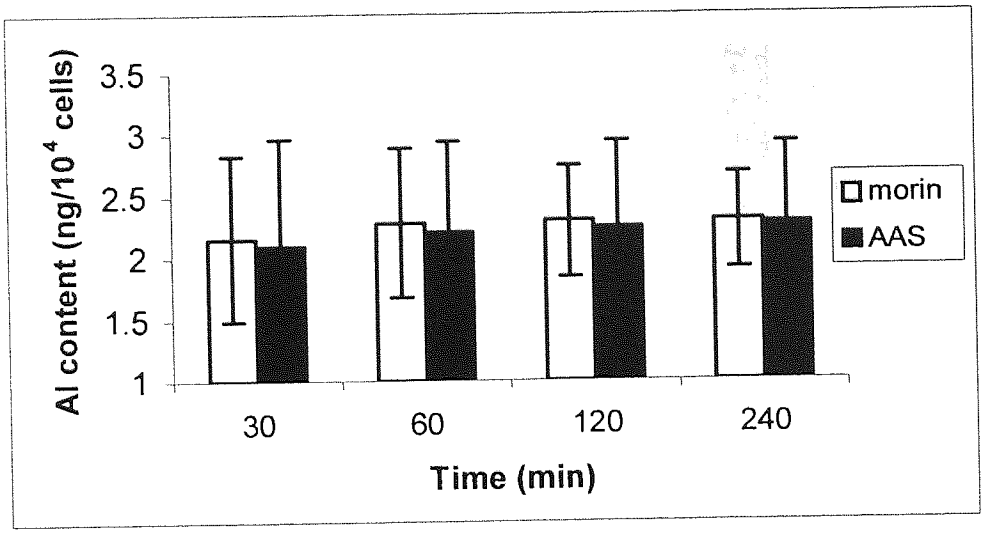


FIGURE 7.22 Graph illustrating the association of Al lactate into U87-MG cells over a 4 hour time period and comparing the morin and AAS methods of Al analysis (n = 4, mean ± SD)

Of the available Al per well (200μL of 100μM Al lactate = 540ng/200μL), approximately 3.7% is associated with the cells, assuming each well contains 0.6 x 10^5 cells/mL (1.2 x 10^4 cells/well) as figure 7.21 suggests.

7.4.6 Effects of temperature and metabolic inhibition on the uptake of Al in U87-MG cells

To investigate the effect of temperature and metabolic inhibitors on the uptake of Al, cell uptake was tested over a 4 hour time period in U87-MG cells as described in sections 2.7.3 and 2.7.4. The results of these experiments are demonstrated in figure 7.22 which shows the percentage of added Al that became associated to cells, which were incubated either at 4°C throughout, or were treated with sodium azide and 2-deoxyglucose and incubated at 37°C, compared with the control. The control sample represents the percentage of Al that became associated with U87-MG cells that were incubated at 37°C throughout and were not treated with any metabolic inhibitor.

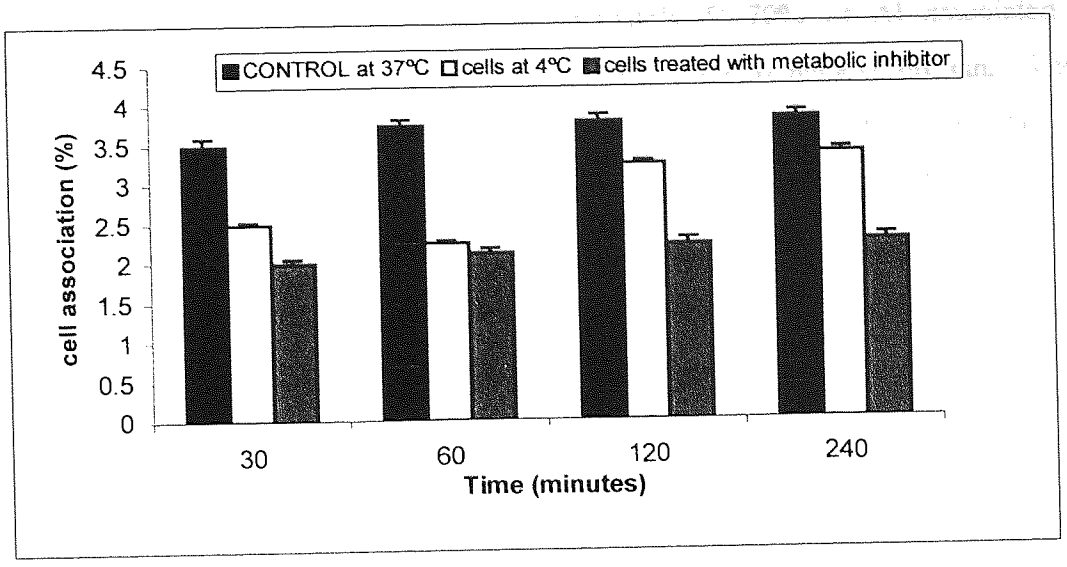


FIGURE 7.23 Effect of reduced temperature and metabolic inhibition on the % cell association of Al in U87-MG cells as a function of time compared with the control (n = 8, mean ±SD)

Cell association of Al was reduced but not completely inhibited at low temperature (4°C) at all time points tested ($P<0.006$, considered extremely significant). After 4 hours cell association was inhibited by almost 40%. An increase in cell association of Al after 60 minutes suggests that initial association is due to adsorption of Al on the cell surface s opposed to internalisation.

Metabolic inhibition also reduced the extent of Al cell association compared with the control at all time points tested ($P<0.0012$, considered very significant). Metabolic inhibition reduced cell association from 3.85% in the control to 2.25% after 4 hours and this effect was similar to that of a reduction in temperature.

The reduced cell association at low temperatures and in the presence of metabolic inhibitors indicates that to a degree, association involves cellular energy. The lack of complete inhibition of cell association could be due to energy-independent surface binding of the Al in the absence of internalisation (adsorption). Alternatively, in the case of the metabolic inhibitors, it could be due to incomplete ATP depletion by the sodium azide/2-deoxyglucose combination.

Dobson *et al* (1998) have reported approximately 50-70% of Al associated to neuroblastoma cells is present in the cytosol, and 20% to nuclear protein. These studies used ^{26}Al, a method capable of measuring pecogram quantities of Al, thus superior to the morin method. Attempts at establishing the quantity of Al adsorbed onto the cell surface using EDTA solutions proved to be unsuccessful due to the excessive Al content already associated with the EDTA.

7.4.7 Influence of chelators on the association of Al U87-MG

This study was undertaken to identify the influence of chelators on the association of Al into the cells. All chelators used in this study possess oxygen donor sites for Al complexation.

As with previous studies a 100μM Al concentration was used. Al lactate and acetylacetonate were obtained as 3:1 complexes (Aldrich). For controls free 300μM DL-lactic acid and acetylacetone was used. Desferrioxamine, DFO (Aldrich), and EDTA were used in 100μM concentrations with and without Al assuming a 1:1 complex would form. All other chelators were used at 300μM concentrations without an Al source, acting as controls and with $AlCl_3.6(H_20)$ to make 3:1 complexes. Professor Hider, Kings College, London, UK generously donated CP20, CP21 and CP94, (structures shown in figure 5.20). All chelator/Al solutions were made up as aqueous solutions and were mixed an hour prior to addition with serum free/phenol red free media to ensure pre-chelation equilibration. The study was carried out as shown in section 2.7.2 and analysed for Al using the morin assay as described in section 2.5.1. The subsequent results were expressed in terms of % control (i.e. 100μM $AlCl_3.6(H_20)$ without chelator present).

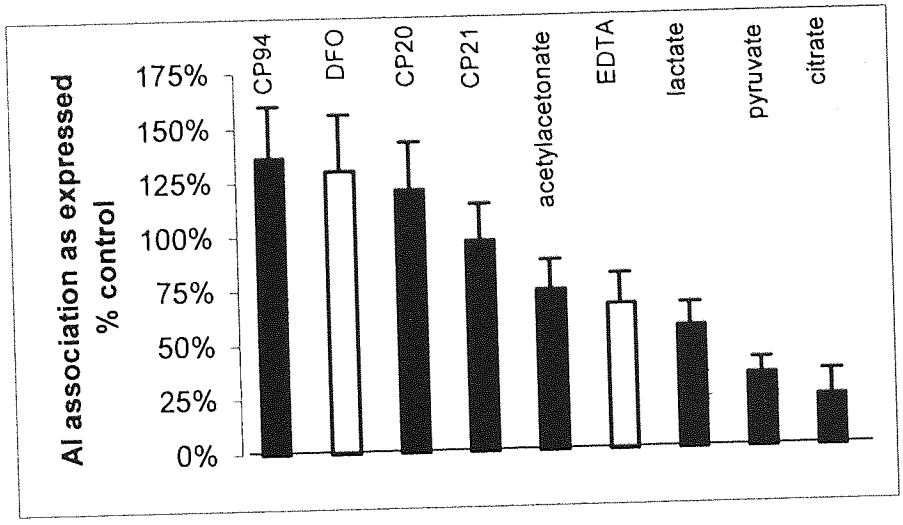


FIGURE 7.24 Influence of chelators on the association of Al to U87-MG cells relative to control. Clear and shaded bars indicate 1:1 and 3:1 ratios of ligand:Al, respectively (n = 4, mean ±SD)

The aliphatic carboxylic acids prove to inhibit association of Al. This may result from complexation forming less lipophilic compounds, which are unable to penetrate the cell membrane. Citrate shows the most marked influence with 77% reduction in association relative to the control, a value similar to that reported by Vitorello *et al* (1996) who showed an 85% reduction in Al uptake by neuroblastoma cells using a 20:1 ratio of citrate:Al (5mM:20μM).

Only the hydroxypyridinones CP94 enhance the association of Al on U87-MG cells relative to the model chelator, DFO, probably because the resultant complexes after pre-chelation with these ligands form more lipophilic compounds which are better able to pass through cell membranes.

7.5 CONCLUDING REMARKS

These studies have shown a simple and inexpensive method of Al quantification that can be used on models for the evaluation of potential Al chelating agents. The morin assay was optimised and ultimately capable of measuring up to ng quantities of Al. The morin results were also comparable to the more routinely used and expensive AAS method of Al analysis. Studies using *E. coli* have identified that ciprofloxacin activity is inhibited by complexation with Al, rendering the complex itself ineffective. The U87-MG cell line proved to be an effective model showing statistically significant changes in Al association upon variation of chelating agents, ultimately identifying only CP94 as an improvement over the model chelator in this study, DFO. This may be attributable to the fact that the 3:1 complex of CP94 with Al has a reported octanol/water partition coefficient of 2.6, making it lipophilic, hence more favourable to pass through cell membranes, while that of aluminoxamine is reported to be <0.0006, making this complex extremely lipophobic (Yokel, 1991). Cable and Lloyd (1999) have also shown that the CP94:Al complex can pass readily and more rapidly through the cell membrane, while the more lipophobic aluminoxamine complex enters rat visceral cells slowly via endocytosis as it is unable to pass through the cell membrane.

CONCLUSION

The work in this thesis concentrated on developing both a theoretical and a practical approach towards designing Al chelators. Preliminary studies involving CSD searches identified that Al prefers to bind in a six co-ordinate manner to bidentate ligands possessing oxygen as the exclusive donating atom to form 3:1 complexes containing five and six membered chelate ring systems. Approximately 76% of this type of complexes exhibited in deprotonation at the point of ligation. This result is most likely attributable to the repulsive forces between the proton and the high positive charge density of the Al ion. The CSD studies also identified differences in binding trends of Al and other trivalent metal ions, in particular the ferric ion (Fe), an ion with the same charge as Al and relatively similar ionic radius. Fe prefers to bind to ligands possessing the 'softer' donating atom, nitrogen, again resulting in the formation of complexes possessing five and six membered chelate ring systems. Al-O distances were significantly shorter than Fe-O distances, with five membered chelate systems having mean distances of 1.909 Å and 2.014Å respectively, and six membered chelate ring systems having mean distances of 1.888Å and 1.996Å respectively. Ultimately, MO calculations concentrated on six co-ordinate Al complexes with bidentate oxygen containing ligands.

A crystallographic theme was also inherent, as X-ray crystallography is still considered an important aspect of the drug design process, as demonstrated by the CSD work. These studies solved novel structures of anhydrous DL tartaric acid (ALTAR), dimethylcitrate monohydrate (CITXL) and butylciprofloxacin (BUCIP4), while previously reported structures of aluminium chloride hexahydrate (ALPXL) and anhydrous tricarballylic acid (TRIC2XL) have been bettered.

Preliminary MO studies involved the identification of the most suitable semi-empirical method for the calculation of organoaluminium complexes. Studies began with geometric comparisons of 3:1 complexes of Al with oxalate, glyoxalate and glycolate. Since these complexes have no more than about twenty atoms, *ab initio* MO calculations with the powerful 6-31G basis set were feasible. Using these

results as the benchmark, the PM3 Hamiltonian was identified as the most suitable, and was consequently used for optimisation of complexes involving a greater number of atoms within the complex. Although no correlation was generally observed between published log stability constants and output data from MO calculations, promise was shown when comparing similar types of molecules. In these studies, the dicarboxylic ligands, oxalate, malonate and succinate produced a correlation of 0.961 showing promise for affinity prediction. An obstacle to perfect correlation may be the fact that the chelate ring size changes to five, six and seven as the ligand changes from oxalate to malonate and finally succinate. The increase in chelate ring number results in an increase in the 'chelate effect', ultimately influencing the stability of the complex, a factor not considered in the parameterisation of the PM3 Hamiltonian. These parameters are based on a limited number of Al oxides and halides that differ considerably from the ligands used in these studies. This suggests that a broader ranger of organoaluminium complexes need to be included in the PM3 parameterisation of Al to give more meaningful results. The advances in computer technology may allow larger complexes of Al to be calculated with the use of *ab initio* methods, which would ultimately aid the parameterisation of semi-empirical methods. Finally, semi-empirical methods are parameterised for predicting enthalpies, but neglect an entropy term that must also be considered in Gibbs free energy calculations. This may prove to be the limiting factor in the predictive ability of semi-empirical calculations on chelators with Al.

The morin assay, involving a flavone type molecule which fluoresce upon complexation with Al, was developed and optimised so that it could be used as a quantitative measure of Al content for subsequent studies involving *E. coli* and U87-MG glioblastoma cells. The method proved to be very useful and produced results comparable to the more conventional but expensive method used for Al analysis, graphite furnace atomic absorption spectroscopy (GFAAS).

Studies involving *E. coli* and ciprofloxacin identified that complexation of the antibiotic with Al rendered the antibiotic ineffective. Most probably this activity is due to the Al binding tightly to the active sites of the ciprofloxacin molecule, thereby hindering the binding of ciprofloxacin to DNA gyrase. *E. coli* cells differ somewhat from mammalian cells in terms of possessing a cell wall, consequently, U87-MG

cells were then investigated. Applying the same principles as those used with the bacterial studies, the influence of chelators on the association, in terms of Al influx or adsorption to cells was studied. The study showed that of the chelators under investigation, the 1,2-diethylhydroxypyridinone ligand exhibits better efficacy than the model drug DFO. This study does have one major drawback, in that it is only measuring the association of a complex onto cells. Ideally, a protocol needs to be established for loading Al into cells and investigating the influence of a ligand on the efflux of Al. This is unlikely to be achieved with the analytical method used in these studies, namely the morin assay, as this is only capable of measurement down to nanogram quantities of Al. For this to become more practical, a more sensitive method needs to be adopted such as the use of the radioisotope ^{26}Al, which is about three orders of magnitude more sensitive than the morin assay.

REFERENCES

Achari, A. and Neidle S., (1976), Nalidixic acid, *Acta Crystallographica,* **B32**, 600.

Acho, J.A., Doerrer, L.H. and Lippard, S.J., (1995), Pentamethylcyclopentadienyl and Cyclopentadienyl Tantalum and Niobium Calixarene Compounds and their Acetonitrile Inclusion Complexes, *Inorg. Chem.*, **34**, 2542.

Ackley, D.C. and Yokel R.A., (1997), Aluminum citrate is transported from brain into blood via the monocarboxylic acid transporter located at the blood-brain barrier, *Toxicology,* **120**, 89.

Ahmed, M.J. and Hossan J., (1995), Spectrophotometric Determination Of Aluminum By Morin, *Talanta,* **42**, 1135.

Albert, A., (1984), *The determination of ionization constants. A laboratory manual*, 3rd ed., Chapman.

Albertsson, J., Oskarsson A. and Stahl K., (1979), A Liquid-Helium Cryostat for Collection of Three-Dimensional X-ray Intensity Data down to 20 K. The Crystal Structure of D(+)-Tartaric Acid at 35, 105, 160 and 295K, *Journal of Applied Crystallography,* **12**, 537.

Allen, F.H., (1984), The Current Status Of Crystallographic Databases, *Acta Crystallographica Section A,* **40**, C441.

Allen, F.H., (1998), The development, status and scientific impact of crystallographic databases, *Acta Crystallographica Section A,* **54**, 758.

Allen, F.H. and Kennard O., (1983), The Cambridge Database Of Molecular-Structures, *Perspectives In Computing,* **3**, 28.

Allen, F.H., Kennard O., Watson D.G. and Crennell K.M., (1982), Cambridge Crystallographic Data Center .6. Preparation and Computer Typesetting Of Molecular-Structures and Dimensions Bibliographic Volumes, *Journal Of Chemical Information and Computer Sciences,* **22**, 129.

Alvarezhernandez, X., Madigosky S.R., Stewart B. and Glass J., (1994), Iron Status Affects Aluminum Uptake and Transport By Caco-2 Cells, *Journal Of Nutrition,* **124**, 1574.

Alzheimer, A., (1907), Ueber eine eigenatige Erkrankung der Hirinde`, *Allgemeine Zeitschrift fur Psychiatrie und Psychisch-Gerichtlich Medicin,* **64**, 146.

Anane, R., Bonini M., Grafeille J.M. and Creppy E.E., (1995), Bioaccumulation Of Water-Soluble Aluminum-Chloride In the Hippocampus After Transdermal Uptake In Mice, *Archives Of Toxicology,* **69**, 568.

Andress, K.R. and Carpenter C., (1934), Die Struktur vom Chromchloride- und Aluminiumchloridhexahydrat, *Kristallhydrate. II.*, 446.

Armstrong, R.A., Winsper S.J. and Blair J.A., (1995), Hypothesis - Is Alzheimers-Disease a Metal-Induced Immune Disorder, *Neurodegeneration,* **4**, 107.

Armstrong, R.A., Winsper S.J. and. Blair J.A, (1996), Aluminium and Alzheimer's disease: Review of possible pathogenic mechanisms, *Dementia,* 7, 1.

Ashton, J.F. and Laura R.S., (1989), The Risks Of Dietary Aluminum, *Search,* **20**, 180.

Atkari, K., Kiss T., Bertani R. and Martin R.B., (1996a), Interaction of aluminium(III) with biologically important phosphates, *Magyar Kemiai Folyoirat,* **102**, 229.

Atkari, K., T. Kiss, Bertani R. and Martin R.B., (1996b), Interactions of aluminum(III) with phosphates, *Inorganic Chemistry,* **35**, 7089.

Atwood, J.L., Gardiner M.G., Jones C., Raston C.L., Skelton B.W. and White A.H., (1996), Trimethyl-aluminium and -gallium derivatives of calix[4]arenes: Cone (mono-metallic) or doubly flattened partial cone (tetrametallic) conformations, *Chemical Communications*, 2487.

Banin, E. and Meiri H., (1990), Toxic Effects Of Aluminosilicates On Nerve-Cells, *Neuroscience,* **39**, 171.

Banks, W.A. and Kastin A.J., (1983), Aluminium increases permeability of the blood brain barrier to labelled DSIP and B-endorphin: possible implications for senile and dialysis dementia, *Lancet,* **2**, 1227.

Banks, W.A., Kastin A.J. and Fasold M.B., (1988), Differential effect of aluminium on the blood-brain barrier, transport of peptides, techtenium and albumin, *J. Pharmacol. Exp. Ther.,* **244**, 579.

Barlow, D.J., Hider R.C., Singh S. and Webley K.S., (1988), Computer aided modelling of the structures and metal ion affinities of chelating agents, *Biochemical Society Transactions,* **16**, 835 836.

Barnes, J.C. and Paton J.D., (1988), Propane-1,2,3-tricarboxylic Acid (Tricarballylic Acid), *Acta Crystallographica,* **C44**, 758.

Barreiro, E.J., Rodrigues C.R., Albuquerque M.G., deSantAnna C.M.R. and deAlencastro R.B., (1997), Molecular modeling: A tool for rational drug design in medicinal chemistry, *Quimica Nova,* **20**, 300.

Bierer, L.M., Perl D.P., Haroutunian V., Mohs R.C. and Davis K.L., (1990), Neurofibrillary Tangles, Alzheimers-Disease, and Lewy Bodies, *Lancet,* **335**, 163.

Binkley, J., Pople J. and Hehre W., (1980), *Journal of the American Chemical Society,* **104**, 2797.

Birchall, J.D. and Chappell J.S., (1988a), Aluminum, Chemical Physiology, and Alzheimers-Disease, *Lancet,* **2**, 1008.

Birchall, J.D. and Chappell J.S., (1988b), The Chemistry Of Aluminum and Silicon In Relation to Alzheimers- Disease, *Clinical Chemistry,* **34**, 265.

Bollinger, J.E., Mague J.T., Banks W.A., Kastin A.J. and Roundhill D.M., (1995), Lipophilic Hexadentate Aluminum Complexes Of New Phenolate- Derivatized Cyclohexanetriamine Ligands and Their Effect On the Peptide-Transport System (Pts-1), *Inorganic Chemistry,* **34**, 2143.

Bondy, S.C., Tseng H. and Orvig C., (1998), Active oxygen species formation in synaptosomes exposed to an aluminum chelator, *Neurotoxicology and Teratology,* **20**, 317.

Bootsma, G.A. and Schoone J.C., (1966), Crystal Structures of *Meso* tartaric Acid, *Acta Crystallographica,* **22**, 522.

Bott, R.C., Sagatys D.S., Lynch D.E., Smith G. and Kennard C.H.L., (1993), Structure Of Sodium-Hydrogen (+)-Tartrate Monohydrate, *Acta Crystallographica Section C-Crystal Structure Communications,* **49**, 1150.

Bragg, L., (1968), X-ray crystallography, *Scientific American,* **219**, 58.

Brenner, S.R. and Yoon K.W., (1994), Aluminum Toxicity In Rat Hippocampal-Neurons, *Neuroscience Letters,* **178**, 260.

Breuer, M. and Hagele G., (1989), Determination of approximate force field parameters, *Computers Chem.,* **13**, 123 128.

Briggs, J.M., Marrone T.J. and McCammon J.A., (1996), Computational science new horizons and relevance to pharmaceutical design, *Trends In Cardiovascular Medicine,* **6**, 198.

British National Formulary, (1999), **38**, British Medical Association and Royal Pharmaceutical Society of Great Britain, London.

Brookhaven National Laboratory; Univ. of Birmingham 1986, DATREDXL. Univ. of Birmingham, England.

Brouwers, J., (1992), Drug-Interactions With Quinolone Antibacterials, *Drug Safety,* 7, 268.

Buchanan, D.R. and Harris, P.M. (1982??1968), *Acta Crystallographica*, **B24**, ????

Bulc, N., Golic, L. and Siftar, J., (1984), Structure of ammonium tris (oxalato) gallate (III) trihydrate, (I) $(NH_4)_3[Ga(C_2O_4)_3].3H_2O$, and ammonium tris (oxalato)aluminate (III) trihydrate, (II) $(NH_4)_3$ [Al $(C_2O_4)_3$]. $3H_2O$, *Acta Crystallographica*, **C40**, 1829.

Burns, A., Howard R. and Pettit W., (1997), Alzheimer's Disease. A medical companion Blackwell Science Ltd, Oxford p. 163.

Cable, H. and Lloyd J.B., (1999), Cellular uptake and release of two contrasting iron chelators, *Journal Of Pharmacy and Pharmacology,* **51**, 131.

Caira, M.R., Nassimbeni L.R., Scott J.L. and Wildervanck A.F., (1996), Resolution of optical isomers of 4-amino-p-chlorobutyric acid lactam by co-crystallization, *Journal Of Chemical Crystallography,* **26**, 117.

Canavese, C., Gurioli L., Damicone M., Cardelli R., Caligaris F., Bongiorno P., Arnaud A., Mattiello G. and Marchiori M., (1992), Kinetics Of Aluminoxamine and Feroxamine Chelates In Dialysis Patients, *Nephron,* **60**, 411.

Candy, J.M., McArthur F.K., Oakley A.E., Taylor G.A., Chen C., Mountfort S.A.,. Thompson J.E, Chalker P.R., Bishop H.E., Beyreuther K., Perry G., Ward M.K.,. Martyn C.N and Edwardson J.A., (1992), Aluminum Accumulation In Relation to Senile Plaque and Neurofibrillary Tangle Formation In the Brains of Patients With Renal-Failure, *Journal Of the Neurological Sciences,* **107**, 210.

Caravan, P., S.J. Rettig and C. Orvig, (1997), Effect of pyridyl donors in the chelation of aluminum(III), gallium(III), and indium(III), *Inorganic Chemistry,* **36**, 1306.

Carbo, R., (1980), *Int. J. Quan. Chem.*, **17**, 1185.

Clark, D.E., (1993), Computer-Aided Drug Design, *Chemistry & Industry*, 444.

Clauberg, M. and J.G. Joshi, (1993), Regulation Of Serine Protease Activity By Aluminum - Implications For Alzheimer-Disease, *Proceedings Of the National Academy Of Sciences Of the United States Of America,* **90**, 1009.

Clevette, D.J., W.O. Nelson, A. Nordin, C. Orvig and S. Sjoberg, (1989), Equilibrium and Structural Studies Of Silicon(Iv) and Aluminum(Iii) In Aqueous-Solution .18. Complexation Of Aluminum With N-Substituted 3-Hydroxy-4-Pyridinones, *Inorganic Chemistry,* **28**, 2079.

Chem-X molecular modelling software (1991), Chemical Design Ltd, Roundway House, Cromwell Park, Chipping Norton, Oxford.

Cohen, S.M., M. Meyer and K.N. Raymond, (1998), Enterobactin protonation and iron release: Hexadentate tris- salicylate ligands as models for triprotonated ferric enterobactin, *Journal Of the American Chemical Society,* **120**, 6277.

Corain, B., M. Nicolini and P. Zatta, (1992), Aspects Of the Bioinorganic Chemistry Of Aluminum(Iii) Relevant to the Metal Toxicity, *Coordination Chemistry Reviews,* **112**, 33.

Cotton, F.A. and Wilkinson G., (1980), Advanced Inorganic Chemistry. A Comprehensive Guide, John Wiley and Sons, New York.

Cramer, R.D., Pattterson D.E. and Bunce J.D., (1988), Effect of Shape Binding of Steroids to Carrier Proteins, *Journal of the American Chemical Society,* **170**, 5959.

Crapper, D.R., Krishnan S.S. and Dalton A.J., (1973), Brain Aluminium Distribution in Alzheimer's Disease and Experimental Neurofibrillary Degeneration, *Science,* **180**.

Crapper, D.R., Quittkat S. and Krishnan S.S., (1980), Intranuclear aluminium content in Alzheimer's disease: dialysis encephalopathy, *Acta. Neuropathol. (Berl),* **50**, 19.

Crapper McLachlan, D.R., Dalton A.J. and Kruck T.P.A., (1991), Intramuscular desferrioxamine in patients with Alzheimer's disease, *Lancet,* **337**, 1034.

Crapper McLachlan, D.R., Dam T.V. and Farnel B.J., (1983), Aluminium inhibition of ADP-ribosylation in vivo and in vitro, *Neurobehav. Toxicol. Teratol.,* **5**, 645.

CRC Handbook of Chemistry and Physics, (1988), 69th ed, Chemical Rubber Publishing Press, Florida.

Das, A.K., R. Chakraborty, M.L. Cervera and M. delaGuardia, (1996), Metal speciation in biological fluids - A review, *Mikrochimica Acta,* **122**, 209.

DeAlmeida, W.B., H.F. DosSantos and M.C. Zerner, (1998), A theoretical study of the interaction of anhydrotetracycline with Al(III), *Journal Of Pharmaceutical Sciences,* **87**, 1101.

DeBoni, U., A. Otvos, J.W. Scott and D.R. Crapper, (1976), *Acta neuropathalogy,* **35**, 285.

Deleers, M., (1985), Cationic Atmosphere and Cation Competition Binding At Negatively Charged Membranes - Pathological Implications Of Aluminum, *Research Communications In Chemical Pathology and Pharmacology,* **49**, 277.

Deleon, M.J., T. McRae, J.R. Tsai, A.E. George, D.L. Marcus, M. Freedman, A.P. Wolf and B. McEwen, (1988), Abnormal Cortisol Response In Alzheimers-Disease Linked to Hippocampal Atrophy, *Lancet,* **2**, 391.

Delhaize, E. and P.R. Ryan, (1995), Aluminum Toxicity and Tolerance In Plants, *Plant Physiology*, **107**, 315.

Deloncle, R. and O. Guillard, (1990), Mechanism Of Alzheimers-Disease - Arguments For a Neurotransmitter Aluminum-Complex Implication - Comment, *Neurochemical Research*, **15**, 1239.

Demiguel, A.V., Gomez M., Isobe K., Taylor B.F., Mann B.E. and Maitilis P.M., (1983), Reactions Of Dichlorobis(Mu- Chloro)Bis(Pentamethylcyclopentadienyl) Dirhodium and Diiridium With Hexamethyldialuminum, *Organometallics*, **2**, 1724.

Denizli, A., Salih B. and Piskin E., (1998), New chelate-forming polymer microspheres carrying dyes as chelators for iron overload, *Journal Of Biomaterials Science-Polymer Edition*, **9**, 175.

Depablos, F., Ariza J.L.G. and Pino F., (1986), N-Oxalylamine(Salicylaldehyde Hydrazone) As an Analytical Fluorometric Reagent For the Determination Of Nanogram Amounts Of Aluminum, *Analyst*, **111**, 1159.

Derrissen, J.L. and Smit P.H., (1974), Refinement of the Crystal Structures of Anhydrous a- and b-Oxalic acids, *Acta Crystallographica*, **B30**, 2240.

Deuis, R.L., Subramanian C. and Yellup J.M., (1996), Abrasive wear of aluminium composites - A review, *Wear*, **201**, 132.

Devoto, E. and Yokel R.A., (1994), The Biological Speciation and Toxicokinetics Of Aluminum, *Environmental Health Perspectives*, **102**, 940.

Dewar, M.J. and Holder A., (1990), AM1 Parameters dor Aluminium, *Organometallics*, **9**, 508.

Dewar, M.J.S. and McKee M.L., (1977), Ground States of Molecules. 41. MNDO Results for Molecules containing Boron, *Journal of the American Chemical Society*, 99, 5231.

Dick van der Helm, J.R., Baker R.A., Loghry R.A. and Ekstrand J.D., (1981), Structures of Alumichrome A and Ferrichrome A at Low Temperature, *Acta Crystallographica,* **B37**, 323.

Dobson, C.B., Day J.P., King S.J. and Itzhaki R.F., (1998), Location of aluminium and gallium in human neuroblastoma cells treated with metal-chelating agent complexes, *Toxicology and Applied Pharmacology,* **152**, 145.

Doedens, R.J., (1970), Structural studies on organonitrogen compounds of the transition elements. IV. The crystal and molecular structure of benzo [*c*] cinnolinebis (tricarbonyliron), $C_{12}H_5N_2Fe_2(CO)_6$, *Inorganic Chemistry*, **9**, 429.

Doll, R., (1993), Alzheimers-Disease and Environmental Aluminum, *Age and Ageing,* **22**, 138.

Drew, M.G.B. and Yates P.C., (1987), Molecular Mechanics Studies Of a Series Of Dicopper Complexes Of a 20-Membered Macrocycle Containing Differing Types Of Bridges Between the Metal Centers, *Journal Of the Chemical Society-Dalton Transactions*, 2563.

Ehmann, W.D., Markesbery W.R., Alauddin M., Hossain T.I.M. and Brubaker E.H., (1986), Brain Trace-Elements In Alzheimers-Disease, *Neurotoxicology,* 7, 197.

Engelter, C., G.E. Jackson, C.L. Knight and D.A. Thornton, (1989), Complexes Of 8-Aminoquinoline .1. the Infrared-Spectra Of the Ligand, the Tris Complexes Of Iron, Cobalt and Nickel Perchlorates and Their Nd2 Analogs, *Journal Of Coordination Chemistry,***20**, 289.

Enraf-Nonius 1989, CAD-4 Software. Version 5.0. Enraf-Nonius, Delft, The Netherlands.

Erman, L.Y., Mindrul V.F., Mikhaleva I.L., Pankov D.I. and Kurochkin V.K., (1994), Crystal and Molecular-Structure Of 3-Quinuclidinol Bis-Tartrate, *Journal Of Structural Chemistry,* **35**, 418.

Evers, A., Hancock R.D., Martell A.E. and Motekaitis R.J., (1989), Metal-Ion Recognition In Ligands With Negatively Charged Oxygen Donor Groups - Complexation Of Fe(III), Ga(III), In(III), Al(III), and Other Highly Charged Metal-Ions, *Inorganic Chemistry,* **28**, 2189.

Exley, C. and Birchall J.D., (1992), The Cellular Toxicity Of Aluminum, *Journal Of Theoretical Biology,* **159**, 83.

Exley, C., Schley L., Murray S., Hackney C.M. and Birchall J.D., (1995), Aluminum, Beta-Amyloid and Nonenzymatic Glycosylation, *Febs Letters,* **364**, 182.

Farnell, B.J., McLachlan D.R.C., Baimbridge K., DeBoni U., Wong L. and Wood P.L., (1985), Calcium-Metabolism In Aluminum Encephalopathy, *Experimental Neurology,* **88**, 68.

Fasman, G.D., (1996), Aluminum and Alzheimer's disease: Model studies, *Coordination Chemistry Reviews,* **149**, 125.

Favarato, M. and Zatta P.F., (1993), Differential Aluminum Lactate Toxicity In Rabbits Using Either Aqueous-Solutions or Liposomal Suspensions, *Toxicology Letters,* **66**, 133.

Feng, T.L., Gurian P.L., Healy M.D. and Barron A.R., (1990), Aluminium Citrate: Isolation and Structural Characterization of a Stable Trinuclear Complex, *Inorg. Chem.,* **29**, 408.

Findlow, J.A., Duffield J.R., Evans D.A. and Williams D.R., (1987), Speciation Of Aluminum In Human and Bovine-Milk, *Recueil Des Travaux Chimiques Des Pays-Bas-Journal Of the Royal Netherlands Chemical Society,* **106**, 403.

Flaten, T.P., (1990), Geographical Associations Between Aluminum In Drinking-Water and Death Rates With Dementia (Including Alzheimers-Disease), Parkinsons- Disease and Amyotrophic Lateral Sclerosis In Norway, *Environmental Geochemistry and Health,* **12**, 152.

Florence, A.L., A. Gauthier, C. Ponsar, P.V. Deaguilar and R.R. Crichton, (1994), An Experimental Animal-Model Of Aluminum Overload, *Neurodegeneration,***3**, 315.

Forbes, W.F., Smith L.F., Nieboer E. and Gibson B.L., (1995), Public-Health Role, Aluminum and Alzheimers-Disease - Discussion, *Environmetrics,* **6**, 286.

Foy, C.D., Chaney R.L. and White M.C., (1978), The physiology of metal toxicity in plants, *Annu. Rev. Plant Physiol.,* **29**, 511.

Fraga, C.G., Oteiza P.I., Golub M.S., Gershwin M.E. and Keen C.L., (1990), Effects Of Aluminum On Brain Lipid-Peroxidation, *Toxicology Letters,* **51**, 213.

Freedman, M.H., Boyden M., Taylor M. and Skarf B., (1988), Neurotoxicity Associated With Deferoxamine Therapy, *Toxicology,* **49**, 283.

Gallego, M., Valcarcel M. and Garciavargas M., (1983), Spectrofluorimetric and Spectrophotometric Determination Of Aluminum With the Salicyloylhydrazones Of Pyridine-2-Aldehyde and Pyridoxal, *Analyst,* **108**, 92.

Ganrot, P.O., (1986), Metabolism and Possible Health-Effects Of Aluminum, *Environmental Health Perspectives,* **65**, 363.

Gans, P., Sabatini A. and Vacca A., (1985a), Superquad - an Improved General Program For Computation Of Formation- Constants From Potentiometric Data, *Journal Of the Chemical Society-Dalton Transactions*, 1195.

Gans, P., Sabatini A. and Vacca A., (1985b), SUPERQUAD - an Improved General Program For Computation Of Formation- Constants From Potentiometric Data, *Journal Of the Chemical Society-Dalton Transactions*, 1195.

Gearing, M., Mirra S.S., Hedreen J.C., Sumi S.M., Hansen L.A. and Heyman A., (1995), The Consortium to Establish a Registry For Alzheimers-Disease (Cerad) .10. Neuropathology Confirmation Of the Clinical-Diagnosis Of Alzheimers-Disease, *Neurology*, **45**, 461.

Geldmacher, D.S. and Whitehouse P.J., (1997), Differential diagnosis of Alzheimer's disease, *Neurology*, **48**, S2.

Gilman, S., (1997), Alzheimer's disease, *Perspectives In Biology and Medicine*, **40**, 230.

Glusker, J.P., Minkin J.A. and Patterson A.L., (1969), X-ray Crystal Analysis of the Substrates of Aconites. IX. A Refinement of the Structure of Anhydrous Citric Acid, *Acta Crystallographica*, **B25**, 1066.

Glusker, J.P. and Trueblood K.N., (1972), Crystal Structure Analysis: A Primer Oxford University Press, New York.

Gomez, M., Esparza J.L., Domingo J.L., Singh P.K. and Jones M.M., (1998), Comparative aluminium mobilizing actions of deferoxamine and four 3- hydroxypyrid-4-ones in aluminium-loaded rats, *Toxicology*, **130**, 175.

Gomez, M., Yarrow P.I.W., Demiguel A.V. and Maitlis P.M., (1983), Reactions Of Dimethyl(Dimethylsulphoxide)Pentamethylcyclopentadienyl- Rhodium and "Pentamethylcyclopentadienyl-Iridium With Acids, *Journal Of Organometallic Chemistry*, **259**, 237.

Good, P.F. and Perl D.P., (1993), Aluminum In Alzheimers, *Nature*, **362**, 418.

Good, P.F. and Perl D.P., (1994), A Quantitative Comparison Of Aluminum Concentration In Neurofibrillary Tangles Of Alzheimers-Disease and Parkinsonian Dementia Complex Of Guam By Laser Microprobe Mass Analysis, *Neurobiology of Aging*, **15**, S28.

Good, P.F., Perl D.P., Bierer L.M. and Schmeidler J., (1992), Selective Accumulation Of Aluminum and Iron In the Neurofibrillary Tangles Of Alzheimers-Disease - a Laser Microprobe (Lamma) Study, *Annals Of Neurology,* **31**, 286.

Gordon, M., Binkley J., Pople J., Pietro W.and Hehre W., (1982a), *Journal of the American Chemical Society,* **104**, 2797.

Gordon, M., Binkley J., Pople J., Pietro W.and Hehre W., (1982b), Self-Consistent Molecular-Orbital Methods. 22. Small Split-Valence Basis Sets for Second-Row Elements, *Journal of the American Chemical Society,* **104**, 2797.

Graff, L., Muller G. and Bumel D., (1995a), In-Vitro and In-Vivo Comparative-Studies On Chelation Of Aluminum By Some Polyaminocarboxylic Acids, *Research Communications In Molecular Pathology and Pharmacology,* **88**, 271.

Graff, L., Muller G. and Burnel D., (1995b), In-Vitro and In-Vivo Evaluation Of Potential Aluminum Chelators, *Veterinary and Human Toxicology,* **37**, 455.

Greger, J.L., (1993), Aluminum Metabolism, *Annual Review Of Nutrition,* **13**, 43.

Greger, J.L. and Sutherland J.E., (1997), Aluminum exposure and metabolism, *Critical Reviews In Clinical Laboratory Sciences,* **34**, 439.

GromyszKalkowska, K. and Szubartowska E., (1999), Aluminium - its ecological role and toxicity for animals, *Medycyna Weterynaryjna,* **55**, 229.

Guest, M.F., and Kendrick, J., (1986), GAMESS User Manual, Pt. 1, An introductory guide to GAMESS, *Computational Science Group*, SERC, Daresbury Lab., Warrington.

Guida, L., Saidi Z., Hughes M.N. and Poole R.K., (1991), Aluminum Toxicity and Binding to Escherichia-Coli, *Archives Of Microbiology,* **156**, 507.

Gurian, P.L., Cheatham L.K., Ziller J.W. and Barron A.R., (1991), Aluminum Complexes Of N,N'-Ethylenebis(Salicylideneimine)Mu(H2salen) - X-Ray Crystal-Structures Of [[Al(Salen)]2(Mu-O)].Mecn and [Al(Oc6h2me3-2,4,6)(Salen)], *Journal Of the Chemical Society-Dalton Transactions*, 1449.

Gutteridge, J.M.C., Quinlan G.J. and Clark I., (1985), Aluminium salts accelerate peroxidation of membrane lipids stimulated by iron salts, *Biochim. Biophys. Acta.*, **835**, 441.

Guy, S.P., Jones D., Mann D.M.A. and Itzhaki R.F., (1991), Human Neuroblastoma-Cells Treated With Aluminum Express an Epitope Associated With Alzheimers-Disease Neurofibrillary Tangles, *Neuroscience Letters*, **121**, 166.

Guy, S.P., Seabright P., Day J.P. and Itzhaki R.F., (1990), Uptake Of Aluminum By Human Neuroblastoma-Cells, *Journal Of Trace Elements and Electrolytes In Health and Disease*, **4**, 183.

Harris, W.R., (1992), Equilibrium-Model For Speciation Of Aluminum In Serum, *Clinical Chemistry*, **38**, 1809.

Harrowfield, J.M., Ogden M.I., Richmond W.R., Skelton B.W. and White A.H., (1993), Cation Calixarene Interactions - Tetraalkylammonium Cation-Binding By Calixarene Anions, *Journal Of the Chemical Society-Perkin Transactions 2*, 2183.

Harvey, R.J., (1998), Young Onset Dementia: Epidemiology, clinical symptoms, family burden, support and outcome. NHS Executive (North Thames), London.

Haug, A., Shi B. and Vitorello V., (1994), Aluminum Interaction With Phosphoinositide-Associated Signal- Transduction, *Archives Of Toxicology*, **68**, 1.

Hedlund, T. and Ohman L.O., (1988), Equilibrium and Structural Studies Of Silicon(Iv) and Aluminum(Iii) In Aqueous-Solution .19. Composition and Stability Of Aluminum Complexes With Kojic Acid and Maltol, *Acta Chemica Scandinavica Series a-Physical and Inorganic Chemistry*, **42**, 702.

Hehre, W.J., (1995), Practical Strategies for Electronic Structure Calculations Wavefunction, Irvine, California, USA, 241.

Helena, M., Teixeira S.F., Vilas-Boas L.F., Gil V.M.S. and Teixeira F., (1995), Complexes o ciprofloxacin with metal ions contained in antacid drugs, *Journal of Chemotherapy,* **7**, 126.

Hewitt, C.D., Poole C.L., Westervelt F.B., Savory J. and Wills M.R., (1988), Risks of Simultaneous Therapy with Oral Aluminum and Citrate Compounds, *Lancet,* **2**, 849.

Hider, R.C., Singh S.and Porter J.B., (1992), Iron Chelating-Agents With Clinical Potential, *Proceedings Of the Royal Society Of Edinburgh Section B-Biological Sciences,* **99**, 137.

Hider, R.C., Taylor P.D., Walkinshaw M., Wang J.L. and Vanderhelm D., (1990), Crystal-Structures Of 3-Hydroxy-1,2-Dimethylpyridin-4-One - an Iron(III) Chelation Study, *Journal Of Chemical Research-S*, 316.

Hider, R.C., and Hall, A.D., (1991), Clinically useful chelators of tripositive elements, *Prog. Med. Chem.* **28**, 41.

Hodgkin, E.E. and Richards W.G., (1988), Molecular Similarity *Chem. in Brit.,* **24**, 1141.

Hodgkin, E.E. and Richards W.G., (1987), Molecular Similarity Based On Electrostatic Potential and Electric- Field, *International Journal Of Quantum Chemistry*, 105.

Hope, H. and De La Camp U., (1972), Anomalous Scattering by Oxygen: Measurement s on (+)-Tartaric Acid, *Acta Crystallographica,* **A28**, 201.

Hossain, M.B., Jalal M.A.F. and Vanderhelm D., (1986), The Structure Of Ferrioxamine D1 Ethanol Water (1/2/1), *Acta Crystallographica Section C-Crystal Structure Communications,* **42**, 1305.

Hu, X.C. and. Boyer G.L, (1996), Siderophore-mediated aluminum uptake by Bacillus megaterium ATCC 19213, *Applied and Environmental Microbiology,* **62**, 4044.

Huang, Y., Savory J., Herman M.M., Nicholson J.R., Reyes M.R., Boyd J.C. and Wills M.R., (1995), Quantitative-Evaluation Of Al Maltolate-Induced Neurodegeneration With Subsequent Al Removal By Desferrioxamine Treatment, *Neurotoxicology,* **16**, 291.

Huber, C.P., Gowda D.S. and Achaya K.R., (1980), Refinement of the structure of nalidixic acid, *Acta Crystallographica,* **B36**, 497.

Hue, N.V., Craddock G.R. and Adams F., (1986), Effect Of Organic-Acids On Aluminum Toxicity In Subsoils, *Soil Science Society Of America Journal,* **50**, 28.

Hussain, S.A., Sharma A.H. and Perkins M.J., (1979), Oxidation of N-Alkylhydroxamic Acids: Interception of N-Acyl Nitrones, *Journal of the Chemical Society. Chemical Communications*, 289.

Iball, J. and Morgan C.H., (1967), A Refinement of the crystal of Ferric Acetylacetonate, *Acta Crystallographica,* **23**, 29.

Idem:, (1986), Neurotoxic cations induce membrane rigidification and membrane fusion at micromolar concentrations, *Biophys. Acta,* **855**, 271.

International tables for Crystallography, (1996), Volume 4. Space Group Symmetry, edited by Theo Hahn Pub. for IUCr by Kluwe Academic Publishers, London.

Ittel, T.H., (1993), Determinants Of Gastrointestinal Absorption and Distribution Of Aluminum In Health and Uremia, *Nephrology Dialysis Transplantation,* **8**, 17.

Ivanov, M.A. and Kosoy A.L., (1975a), The Structure of the Iron(III) Complex with Sodium Tartrate (FeTNa), *Acta Crystallographica,* **B31**, 2843.

Jackson, G.E., (1982), Studies On the Chelation Of Aluminum For Biological Application .1. Citric-Acid, *South African Journal Of Chemistry,* **35**, 89.

Jackson, G.E. and Cosgrove A., (1982), Studies On the Chelation Of Aluminum For Biological Application .2. Oxalic, Malonic, and Succinic Acids, *South African Journal Of Chemistry,* **35**, 93.

Jackson, G.E. and Voyi K.V., (1987), Studies On the Chelation Of Aluminum For Biological Application .4. AMP, ADP and ATP, *Polyhedron,* **6**, 2095.

Jiang, C., Tag B., Wang C.and Zhang X., (1996), Spectrofluorimetric determination of trace amounts of aluminium with salicylhydrazone, *Analyst,* **121**, 317.

Jiang, C.Q., Tang B., Wang R.Y. and Yen J.C., (1997), Spectrofluorimetric determination of trace amounts of aluminium with 5-bromo-salicylaldehyde salicyloylhydrazone, *Talanta,* **44**, 197.

Johnson, G.V.M. and Jope R.S., (1987), Cytoskeletal protein phosphorylation is altered in the brains of aluminium treated rats, in: Annual Meeting of the Society for Neurosciences, **13**, New Orleans, A366.10.

Joshi, J.G., Dhar M., Clauberg M. and Chauthaiwale V., (1994), Iron and Aluminum Homeostasis In Neural Disorders, *Environmental Health Perspectives,* **102**, 207.

Kabak, M., Elmali A., Ozbey S., Atakol O. and Kenar A., (1996), Redetermination of the crystal structure of tris(acetylacetonato)iron(III) (ferric acetylacetonate), *Zeitschrift Fur Kristallographie,* **211**, 831.

Karlik, S.J., G.L. Eichorn and D.R. Crapper, (1980), Interactions of aluminium with deoxyribnucleic acid, *Biochemistry,* **19**, 5991.

Kennard, O., Allen F.H., Bellard S., Davies J.E., Galloy J., McMeeking R.F., Taylor R. and Watson D.G., (1984), Current Developments In the Cambridge Structural Database, *Acta Crystallographica Section A,* **40**, C445.

Kiss, T., Atkari K., Jezowskabojczuk M. and Decock P., (1993), Complexes Of Al(Iii) With Hydroxyaromatic Ligands, *Journal Of Coordination Chemistry*, **29**, 81.

Kiss, T., S. I. and Martin , (1991a), Al Binding by Adenosine 5'-Phosphates: AMP, ADP, and ATP, *Inorg. Chem.*, **30**, 2130.

Kiss, T., Sovago I. and Martin R.B., (1989), Complexes Of 3,4-Dihydroxyphenyl Derivatives .9. Al-3+ Binding to Catecholamines and Tiron, *Journal Of the American Chemical Society*, **111**, 3611.

Kiss, T., Sovago I. and Martin R.B., (1991b), Al^{3+} Binding By Adenosine 5'-Phosphates - AMP, ADP, and ATP, *Inorganic Chemistry*, **30**, 2130.

Kiss, T., Sovago I., Martin R.B. and Pursiainen J., (1994), Ternary Complex-Formation Between Al(Iii)-Adenosine-5'-Phosphates and Carboxylic-Acid Derivatives, *Journal Of Inorganic Biochemistry* ,**55**, 53.

Kiss, T., Zatta P. and Corain B., (1996), Interaction of aluminium(III) with phosphate-binding sites: Biological aspects and implications, *Coordination Chemistry Reviews*, **149**, 329.

Klemm, A., Sperschneider H., Winnefeld K., Gunther K. and Stein G., (1997), Removal of aluminoxamine and protein bound aluminum during hemodialysis and hemofiltration in end-stage renal failure patients after desferrioxamine infusion, *Trace Elements and Electrolytes*, **14**, 38.

Kontoghiorghes, G.J., (1995), New Concepts Of Iron and Aluminum Chelation-Therapy With Oral L1 (Deferiprone) and Other Chelators - a Review, *Analyst*, **120**, 845.

Krishnan, S.S., D.R. McLachlan, B. Krishnan, S.S.A. Fenton and J.E. Harrison, (1988), Aluminum Toxicity to the Brain, *Science Of the Total Environment*, **71**, 59.

Kruck, T.P.A. and McLachlan D.R., (1988), Mechanisms Of Aluminum Neurotoxicity - Relevance to Human-Disease, *Metal Ions In Biological Systems,* **24**, 285.

Landsberg, J.P., McDonald B. and Watt F., (1992), Absence Of Aluminum In Neuritic Plaque Cores In Alzheimers-Disease, *Nature,* **360**, 65.

Levesque, L., Fraser P.E. and McLachlan D.R., (1997), Differential uptake of aluminum by astrocytes and neuronal cells, *Journal Of Neurochemistry,* **69**, S43.

Lide, D.R., (1962), A survey of carbon-carbon bond, *Tetrahedron,* **17**, 125.

Little, R.G. and Doedens, R.J. (1972), Structural studies of orgnonitrogen compounds of the transition elements V. The structure of μ-2,3-[2,3-diazobicyclo [2.2.1] heptane] diyl-bis (tricarbonyliron) $C_5H_8N_2Fe_2(CO)_6$, an iron carbonyl complex of a bicyclic aliphatic azo compound. *Inorganic Chemistry*, 11, 1392.

Liu, J.M., (1999), Spectrophotometric determination of trace aluminium and polyacrylamide by morin, *Chinese Journal Of Analytical Chemistry,* **27**, 972.

Liu, S., Wong E., Karunaratne V., Rettig S.J. and Orvig C., (1993), Highly Flexible Chelating Ligands For Group 13 Metals - Design and Synthesis Of Hexadentate Tripodal Amine Phenol Ligand Complexes Of Aluminum, Gallium, and Indium, *Inorg. Chem.* **32**, 1756.

Lukiw, W.J., Krishnan B., Wong L., Kruck T.P.A., Bergeron C.and McLachlan D.R.C., (1992), Nuclear Compartmentalization Of Aluminum In Alzheimers-Disease (Ad), *Neurobiology Of Aging,* **13**, 115.

Lukiw, W.J., Kruck T.P.A. and McLachlan D.R.C., (1989), Aluminum and the Nucleus Of Nerve-Cells, *Lancet,* **1**, 781.

Ma, R., Reibenspies J.J. and Martell A.E., (1994), Stabilities Of 1,2-Diethyl-3-Hydroxy-4-Pyridinone Chelates Of Divalent and Trivalent Metal-Ions, *Inorganica Chimica Acta,* **223**, 21.

Main, P., Hull H.S. Lessinger L. Germain G. Declercq J.P. and Woolfson., 1978, MULTAN78. A system of computer programs for the automatic solution of crystal structures from X-ray diffraction data.

Mantyh, P.W., Ghilardi J.R., Rogers S., Demaster E., Allen C.J., Stimson E.R. and Maggio J.E., (1993), Aluminum, Iron, and Zinc Ions Promote Aggregation Of Physiological Concentrations Of Beta-Amyloid Peptide, *Journal Of Neurochemistry,* **61**, 1171.

Marklund, E. and Ohman L.O., (1990), Equilibrium and Structural Studies Of Silicon(Iv) and Aluminum(Iii) In Aqueous-Solution .22. a Potentiometric Study Of Mononuclear and Polynuclear Aluminum(Iii) Tartrates, *Journal Of the Chemical Society-Dalton Transactions*, 755.

Marklund, E., Ohman L.O. and Sjoberg S., (1989), Equilibrium and Structural Studies Of Silicon(IV) and Aluminum(III) In Aqueous-Solution .20. Composition and Stability Of Aluminum Complexes With Propionic-Acid and Acetic-Acid, *Acta Chemica Scandinavica,* **43**, 641.

Marquis, J.K., (1982), Aluminum Neurotoxicity - an Experimental Perspective, *Bulletin Of Environmental Contamination and Toxicology,* **29**, 43.

Martell, A.E., Hancock R.D., Smith R.M. and Motekaitis R.J., (1996), Coordination of Al(III) in the environment and in biological systems, *Coordination Chemistry Reviews,* **149**, 311.

Martell, A.E., Motekaitis R.J. and Smith R.M., (1990), Aluminum Complexes Of Hydroxyaliphatic and Hydroxyaromatic Ligands In Aqueous Systems - Some Problems and Solutions, *Polyhedron,* **9**, 171.

Martell, A.E. and Smith R.M., (1974-1977), *Critical Stability Constants*, Vol. 1-5 Plenum Press, New York.

Martin, R.B., (1986), Citrate Binding Of Al-3+ and Fe-3+, *Journal Of Inorganic Biochemistry*, **28**, 181.

Martin, R.B., (1990), Aluminosilicate Stabilities Under Blood-Plasma Conditions, *Polyhedron*, **9**, 193.

Martin, R.B., J. Savory, S. Brown, R.L. Bertholf and M.R. Wills, (1987), Transferrin Binding Of Al-3+ and Fe-3+, *Clinical Chemistry*, **33**, 405.

Martyn, C.N., Osmond C., Edwardson J.A., Barker D.J.P., Harris E.C. and Lacey R.F., (1989), Geographical Relation Between Alzheimers-Disease and Aluminum In Drinking-Water, *Lancet*, **1**, 59.

McLachlan, D.R.C., Lukiw W.J. and Kruck T.P.A., (1989), New Evidence For an Active-Role Of Aluminum In Alzheimers-Disease, *Canadian Journal Of Neurological Sciences*, **16**, 490.

Melograna, J.M. and Yokel R.A., (1983), Effect Of the Chelator Desferrioxamine On Aluminum Elimination In Rabbits, *Research Communications In Chemical Pathology and Pharmacology*, **40**, 497.

Miller, C.A. and Levine E.M., (1974), Affects of aluminium salts on cultured neuroblastoma cells, *J. Neurochem.*, **22**, 751.

Moan, J., Berg K., Anholt H. and Madslien K., (1994), Sulfonated Aluminum Phthalocyanines As Sensitizers For Photochemotherapy - Effects Of Small Light Doses On Localization, Dye Fluorescence and Photosensitivity In V79 Cells, *International Journal Of Cancer*, **58**, 865.

Mocker, M., Robl C. and Schnockel H., (1994a), Donor-Stabilized Aluminum(I) Bromide, *Angewandte Chemie-International Edition In English*, **33**, 1754.

Mocker, M., Robl C. and Schnockel H., (1994b), Donor-Stabilized Aluminum(II) Bromide, *Angewandte Chemie-International Edition In English,* **33**, 862.

Morrison, A. and Cozzarelli N.P., (1979), Site specific cleavage of DNA by *E. coli* DNA gyrase, *Cell,* **17**, 175.

Motekaitis, R.J. and Martell A.E., (1982), Best - a New Program For Rigorous Calculation Of Equilibrium Parameters Of Complex Multicomponent Systems, *Canadian Journal Of Chemistry-Revue Canadienne De Chimie,* **60**, 2403.

Motekaitis, R.J. and Martell A.E., (1984), Complexes Of Aluminum(III) With Hydroxy Carboxylic-Acids, *Inorg. Chem.,* **23**, 18.

Motekaitis, R.J. and Martell A.E., (1991), Stabilities Of the Iron(III) Chelates Of 1,2-Dimethyl-3-Hydroxy-4- Pyridinone and Related Ligands, *Inorganica Chimica Acta,* **183**, 71.

Muller, M., M. Anke and H. IllingGunther, (1997), Availability of aluminium from tea and coffee, *Zeitschrift Fur Lebensmittel-Untersuchung Und-Forschung a-Food Research and Technology,***205**, 170.

Muller, M., Anke M. and IllingGunther H., (1998), Aluminium in foodstuffs, *Food Chemistry,* **61**, 419.

Munoz-Garcia, D., Pendlebury W.W. and Kessler J.B., (1986), An immunocytochemical comparison of cytoskeletal proteins in aluminium-induced and Alzheimer-type neurofibriallry tangles, *Acta. Neuropathol. (Berl.),* **70**, 243.

Neill, D., Leake A., Hughes D., Keith A.B., Taylor G.A., Allsop D., Rima B.K., Morris C., Candy J.M. and Edwardson J.A., (1996), Effect of aluminium on expression and processing of amyloid precursor protein, *Journal Of Neuroscience Research,* **46**, 395.

Nelson, W.O., Karpishin T.B., Rettig S.J. and Orvig C., (1988), Aluminium and Gallium Compounds of 3-Hydroxy-4-pyridinones: Synthesis, Characterization, and Crystallography of Biologically Active Complexes with Unusual Hydrogen Bonding, *Inorganic Chemistry,* **27**, 1045.

Nelson, W.O., Rettig S.J. and Orvig C., (1989), Aluminium and Gallium Complexes of 1-Ethyl-3-hydroxy-2-methyl-4-pyrdinone: A New Exoclathrate Matrix, *Inorganic Chemistry,* **28**, 3153.

Ohm, T.G., Scharnagl H.and Marz W., (1997), Apolipoprotein E and neurofibrillary tangles in Alzheimer's disease, *Bibliotheca Psychiatrica*, 119.

Ohman, L.O., (1988), Equilibrium and Structural Studies Of Silicon(IV) and Aluminum(III) In Aqueous-Solution .17. Stable and Metastable Complexes In the System H+-Al-3+-Citric Acid, *Inorg. Chem.,* **27**, 2565.

Ohman, L.O. and Martin R.B., (1994), Citrate As the Main Small-Molecule Binding Al^{3+} In Serum, *Clinical Chemistry,* **40**, 598.

Ohman, L.O. and Sjoberg S., (1996), The experimental determination of thermodynamic properties for aqueous aluminium complexes, *Coordination Chemistry Reviews,* **149**, 33.

Okaya, Y., Stemple N.R. and Kay M.I., (1966), *Acta Cryst.,* **21**, 237.

Orvig, C., (1985), A Simple Method to Perform a Liquid Diffusion Crystallization, *Journal Of Chemical Education,* **62**, 84.

Pailler, F.M., D. Bequet, H. Corbe and C.P. Giudicelli, (1995), Aluminum In Alzheimers-Disease, *Presse Medicale,***24**, 489.

Parry, G.S., (1951), The Crystal Structure of Hydrate Racemic Acid, *Acta Crystallographica,* **4**, 131.

Pasteur, L., (1848), Recherches sur les relations qui peuvent exister entre la forme crystalline, *Annales de Chimie et de Physique,* **24**, 28.

Perl, D.P., (1985), Relationship Of Aluminum to Alzheimers-Disease, *Environmental Health Perspectives,* **63**, 149.

Perl, D.P., (1986), The Aluminum Hypothesis Of Alzheimers-Disease - a Personal View Based On Microprobe Analysis, *Neurobiology Of Aging,* 7, 550.

Perl, D.P. and Good P.F., (1987), The Association Of Aluminum, Alzheimers-Disease, and Neurofibrillary Tangles, *Journal Of Neural Transmission*, 205.

Perl, D.P. and. Good P.F, (1988), Aluminum, Environment and Central Nervous-System Disease, *Environmental Technology Letters* ,**9**, 901.

Perl, D.P. and Pendlebury W.W., (1986), Aluminum Neurotoxicity - Potential Role In the Pathogenesis Of Neurofibrillary Tangle Formation, *Canadian Journal Of Neurological Sciences,* **13**, 441.

Pina, R.G. and Cervantes C., (1996), Microbial interactions with aluminium, *Biometals,* **9**, 311.

Pople, J.A., (1976), In modern theoretical chemistry, Vol. 4 (Plenum, New York).

Porter, J.B., Jaswon M.S., Huehns E.R., East C.A. and. Hazell J.W.P, (1989), Desferrioxamine Ototoxicity - Evaluation Of Risk-Factors In Thalassemic Patients and Guidelines For Safe Dosage, *British Journal Of Haematology,* **73**, 403.

Powell, A.K. and Heath S.L., (1996), X-ray structural analysis of biologically relevant aluminium(III) complexes, *Coordination Chemistry Reviews,* **149**, 59.

Raggi, M.A., Sabbioni C., Mandrioli R., Zini Q. and Forti G.C., (1999), Fluorimetric determination of aluminum traces in hemodialysis solutions using Mordant Red 19, *Journal Of Analytical Toxicology,* **23**, 94.

Rahman, A., Ahmed S.N., Khair M.A., Zanrando E. and Randaccio L., (1990), The crystal structure of tris(acetylacetonate)aluminium (III), *Journal of Bangladesh Sciences,* **14**, 161.

Rajan, K.S., Mainer S., Rajan N.L. and Davis J.M., (1978), Studies on the chelation of L-Dopa with metal ions and ATP systems, *Bioinorganic chemistry,* **9**, 187.

Rajwanshi, P., Singh V., Gupta M.K. and Dass S., (1997), Leaching of aluminium from cookwares - A review, *Environmental Geochemistry and Health,* **19**, 1.

Rocca, W.A., Hofman A., Brayne C., Breteler M.M.B., Clarke M., Copeland J.R.M., Dartigues J.F., Engedal K., Hagnell O., Heeren T.J., Jonker C., Lindesay J., Lobo A., Mann A.H., Molsa P.K., Morgan K., Oconnor D.W., Droux A.D., Sulkava R., D.W.K. Kay and Amaducci L., (1991), Frequency and Distribution Of Alzheimers-Disease In Europe - a Collaborative Study Of 1980-1990 Prevalence Findings, *Annals Of Neurology,* **30**, 381.

Rogers, H.G., (1978), England, patent number 18003/78.

Rorison, I.H., (1965), The effect of aluminium on the uptake and incorporation of phophate by excised sanfoin roots, *New Physiol.,* **64**, 23.

Sampson, M., Clarkson D. and Davies D.D., (1965), DNA synthesis in aluminium treated roots of barley, *Science,* **148**, 1476.

Sarkander, H.I., Balb G. and Schlosser H., (1983), Blockade of neuronal brain RNA initiation sites by aluminium: a primary molecular mechanism of aluminium induced neurofibriallary changes, Raven, New York, 645.

Sato, M., Yoshimura H., Shimmura T., Obi H., Hatakeyama S., Kaneko E., Hoshino H. and Yotsuyanagi T., (1997), Fluorometric determination of serum and urinary aluminium with 8- quinolinol by kinetic-differentiation-mode micellar chromatography, *Journal Of Chromatography,* **789**, 361.

Savory, J., Exley C., Forbes W.F., Huang Y., Joshi J.G., Kruck T., McLachlan D.R.C. and Wakayama I., (1996), Can the controversy of the role of aluminum in Alzheimer's disease be resolved? What are the suggested approaches to this controversy and methodological issues to be considered?, *Journal Of Toxicology and Environmental Health,* **48**, 615.

Savory, J., Huang Y., Wills M.R. and Herman M.M., (1998), Reversal by desferrioxamine of tau protein aggregates following two days of treatment in aluminum-induced neurofibrillary degeneration in rabbit: Implications for clinical trials in Alzheimer's disease, *Neurotoxicology,* **19**, 209.

Schmidt, M.W., Baldridge K.K., Boatz J.A., Elbert S.T., Gordon M.S., Jensen J.H., Koseki S., Matsunaga N., Nguyen K.A., Su S.J., Windus T.L., Dupuis M. and Montgomery J.A., (1993), General Atomic and Molecular Electronic-Structure System, *Journal Of Computational Chemistry,* **14**, 1347.

Shea, T.B., Beermann M.L. and Nixon R.A., (1995), Aluminum Treatment Of Intact Neuroblastoma-Cells Alters Neurofilament Subunit Phosphorylation, Solubility, and Proteolysis, *Molecular and Chemical Neuropathology,* **26**, 1.

Sheldrick, G.M., (1993), SHELXL-93. Program for Crystal Structure Refinement, University of Göttingen, Germany.

Shen, L.L., Mitscher L.A., Sharma P.N., Odonnell T.J., Chu D.W.T., Cooper C.S., Rosen T. and Pernet A.G., (1989), Mechanism Of Inhibition Of DNA Gyrase By Quinolone Antibacterials - a Cooperative Drug-DNA Binding Model, *Biochemistry,* **28**, 3886.

Shi, B. and Haug A., (1990), Aluminum Uptake By Neuroblastoma-Cells, *Journal Of Neurochemistry,* **55**, 551.

Shoop, D.M., Lambrecht R.M. and Rack E.P., (1996), Radiochemistry of aluminium, *Journal Of Radioanalytical and Nuclear Chemistry-Articles,* **211**, 485.

Slanina, P., Frech W., Ekstrom L.G., Loof L., Slorach S. and Cedergren A., (1986), Dietary Citric-Acid Enhances Absorption Of Aluminum In Antacids, *Clinical Chemistry,* **32**, 539.

Sobow, T., (1996), An ultra structural and molecular perspective of the pathological hallmarks of Alzheimer's disease, *J. Folia. neuropath.,* **34**, 55.

Stern, F. and Beevers A., (1950), The Crystal Structure of Tartaric Acid, *Acta Crystallographica,* **3**, 341.

Stewart, J.J.P., (1989a), Optimization Of Parameters For Semiempirical Methods .1. Method, *Journal Of Computational Chemistry,* **10**, 209.

Stewart, J.J.P., (1989b), Optimization Of Parameters For Semiempirical Methods .2. Applications, *Journal Of Computational Chemistry,* **10**, 221.

Stewart, J.J.P., (1990), Comments On a Comparison Of Am1 With the Recently Developed PM3 Method - Reply, *Journal Of Computational Chemistry,* **11**, 543.

Stewart, J.J.P., and Fujitsu Ltd., (1993), MOPAC93. QCPE455, Dept. of Chemistry, Creative Arts Bldg. 181, Indiana University, Bloomington, IN 47405, USA.

Still, C.N. and Kelly P., (1980), On the incidence of primary degenerative dementia vs. water fluoride content in South Carolina, *Neurotoxicology,* **4**, 125.

Stout, G.H. and Jensen L.H., (1989), X-ray Structure Determination John Wiley and Sons, New York.

Sturman, J.A., Wisnieski H.M. and Shek J.W., (1983), High affinity uptake of GABA and glycine by rabbits with aluminium induced neurofibrillary degeneration, *Neurochem. Res.,* **8**, 1097.

Summers, J.B., Gunn B.P., Martin J.G., Martin M.B., Mazdiyasni H., Stewart A.O., Young P.R., Bouska J.B., Goetze A.M., Dyer R.D., Brooks D.W. and Carter G.W., (1988), Structure-Activity Analysis Of a Class Of Orally Active Hydroxamic Acid Inhibitors Of Leukotriene Biosynthesis, *Journal Of Medicinal Chemistry,* **31**, 1960.

Taylor, G.A., Ferrier I.N., McLoughlin I.J., Fairbairn A.F., McKeith I.G., Lett D. and Edwardson J.A., (1992), Gastrointestinal Absorption Of Aluminum In Alzheimers-Disease - Response to Aluminum Citrate, *Age and Ageing,* **21**, 81.

Thiel, W. and Voityuk A.A., (1996), Extension of MNDO to d orbitals: Parameters and results for the second-row elements and for the zinc group, *Journal Of Physical Chemistry,* **100**, 616.

Trapp, G.A., (1980), Studies of aluminium interaction with enzymes and proteins: the inhibition of hexokinase, *Neurotoxicology,* **1**, 89.

Venema, F.R., Koningsveld, H. van, Peters, J.A., Bekkum, H. van, (1990) Co-operative hydrogen bonding with short O...O distances in a binuclear Al(III)-glycolate complex, *Journal of the Chemical Society, Chemical Communications*, 699.

Viestra, R. and A. Haug, (1978), The effect of aluminium on the physical properties of membranes in *Thermoplasma ophilum*, *Biochem. Biophys. Res. Commun.*,**84**, 134.

Vitorello, V.A. and Haug A., (1996), Short-term aluminium uptake by tobacco cells: Growth dependence and evidence for internalization in a discrete peripheral region, *Physiologia Plantarum,* **97**, 536.

Vitorello, V.A. and Haug A., (1997), An aluminum-morin fluorescence assay for the visualization and determination of aluminum in cultured cells of Nicotiana tabacum L cv BY-2, *Plant Science,* **122**, 35.

Vogt, T., (1986), Water quality and health-study of a possible relationship between aluminium in drinking water and dementia, in: Bureau of Statistics of Norway Oslo.

Wang, X.G., Nelson D.J., Trindle C.and Martin R.B., (1997), Experimental and theoretical analysis of Al^{3+} complexation with ADP and ATP, *Journal Of Inorganic Biochemistry,* **68**, 7.

Wettstein, A., Aeppli J., Gautschi K. and Peters M., (1991), Failure to Find a Relationship Between Mnestic Skills Of Octogenarians and Aluminum In Drinking-Water, *International Archives Of Occupational and Environmental Health,* **63**, 97.

Williams, R.J.P., (1996), Aluminium and biological systems: An introduction, *Coordination Chemistry Reviews,* **149**, 1.

Wilson, A.P.R. and Gruneberg R.N., (1997), Cipofloxacin: 10 years of clinical experience, Maxim medical, Oxford.

Wu Pong, S., Weiss T.L. and Hunt C.A., (1992), Antisense C-Myc Oligodeoxyribonucleotide Cellular Uptake, *Pharmaceutical Research,* **9**, 1010.

Wynne, K.J., (1985), 2 Ligand-Bridged Phthalocyanines - Crystal and Molecular-Structure Of Fluoro(Phthalocyaninato)Gallium(III), [Ga(Pc)F]N, and (Mu-Oxo)Bis[(Phthalocyaninato)Aluminum(III)], [Al(Pc)]2o, *Inorg. Chem.* **24**, 1339.

Yates, P.C., (1993), Molecular Mechanics and Semiempirical Molecular-Orbital Calculations On Zinc-Complexes With Amino-Acid Derivatives, *Theochem-Journal Of Molecular Structure,* **100**, 275.

Yates, P.C. and Marsden A.K., (1994), A Modified Mm2 Program For Molecular Mechanics Calculations On Coordination-Compounds, *Computers & Chemistry,* **18**, 89.

Yokel, R.A., (1994), Aluminum Chelation - Chemistry, Clinical, and Experimental Studies and the Search For Alternatives to Desferrioxamine, *Journal Of Toxicology and Environmental Health,* **41**, 131.

Yokel, R.A., (1996), Aluminum chelation by 3-hydroxypyridin-4-ones in the rat demonstrated by microdialysis, *Biological Trace Element Research,* **53**, 193.

Yokel, R.A., Ackrill P., Burgess E., Day J.P., Domingo J.L., Flaten T.P. and Savory J., (1996a), Prevention and treatment of aluminum toxicity including chelation therapy: Status and research needs, *Journal Of Toxicology and Environmental Health,* **48**, 667.

Yokel, R.A., Datta A.K. and Jackson E.G., (1991), Evaluation Of Potential Aluminum Chelators Invitro By Aluminum Solubilization Ability, Aluminum Mobilization From Transferrin and the Octanol Aqueous Distribution Of the Chelators and Their Complexes With Aluminum, *Journal Of Pharmacology and Experimental Therapeutics,* **257**, 100.

Yokel, R.A., Fredenburg A.M., Meurer K.A. and Skinner T.L., (1995), Influence Of Lipophilicity On the Bioavailability and Disposition Of Orally-Active 3-Hydroxypyridin-4-One Metal Chelators, *Drug Metabolism and Disposition,* **23**, 1178.

Yokel, R.A., Meurer K.A., Hong C.B., Dickey K.M., Skinner T.L. and Fredenburg A.M., (1997), Short-term oral 3-hydroxypyridin-4-one dosing increases aluminum excretion and partially reverses aluminum-induced toxicity in the rabbit independent of chelator lipophilicity, *Drug Metabolism and Disposition,* **25**, 182.

Yokel, R.A., K.A. Meurer, T.L. Skinner and A.M. Fredenburg, (1996b), The 3-hydroxypyridin-4-ones more effectively chelate aluminum in a rabbit model of aluminum intoxication than does desferrioxamine, *Drug Metabolism and Disposition,* **24**, 105.

Yoshino, M., Murakami K. and Kawano K., (1998), Interaction of aluminum ion with ATP. Mechanism of the aluminum inhibition of glycerol kinase and its reversal by spermine, *Biometals,* **11**, 63.

Yumoto, S., Nagai H., Imamura M., Matsuzaki H., Hayashi K., Masuda A., Kumazawa H., Ohashi H. and Kobayashi K., (1997), Al-26 uptake and accumulation in the rat

brain, *Nuclear Instruments & Methods In Physics Research Section B-Beam Interactions With Materials and Atoms,* **123**, 279.

Zatta, P., Favarato M. and Nicolini M., (1993), Deposition Of Aluminum In Brain-Tissues Of Rats Exposed to Inhalation Of Aluminum Acetylacetonate, *Neuroreport,* **4**, 1119.

Zatta, P.F., (1995), Aluminum Binds to the Hyperphosphorylated Tau In Alzheimers-Disease - a Hypothesis, *Medical Hypotheses,* **44**, 169.

Zhang, Z.H., Rettig S.J. and Orvig C., (1991), Lipophilic Coordination-Compounds - Aluminum, Gallium, and Indium Complexes Of 1-Aryl-3-Hydroxy-2-Methyl-4-Pyridinones, *Inorganic Chemistry,* **30**, 509.

APPENDIX

A1.0 EXAMPLES OF INPUT FILES

All the examples used are based on the input files for the crystal structure of anhydrous DL tartaric acid discussed in chapter four.

A1.1 North format file (nth)

```
* 0 CELL   4.8879 6.5739 9.1768 74.777 88.465 76.555
* 1 racemic tartaric acid (synthesised)
C1          0.32302  0.89597  0.39557
C2          0.56341   0.8094  0.30368
C3          0.44227   0.7058   0.1946
C4          0.68066   0.6092  0.10509
O1          0.12643  1.04626  0.31105
O2          0.31623  0.82733  0.53261
O3          0.76844  0.65779  0.40556
O4          0.29253  0.55324  0.27016
O5          0.75791  0.41568  0.11764
O6          0.79064  0.75887  0.01704
H1          -0.0182  1.10442  0.36899
H2          0.63517  0.92689   0.2451
H3          0.93954  0.62547   0.3629
H4           0.3128   0.8187  0.12665
H5          0.39792  0.44999  0.33453
H6           0.9413  0.68193  -0.0281
```

A1.2 Crystal Structure Search Retrieval format file (cssr)

```
                ALTARCRYSTA       1.000   1.000   1.000
                90.000  90.000  90.000
 16  1
  2
 4 C4          0         0         0       2   8  15   0   0   0   0   0   0   1
 3 C3          1.52129   0         0       3   1   7  14   0   0   0   0   0   1
 2 C2          2.02302   1.46357   0       4   2   6  13   0   0   0   0   0   1
 1 C1          3.53932   1.42922  -0.057   3   5  12   0   0   0   0   0   0   1
 5 O1          4.05682   0.83794   0.9821  4   9   0   0   0   0   0   0   0   1
 7 O3          1.57542   2.17654  -1.1223  3  10   0   0   0   0   0   0   0   1
 8 O4          2.05422  -0.7461   -1.0633  2  11   0   0   0   0   0   0   0   1
 9 O5         -0.6595   -0.4194   -0.9303  1   0   0   0   0   0   0   0   0   1
11 H1          4.99951   0.85637   0.96363 5   0   0   0   0   0   0   0   0   1
13 H3          0.70088   2.44367  -1.0505  6   0   0   0   0   0   0   0   0   1
15 H5          1.82999  -0.4146   -1.8103  7   0   0   0   0   0   0   0   0   1
 6 O2          4.18013   1.88588  -0.9918  4   0   0   0   0   0   0   0   0   1
12 H2          1.74968   1.87516   0.81382 3   0   0   0   0   0   0   0   0   1
14 H4          1.82606  -0.4015    0.80358 2   0   0   0   0   0   0   0   0   1
10 O6         -0.4851    0.51878   1.10033 1  16   0   0   0   0   0   0   0   1
16 H6         -1.4204    0.51829   0.97594 15  0   0   0   0   0   0   0   0   1
```

A1.3 GAMESS input file

```
$CONTRL SCFTYP=RHF ICHARG=0 RUNTYP=OPTIMIZE COORD=CART
$END
$SYSTEM TIMLIM=99999 MEMORY=1500000 $END
$BASIS GBASIS=N21 NGAUSS=3 $END
$STATPT NSTEP=150 $END
$DATA
3-21G OPT. OF DL TARTARIC ACID, CARTESIAN INPUT
C1
C1          6    -1.88587    0.043144   -0.21235
C2          6    -0.47908    0.337593   -0.64673
C3          6    0.441364    -0.65336   0.061316
C4          6    1.844771    -0.13194   -0.05535
O1          8    -2.25591    -1.19555   -0.57541
O2          8    -2.58824    0.816004   0.382492
O3          8    -0.12977    1.659594   -0.24907
O4          8    0.077121    -0.72261   1.436256
O5          8    2.534848    0.173719   0.880041
O6          8     2.22693    -0.05161   -1.34003
H1          1    -3.13321    -1.44168    -0.2467
H2          1    -0.38606    0.231119   -1.71497
H3          1    -0.81387    2.014326   0.339386
H4          1    0.362298    -1.62545   -0.39711
H5          1     0.75628    -0.28895   1.975714
H6          1    3.100318    0.352015   -1.45222
$END
```

A2.0 ATOMIC CO-ORDINATES AND DISPLACEMENT PARAMETERS OF STRUCTURES SOLVED IN CHAPTER FOUR

2.1 ALP2XL

Atomic co-ordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$ x 10^3) for ALP2XL. U(eq) is defined as one third of the trace of the orthogonalised Uij tensor.

	x	y	z	U(eq)
Cl(1)	-143(2)	4490(2)	7180(2)	31(1)
Al(2)	4678(2)	4678(2)	4678(2)	21(1)
O(1)	2688(2)	3371(3)	5217(3)	28(1)
O(2)	6616(2)	5951(3)	4146(3)	32(1)

Anisotropic displacement parameters ($Å^2$ x 10^3) for ALP2XL. The anisotropic displacement factor exponent takes the form:
$-2\pi^2 [h^2 a^{*2} U11 + ... + 2 h k a^* b^* U12]$

	U11	U22	U33	U23	U13	U12
Cl(1)	30(1)	29(1)	40(1)	12(1)	12(1)	11(1)
Al(2)	22(1)	22(1)	22(1)	9(1)	9(1)	9(1)
O(1)	29(1)	18(1)	44(1)	10(1)	21(1)	4(1)
O(5)	28(1)	33(1)	39(1)	10(1)	14(1)	11(1)

Hydrogen co-ordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) for ALP2XL.

	x	y	z	U(eq)
H(1A)	2643(60)	2432(31)	5165(58)	48(3)
H(1B)	2034(39)	3781(44)	5784(37)	48(3)
H(5B)	6848(60)	6978(32)	4334(60)	48(3)
H(5A)	7356(40)	5596(48)	3849(38)	48(3)

2.2 ALTAR

Atomic co-ordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$ x 10^3) for ALTAR. U(eq) is defined as one third of the trace of the orthogonalised Uij tensor.

	x	y	z	U(eq)
C(1)	3230(4)	8960(3)	3956(2)	21(1)
C(2)	5634(4)	8094(3)	3037(2)	22(1)
C(3)	4423(4)	7058(3)	1946(2)	22(1)
C(4)	6807(4)	6092(3)	1051(2)	22(1)
O(1)	1264(3)	10463(3)	3111(2)	32(1)
O(2)	3162(3)	8273(2)	5326(1)	26(1)
O(3)	7684(3)	6578(3)	4056(2)	29(1)
O(4)	2925(3)	5532(2)	2702(2)	25(1)
O(5)	7579(3)	4157(2)	1176(2)	28(1)
O(6)	7906(3)	7589(2)	170(2)	34(1)

Anisotropic displacement parameters ($Å^2$ x 10^3) for ALTAR. The anisotropic displacement factor exponent takes the form:
$-2\ pi^2\ [\ h^{\wedge 2}\ a^{*2}\ U11 + ... + 2\ h\ k\ a^*\ b^*\ U12\ ]$

	U11	U22	U33	U23	U13	U12
C(1)	20(1)	25(1)	17(1)	-4(1)	7(1)	-4(1)
C(2)	19(1)	28(1)	15(1)	-4(1)	7(1)	-1(1)
C(3)	19(1)	27(1)	14(1)	-3(1)	5(1)	2(1)
C(4)	21(1)	27(1)	12(1)	-4(1)	4(1)	2(1)
O(1)	28(1)	38(1)	19(1)	-3(1)	8(1)	10(1)
O(2)	24(1)	33(1)	15(1)	-4(1)	7(1)	0(1)
O(3)	18(1)	41(1)	20(1)	-4(1)	4(1)	3(1)
O(4)	20(1)	30(1)	22(1)	-3(1)	6(1)	-2(1)
O(5)	26(1)	30(1)	24(1)	-6(1)	9(1)	2(1)
O(6)	38(1)	31(1)	27(1)	-5(1)	21(1)	-2(1)

Hydrogen co-ordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) for ALTAR.

	x	y	z	U(eq)
H(1)	-182(79)	11044(60)	3690(43)	75(11)
H(2)	6352(51)	9269(40)	2451(28)	27(6)
H(3)	9395(87)	6255(64)	3629(43)	78(11)
H(4)	3128(49)	8187(38)	1266(25)	22(5)
H(5)	3979(63)	4500(53)	3345(33)	48(8)
H(6)	9413(84)	6819(64)	-281(43)	82(12)

2.3 ALTXL

Atomic co-ordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$ x 10^3) for ALTXL. U(eq) is defined as one third of the trace of the orthogonalised Uij tensor.

	x	y	z	U(eq)
Na(1)	4107(1)	12075(1)	9266(1)	28(1)
O(1)	5634(2)	7143(2)	8396(1)	26(1)
O(2)	5690(2)	9641(2)	8896(1)	27(1)
C(1)	4883(2)	8436(2)	8646(2)	17(1)
C(2)	2754(2)	8413(2)	8633(2)	15(1)
C(3)	2038(2)	7633(2)	7438(2)	17(1)
C(4)	-70(2)	7685(2)	7378(2)	17(1)
O(3)	-881(2)	8124(2)	6447(1)	29(1)
O(4)	-842(2)	7177(2)	8412(1)	24(1)
O(5)	2120(2)	9945(2)	8710(2)	25(1)
O(6)	2808(2)	8313(2)	6342(1)	26(1)
O(16)	4011(2)	14748(2)	9911(2)	27(1)

Anisotropic displacement parameters ($Å^2$ x 10^3) for ALTXL. The anisotropic displacement factor exponent takes the form:
$-2\ pi^2\ [\ h^2\ a^{*2}\ U11 + ... + 2\ h\ k\ a^*\ b^*\ U12\ ]$

	U11	U22	U33	U23	U13	U12
Na(1)	25(1)	25(1)	33(1)	-4(1)	1(1)	-3(1)
O(1)	12(1)	26(1)	39(1)	-6(1)	1(1)	1(1)
O(2)	17(1)	25(1)	38(1)	-3(1)	-4(1)	-5(1)
C(1)	12(1)	24(1)	16(1)	-1(1)	0(1)	0(1)
C(2)	11(1)	18(1)	17(1)	-1(1)	0(1)	-1(1)
C(3)	14(1)	21(1)	16(1)	-1(1)	2(1)	-1(1)
C(4)	15(1)	16(1)	18(1)	-2(1)	-4(1)	0(1)
O(3)	23(1)	34(1)	30(1)	8(1)	-8(1)	-2(1)
O(4)	12(1)	38(1)	21(1)	1(1)	0(1)	-2(1)
O(5)	16(1)	21(1)	37(1)	-6(1)	4(1)	1(1)
O(6)	26(1)	36(1)	18(1)	1(1)	6(1)	-7(1)
O(16)	18(1)	24(1)	39(1)	-2(1)	3(1)	2(1)

Hydrogen co-ordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) for ALTXL

	x	y	z	U(eq)
H(2)	2353(28)	7793(26)	9345(19)	18(5)
H(1)	2390(26)	6575(25)	7467(19)	15(5)
H(4)	-2032(34)	7197(31)	8308(23)	36(6)
H(5)	1255(40)	9952(32)	9091(27)	35(7)
H(6)	2675(35)	9195(32)	6398(25)	30(7)
H(16A)	3082(38)	15041(30)	10241(24)	32(8)
H(16B)	4348(44)	15370(37)	9339(30)	53(9)

2.4 MEOXAL

Atomic co-ordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$ x 10^3) for MEOXAL. U(eq) is defined as one third of the trace of the orthogonalised Uij tensor.

	x	y	z	U(eq)
C(1)	9031(2)	-549(3)	9485(1)	29(1)
O(2)	9368(1)	605(3)	8516(1)	41(1)
O(3)	7439(1)	-2313(3)	9638(1)	40(1)
O(4)	6314(1)	-1143(3)	6802(1)	40(1)

Anisotropic displacement parameters ($Å^2$ x 10^3) for MEOXAL. The anisotropic displacement factor exponent takes the form:
$-2\ pi^2\ [\ h^2\ a^{*2}\ U11 + ... + 2\ h\ k\ a^*\ b^*\ U12\ ]$

	U11	U22	U33	U23	U13	U12
C(1)	29(1)	30(1)	27(1)	-1(1)	5(1)	-2(1)
O(2)	39(1)	55(1)	26(1)	1(1)	4(1)	-14(1)
O(3)	34(1)	54(1)	31(1)	2(1)	2(1)	-16(1)
O(4)	33(1)	56(1)	29(1)	-4(1)	2(1)	9(1)

Hydrogen co-ordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) for MEOXAL.

	x	y	z	U(eq)
H(2)	8212(32)	-46(57)	7883(17)	66(5)
H(4A)	6800(29)	-1632(51)	6185(18)	56(4)
H(4B)	5258(36)	229(67)	6592(17)	70(6)

2.5 CITXL

Atomic co-ordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$ x 10^3) for CITXL. U(eq) is defined as one third of the trace of the orthogonalised Uij tensor.

	x	y	z	U(eq)
O(1)	-2265(6)	7927(6)	5485(5)	66(1)
O(2)	-1092(5)	5995(5)	6662(4)	49(1)
O(3)	6633(6)	9292(5)	8893(4)	54(1)
O(4)	7371(5)	11266(5)	7521(4)	51(1)
O(5)	2973(5)	7008(4)	9120(4)	44(1)
O(6)	3108(5)	5707(5)	7035(4)	42(1)
O(7)	2429(6)	9747(5)	7925(5)	42(1)
C(1)	-1032(8)	7265(7)	5884(6)	43(1)
C(2)	737(8)	7769(7)	5539(6)	40(1)
C(3)	2604(7)	8426(6)	6980(5)	35(1)
C(4)	4260(8)	9214(8)	6505(6)	39(1)
C(5)	6179(8)	9909(7)	7788(6)	39(1)
C(6)	2901(7)	6971(6)	7837(6)	33(1)
O(8)	4006(7)	3379(6)	8476(5)	72(1)
C(7)	-2740(9)	5440(9)	7096(9)	75(2)
C(8)	9320(10)	11934(9)	8657(8)	75(2)

Anisotropic displacement parameters ($Å^2$ x 10^3) for CITXL. The anisotropic displacement factor exponent takes the form:
$-2\ pi^2\ [\ h^2\ a^{*2}\ U11 + ... + 2\ h\ k\ a^*\ b^*\ U12\ ]$

	U11	U22	U33	U23	U13	U12
O(1)	53(3)	64(3)	92(3)	33(3)	25(3)	36(2)
O(2)	43(2)	49(2)	66(3)	25(2)	24(2)	25(2)
O(3)	55(3)	56(3)	40(2)	16(2)	11(2)	10(2)
O(4)	42(2)	50(2)	58(3)	14(2)	19(2)	8(2)
O(5)	55(2)	47(2)	40(2)	19(2)	21(2)	25(2)
O(6)	51(2)	37(2)	41(2)	9(2)	15(2)	23(2)
O(7)	56(3)	35(2)	38(2)	9(2)	18(2)	22(2)
C(1)	41(3)	39(3)	39(3)	3(3)	7(3)	13(3)
C(2)	45(3)	37(3)	34(3)	5(3)	9(3)	19(3)
C(3)	40(3)	34(3)	31(3)	5(2)	14(2)	12(2)
C(4)	44(3)	46(3)	34(3)	15(3)	15(3)	22(3)
C(5)	40(3)	39(3)	43(3)	10(3)	23(3)	13(3)
C(6)	33(3)	31(3)	35(3)	10(2)	10(2)	11(2)
O(8)	77(3)	47(3)	71(3)	18(2)	3(3)	22(2)
C(7)	51(4)	73(5)	108(6)	38(4)	35(4)	21(4)
C(8)	53(4)	75(5)	86(5)	15(4)	25(4)	8(4)

Hydrogen co-ordinates (x 10^2) and isotropic displacement parameters ($Å^2$ x 10^3) for CITXL.

	x	y	z	U(eq)
H(6)	3569(87)	4802(81)	7568(67)	72(19)
H(7)	2951(96)	9520(89)	8710(77)	78(24)
H(2A)	711(65)	6782(65)	4996(52)	34(14)
H(2B)	782(82)	8942(78)	5000(65)	70(18)
H(4A)	4012(77)	10178(74)	5974(61)	58(17)
H(4B)	4443(72)	8263(69)	5789(58)	51(15)
H(8A)	5444(97)	3463(80)	9424(74)	82(20)
H(8B)	3171(139)	1770(143)	7852(108)	174(38)
H(7A)	-2568(33)	4623(49)	7761(44)	112
H(7B)	-3883(13)	4887(55)	6205(10)	112
H(7C)	-2851(40)	6445(13)	7608(47)	112
H(8C)	10027(21)	12984(35)	8433(31)	113
H(8D)	9927(24)	11066(25)	8644(37)	113
H(8E)	9291(10)	12192(58)	9641(11)	113

2.6 TRIC2XL

Atomic co-ordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$ x 10^3) for TRIC2XL. U(eq) is defined as one third of the trace of the orthogonalised Uij tensor.

	x	y	z	U(eq)
C(1)	8834(2)	4542(1)	-3489(6)	39(1)
C(2)	7926(2)	4180(1)	-2319(8)	39(1)
C(3)	8273(2)	3556(1)	-2150(5)	29(1)
C(4)	7278(2)	3146(1)	-2051(5)	29(1)
C(5)	6459(2)	3227(1)	81(5)	27(1)
C(6)	9110(2)	3453(1)	-51(5)	28(1)
O(1)	9451(2)	4372(1)	-5158(5)	59(1)
O(2)	8870(3)	5051(1)	-2594(6)	61(1)
O(3)	6564(2)	3582(1)	1714(4)	40(1)
O(4)	5610(2)	2868(1)	-9(5)	42(1)
O(5)	9031(2)	3071(1)	1442(4)	39(1)
O(6)	9956(2)	3818(1)	-83(5)	42(1)

Anisotropic displacement parameters ($Å^2$ x 10^3) for TRIC2XL. The anisotropic displacement factor exponent takes the form:
$-2\ pi^2\ [\ h^2\ a^{*2}\ U11 + ... + 2\ h\ k\ a^*\ b^*\ U12\ ]$

	U11	U22	U33	U23	U13	U12
C(1)	33(1)	44(2)	41(2)	7(1)	4(1)	-4(1)
C(2)	24(1)	42(2)	53(2)	8(2)	7(1)	1(1)
C(3)	16(1)	40(1)	30(1)	2(1)	3(1)	-1(1)
C(4)	18(1)	42(2)	28(1)	-1(1)	0(1)	-3(1)
C(5)	15(1)	35(1)	32(1)	5(1)	-1(1)	-1(1)
C(6)	15(1)	36(1)	32(1)	-3(1)	3(1)	0(1)
O(1)	66(2)	55(2)	54(2)	-5(1)	29(1)	-19(1)
O(2)	59(2)	44(1)	78(2)	-3(1)	30(2)	-12(1)
O(3)	24(1)	52(1)	43(1)	-7(1)	7(1)	-8(1)
O(4)	26(1)	52(1)	47(1)	-5(1)	9(1)	-14(1)
O(5)	22(1)	47(1)	47(1)	9(1)	-9(1)	-4(1)
O(6)	28(1)	54(2)	45(1)	7(1)	-8(1)	-15(1)

Hydrogen co-ordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) for TRIC2XL.

	x	y	z	U(eq)
H(2A)	7776(30)	4328(14)	-715(79)	37(9)
H(2B)	7265(39)	4205(17)	-3367(86)	59(12)
H(3)	8716(28)	3441(13)	-3710(62)	29(8)
H(4A)	7576(30)	2737(14)	-1942(66)	37(9)
H(4B)	6904(32)	3183(15)	-3619(74)	43(10)
H(2)	9497(47)	5225(22)	-3319(108)	91
H(4)	5217(47)	2908(24)	1244(111)	86(17)
H(6)	10269(44)	3742(21)	1064(103)	69(16)

2.7 PYRXL

Atomic co-ordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$ x 10^3) for PYRXL. U(eq) is defined as one third of the trace of the orthogonalised Uij tensor.

	x	y	z	U(eq)
O(01)	-28(1)	2686(2)	1578(1)	83(1)
C(11)	-798(2)	2494(2)	1080(1)	69(1)
C(21)	-914(2)	3335(2)	829(1)	67(1)
C(31)	-1642(2)	3116(3)	288(1)	85(1)
C(41)	-2237(3)	2106(4)	10(2)	103(1)
C(51)	-2125(3)	1287(3)	288(2)	100(1)
C(61)	-1418(2)	1456(2)	828(2)	82(1)
C(10)	-1347(3)	528(3)	1148(2)	103(1)
O(02)	-311(2)	1181(2)	2500	97(1)
C(12)	-1402(3)	499(3)	2500	83(1)
C(22)	-1925(2)	153(2)	1852(2)	88(1)
C(32)	-3022(2)	-566(2)	1871(2)	100(1)
C(42)	-3565(4)	-915(3)	2500	107(2)
C(20)	-279(2)	4439(2)	3857(1)	69(1)
O(04)	558(2)	4289(2)	2500	70(1)
C(14)	-300(2)	4469(2)	2500	51(1)
C(24)	-710(2)	4567(2)	3149(1)	54(1)
C(34)	-1540(2)	4782(2)	3131(1)	60(1)
C(44)	-1951(3)	4893(2)	2500	61(1)
N(1)	3333	6667	2500	180(4)
C(12)	3333	6667	3092(5)	161(4)
C(4)	3996(14)	7251(20)	3529(9)	478(15)

Hydrogen co-ordinates (x 10^4) and isotropic displacement parameters($Å^2$ x 10^3) for PYRXL.

	x	y	z	U(eq)
H(01)	199(1)	3285(2)	1744(1)	125
H(31)	-1731(2)	3665(3)	107(1)	102
H(41)	-2710(3)	1979(4)	-362(2)	123
H(51)	-2538(3)	602(3)	106(2)	120
H(10A)	-1647(3)	-63(3)	815(2)	124
H(10B)	-602(3)	742(3)	1217(2)	124
H(02)	-145(2)	1593(2)	2162	146
H(32)	-3393(2)	-813(2)	1446(2)	120
H(42)	-4297(4)	-1385(3)	2500	128
H(20A)	453(2)	4605(2)	3792(1)	83
H(20B)	-275(2)	4951(2)	4192(1)	83
H(04)	545(2)	3972(2)	2136	105
H(34)	-1825(2)	4854(2)	3557(1)	72
H(44)	-2506(3)	5041(2)	2500	73

2.8 BUCIP4

Atomic co-ordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$ x 10^3) for BUCIP4. U(eq) is defined as one third of the trace of the orthogonalised Uij tensor.

	x	y	z	U(eq)
N(1)	7555(10)	7663(5)	3752(2)	38(1)
C(2)	6974(13)	6316(6)	4030(2)	44(2)
C(3)	5194(13)	5313(6)	3832(3)	45(2)
C(4)	3848(14)	5656(6)	3299(3)	45(2)
C(4A)	4564(13)	7094(6)	2994(3)	41(2)
C(5)	3385(13)	7555(6)	2453(3)	45(2)
C(6)	3992(13)	8910(6)	2172(2)	43(2)
C(7)	5786(12)	9962(6)	2388(2)	34(1)
C(8)	6976(12)	9487(6)	2917(2)	39(2)
C(8A)	6347(12)	8087(6)	3216(2)	36(2)
C(9)	4814(17)	3873(7)	4191(3)	59(2)
O(1)	5886(12)	3526(5)	4641(2)	79(2)
O(2)	3067(11)	2938(4)	3966(2)	80(2)
O(3)	2104(10)	4794(4)	3096(2)	63(1)
C(10)	9501(12)	8664(6)	3987(2)	42(2)
C(11)	8174(14)	9954(6)	4195(2)	49(2)
C(12)	9385(14)	8704(6)	4594(2)	57(2)
F(1)	2699(8)	9301(4)	1660(2)	64(1)
N(13)	6118(10)	11378(5)	2105(2)	41(1)
C(14)	7527(13)	12443(6)	2405(2)	48(2)
C(15)	6821(13)	13983(6)	2125(2)	44(2)
N(16)	7785(10)	14253(5)	1542(2)	39(1)
C(17)	6219(13)	13204(6)	1255(2)	44(2)
C(18)	7023(14)	11651(6)	1519(2)	50(2)
C(19)	7025(14)	15773(6)	1296(2)	48(2)
C(20)	7991(15)	16224(6)	696(3)	54(2)
C(21)	7480(16)	17833(6)	488(3)	64(2)
C(22)	8269(17)	18296(7)	-119(3)	82(2)

Anisotropic displacement parameters ($Å^2 \times 10^3$) for BUCIP4. The anisotropic displacement factor exponent takes the form:
$-2\ pi^2\ [\ h^2\ a^{*2}\ U11 + ... + 2\ h\ k\ a^*\ b^*\ U12\ ]$

	U11	U22	U33	U23	U13	U12
N(1)	41(3)	36(3)	36(3)	-1(2)	4(2)	-7(2)
C(2)	49(4)	39(4)	41(4)	-1(3)	2(3)	3(3)
C(3)	56(4)	28(3)	51(5)	-8(3)	22(4)	-5(3)
C(4)	56(4)	37(4)	43(4)	-8(3)	18(3)	-3(3)
C(4A)	43(4)	39(4)	42(4)	-12(3)	2(3)	0(3)
C(5)	44(4)	43(4)	51(4)	-15(3)	-4(3)	-1(3)
C(6)	48(4)	44(4)	37(4)	-2(3)	-4(3)	6(3)
C(7)	29(3)	33(3)	43(4)	-12(3)	-4(3)	1(3)
C(8)	40(4)	35(3)	43(4)	-6(3)	-4(3)	-4(3)
C(8A)	40(4)	37(4)	30(4)	-3(3)	9(3)	0(3)
C(9)	72(5)	40(4)	65(5)	-6(4)	15(4)	-3(4)
O(1)	100(4)	56(3)	72(4)	18(3)	0(3)	-2(3)
O(2)	99(4)	45(3)	91(4)	1(3)	8(3)	-23(3)
O(3)	78(3)	48(3)	67(3)	-21(2)	7(3)	-25(2)
C(10)	36(4)	49(4)	42(4)	-7(3)	1(3)	0(3)
C(11)	55(4)	42(4)	52(4)	-7(3)	-5(3)	-12(3)
C(12)	64(4)	65(4)	40(4)	0(3)	-5(3)	-14(3)
F(1)	84(3)	51(2)	57(3)	-6(2)	-29(2)	1(2)
N(13)	55(3)	33(3)	34(3)	-4(2)	-2(2)	-2(2)
C(14)	66(4)	43(4)	34(4)	-5(3)	-9(3)	-8(3)
C(15)	50(4)	45(4)	37(4)	-7(3)	-9(3)	-6(3)
N(16)	44(3)	33(3)	38(3)	-1(2)	-3(2)	-1(2)
C(17)	54(4)	44(4)	31(4)	-2(3)	-2(3)	0(3)
C(18)	63(4)	49(4)	37(4)	-7(3)	12(3)	4(3)
C(19)	54(4)	38(4)	50(4)	-1(3)	-2(3)	-4(3)
C(20)	62(4)	51(4)	47(4)	1(3)	5(3)	-12(3)
C(21)	81(5)	47(4)	57(5)	16(3)	-5(4)	-7(4)
C(22)	114(6)	68(5)	58(5)	13(4)	-14(4)	-28(4)

Hydrogen co-ordinates (x 10^4) and isotropic displacement parameters (Å^2 x 10^3) for BUCIP4.

	x	y	z	U(eq)
H(2)	7838(13)	6048(6)	4381(2)	52
H(5)	2182(13)	6920(6)	2289(3)	55
H(8)	8221(12)	10113(6)	3076(2)	47
H(2A)	2488(11)	3334(4)	3657(2)	120
H(10)	11533(12)	8815(6)	3814(2)	51
H(11A)	9342(14)	10854(6)	4136(2)	59
H(11B)	5971(14)	10090(6)	4176(2)	59
H(12A)	7922(14)	8075(6)	4818(2)	69
H(12B)	11293(14)	8839(6)	4779(2)	69
H(14A)	9726(13)	12289(6)	2417(2)	57
H(14B)	6762(13)	12303(6)	2786(2)	57
H(15A)	4635(13)	14161(6)	2147(2)	53
H(15B)	7844(13)	14669(6)	2322(2)	53
H(17A)	6820(13)	13361(6)	865(2)	53
H(17B)	4023(13)	13355(6)	1276(2)	53
H(18A)	5992(14)	10966(6)	1323(2)	60
H(18B)	9211(14)	11493(6)	1487(2)	60
H(19A)	7982(14)	16425(6)	1517(2)	58
H(19B)	4828(14)	15911(6)	1323(2)	58
H(20A)	10145(15)	15992(6)	658(3)	65
H(20B)	6849(15)	15659(6)	466(3)	65
H(21A)	5347(16)	18072(6)	547(3)	77
H(21B)	8706(16)	18393(6)	707(3)	77
H(22A)	10393(30)	18093(47)	-179(4)	123
H(22B)	7880(103)	19329(13)	-224(6)	123
H(22C)	7036(77)	17763(38)	-341(3)	123

2.9 NAL3XL

Atomic co-ordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$ x 10^3) for NAL3XL. U(eq) is defined as one third of the trace of the orthogonalised Uij tensor.

	x	y	z	U(eq)
C(1)	1667(7)	842(5)	5813(5)	53(2)
C(2)	1509(6)	110(4)	6993(5)	44(1)
N(1)	1313(4)	633(3)	8360(3)	35(1)
C(3)	2529(5)	755(3)	9427(5)	36(1)
C(4)	2457(5)	1211(3)	10720(4)	34(1)
C(5)	1026(5)	1555(3)	11034(4)	36(1)
C(6)	-254(5)	1447(3)	9863(4)	34(1)
C(7)	-1714(6)	1797(4)	9978(6)	47(1)
C(8)	-2874(6)	1690(4)	8843(6)	49(1)
C(9)	-2609(5)	1231(3)	7571(5)	40(1)
N(2)	-1242(4)	877(3)	7409(4)	37(1)
C(10)	-102(5)	1004(3)	8553(4)	33(1)
C(11)	-3879(7)	1102(6)	6293(7)	58(2)
O(1)	878(4)	1921(2)	12245(3)	47(1)
C(12)	3877(6)	1311(4)	11793(5)	47(1)
O(2)	3721(4)	1735(3)	13042(3)	57(1)
O(3)	5105(4)	1019(3)	11580(4)	63(1)

Anisotropic displacement parameters ($Å^2$ x 10^3) for NAL3XL. The anisotropic displacement factor exponent takes the form:
$-2\ pi^2\ [\ h^2\ a^{*2}\ U11 + ... + 2\ h\ k\ a^*\ b^*\ U12\ ]$

	U11	U22	U33	U23	U13	U12
C(1)	46(3)	73(4)	40(3)	-8(3)	9(3)	7(3)
C(2)	36(3)	49(3)	45(3)	-10(2)	4(2)	7(3)
N(1)	27(2)	41(2)	36(2)	-2(2)	4(2)	7(2)
C(3)	25(3)	42(3)	39(2)	5(2)	2(2)	1(2)
C(4)	28(3)	39(2)	33(2)	6(2)	0(2)	0(2)
C(5)	36(3)	36(2)	35(2)	4(2)	6(2)	0(2)
C(6)	33(3)	32(2)	38(2)	1(2)	7(2)	4(2)
C(7)	42(3)	52(3)	48(3)	-7(2)	5(3)	10(3)
C(8)	23(3)	60(3)	65(3)	0(3)	13(3)	15(3)
C(9)	27(3)	36(3)	55(3)	4(2)	2(2)	0(2)
N(2)	27(2)	41(2)	43(2)	1(2)	1(2)	3(2)
C(10)	26(2)	31(2)	42(2)	5(2)	8(2)	3(2)
C(11)	36(3)	64(4)	67(4)	0(3)	-15(3)	7(3)
O(1)	43(2)	60(2)	37(2)	-1(2)	5(2)	8(2)
C(12)	35(3)	59(3)	44(3)	5(2)	-1(2)	0(3)
O(2)	42(2)	80(3)	46(2)	-12(2)	-2(2)	0(2)
O(3)	30(2)	91(3)	63(2)	-7(2)	-5(2)	10(2)

Hydrogen co-ordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) for NAL3XL.

	x	y	z	U(eq)
H(1)	1877(59)	501(39)	4917(53)	82(18)
H(2)	2583(69)	1309(39)	6120(56)	90(20)
H(3)	755(58)	1203(35)	5531(46)	60(16)
H(4)	2431(52)	-361(33)	7233(41)	48(13)
H(5)	719(55)	-361(36)	6715(47)	61(16)
H(6)	3486(51)	407(32)	9249(41)	52(14)
H(7)	-1814(46)	2082(29)	10823(43)	36(12)
H(8)	-3841(47)	1920(30)	8930(39)	38(12)
H(9)	-4502(61)	1710(37)	6252(50)	71(17)
H(10)	-4311(67)	462(45)	6190(57)	87(21)
H(11)	-3549(65)	1145(41)	5325(62)	95(21)
H(12)	2632(70)	1875(45)	13111(58)	98(21)

A3.0 STRUCTURE FACTOR TABLES

A3.1 ALP2XL

h	k	l	F_c^2	F_o^2	σF_o^2
-1	2	0	6037.18	3512.48	4074.76
0	2	0	704.5	351.51	34.9
-2	3	0	18446.92	16061.99	1776.68
-1	3	0	450.36	538.27	179.58
0	3	0	597.97	742.73	85.22
-3	4	0	3782.28	4301.86	274.17
-2	4	0	148.65	144.12	36.21
-1	4	0	1122.2	1075.21	437.67
0	4	0	6206.84	6078.87	774.36
-4	5	0	1616.76	1786.58	76.52
-3	5	0	789.46	640.12	62.92
-2	5	0	9678.42	7463.89	2415.08
-1	5	0	42.54	54.1	12.06
0	5	0	1312.47	1161.05	101.53
-5	6	0	10.91	48.48	20.77
-4	6	0	1112.74	1075.26	45.46
-3	6	0	991.92	1056.76	216.34
-2	6	0	1767.93	1355.84	379.6
-1	6	0	1260.51	786.76	213.41
0	6	0	3051.84	2599.26	155.19
-6	7	0	20.48	39.83	11.92
-5	7	0	6882.41	6702.21	393.81
-4	7	0	2276.77	2058.01	116.14
-3	7	0	303.57	293.25	30.43
-2	7	0	82.71	121.67	18.99
-1	7	0	2642.96	2378.95	381.04
0	7	0	83.4	83.99	6.85
-7	8	0	2635.78	2555.27	89.19
-6	8	0	2579.8	2763.38	129.15
-5	8	0	1622.48	1676.51	114.92
-4	8	0	401.22	357.49	31.44
-3	8	0	1525.11	1466.44	255.77
-2	8	0	1050.19	1050.89	186.36
-1	8	0	46.26	40.48	5.8
0	8	0	294.13	367.64	18.9
-8	9	0	119.64	118.49	3.54
-7	9	0	1535.7	1644.63	73.69
-6	9	0	7558.61	7662.67	441.11
-5	9	0	311.14	283.49	24.83
-4	9	0	40.09	19.58	6.7
-3	9	0	14.38	1.59	5.94
-2	9	0	506.34	527.07	62.48
-2	9	0	506.34	527.07	62.48
-1	9	0	0.58	-2.54	5.95
0	9	0	0.25	-0.24	6.62
-9	10	0	1018.87	984.9	41.24
-8	10	0	1258.25	1194.23	47.85
-7	10	0	12.46	3.13	3.55
-6	10	0	12.81	6.27	4.49
-5	10	0	464.15	614.5	68.47
-4	10	0	59.71	49.61	7
-3	10	0	138.66	122.97	12.9
-2	10	0	235.23	181.4	23.15
-1	10	0	118.87	101.94	15.46
0	10	0	486.84	494.72	36.06
-10	11	0	73.53	60.26	5.1
-9	11	0	205.66	189.74	6.07
-8	11	0	188.46	173.32	13.36
-7	11	0	6.95	2.9	3.47
-6	11	0	234.21	189.63	21.83
-5	11	0	255.36	295.66	39.35
-4	11	0	707.14	661.39	114.23
-3	11	0	2287.38	2051.02	248.79
-2	11	0	162.76	148.57	13.88
-1	11	0	0.51	-10.51	7.27
0	11	0	58.32	47.06	4.15
-11	12	0	2.13	3.19	7.37
-10	12	0	202.73	233.7	7.25
-9	12	0	691.21	656.39	14.77
-8	12	0	8.91	11.91	4.31
-7	12	0	388.85	376.65	48.27
-6	12	0	105.18	99.6	6.96
-5	12	0	245.98	218.28	28.1
-4	12	0	248.14	203.98	29.91
-3	12	0	344.41	293.44	24.02
-2	12	0	7.72	10.28	3.2
-1	12	0	7.68	11.48	3.05
0	12	0	46.24	40.87	2.4
-12	13	0	111.16	99.67	8.17
-11	13	0	104.31	121.36	5.18
-10	13	0	0.38	-4.1	7.47
-9	13	0	606.28	596.97	18.14
-8	13	0	65.57	67.96	9.88
-7	13	0	4.05	9.06	7.2
-6	13	0	114.46	115.29	8.75
-5	13	0	3.88	3.02	3.07
-4	13	0	74.88	75.13	8.42
-3	13	0	1.7	-0.94	4.35
-2	13	0	82.03	88.91	7.05
-1	13	0	396.58	355.6	27.83
0	13	0	13.96	19.42	2.79
-13	14	0	42.83	47.75	4.01
-12	14	0	74.71	53.41	3.08
-11	14	0	11.51	9.2	4.36
-10	14	0	215.64	200.47	6.4
-9	14	0	79.5	90.93	5.69
-8	14	0	10.54	-9.87	7.77
-7	14	0	1.2	-3.26	4.82
-6	14	0	1.38	-5.63	4.24
-5	14	0	47.87	43.9	9.8
-4	14	0	114.68	113.87	14.9
-3	14	0	181.95	145.35	14.37
-2	14	0	261.68	231.02	21.62
-1	14	0	4.27	-0.71	4.68
0	14	0	20.21	19.88	3.15
-14	15	0	3.27	-0.77	8.74
-13	15	0	57.55	37.58	3.32
-12	15	0	7.32	17.05	3.59
-11	15	0	54.26	56.61	5.02
-10	15	0	120.6	113.73	6.61
-9	15	0	118.05	95.1	4.27
-8	15	0	0.02	1.4	4.28
-7	15	0	59.39	66.26	11.58
-6	15	0	107.77	95.5	26.09
-5	15	0	1.09	12.19	3.55
-4	15	0	210.68	193.55	20.36
-3	15	0	204.61	180.94	12.3
-2	15	0	45.77	37.46	3.38
-1	15	0	120.39	138.75	12.25
0	15	0	68.31	60.3	8.29
-15	16	0	0.33	7.29	5.43
-14	16	0	25.98	28.32	3.49
-13	16	0	46.07	37.74	3.53
-12	16	0	1.3	4.1	5.01
-11	16	0	49.01	45.04	7.79
-10	16	0	39.66	28.77	8.48
-9	16	0	0.82	4.44	8.69
-8	16	0	1.11	3.35	6.51
-7	16	0	142.97	143.47	31.27
-6	16	0	9.28	12.38	8.05
-5	16	0	7.61	7.03	7.86
-4	16	0	23.37	21.54	4.64
-3	16	0	1.7	2.77	3.89
-2	16	0	1.34	-2.59	9.32
-1	16	0	51.21	48.01	6.8
-14	17	0	3.2	7.19	5.45
-13	17	0	0	-1.85	7.43
-12	17	0	11.01	12.86	9.29
-11	17	0	64.54	61.1	8.04
-10	17	0	0.13	-8.18	9.13
-9	17	0	37.77	31.64	3.66
-8	17	0	18.51	18.04	8.94
-7	17	0	0.82	6.16	9.22
-6	17	0	10.17	-1.56	9.11
-5	17	0	3.49	-6.72	9.23
-4	17	0	19.78	16.53	4.07
-3	17	0	0.2	-13.18	9.59
-12	18	0	18.14	22.44	5.8
-11	18	0	0.26	3.54	8.92
-10	18	0	3.13	0.6	5.36
-9	18	0	0.38	-11.29	9.84
-8	18	0	111.66	104.26	13.56
-7	18	0	1.79	12.39	5.54
-6	18	0	10.45	5.1	9.73
-1	2	1	1678.04	2002.72	34.35
0	2	1	9117.61	7302.52	118.98
-2	3	1	13850.35	15460.34	413.12
-1	3	1	5.09	6.12	2.41
0	3	1	16694.95	18495.66	808.66
-3	4	1	19457.22	20598.33	442.24
-2	4	1	13931.98	11866.69	615.45
-1	4	1	1420.29	1198.1	251.34
0	4	1	223.6	242.96	12.14
-4	5	1	544.39	533.37	8.51
-3	5	1	679.53	503.62	24.37
-2	5	1	1864.94	1882.14	131.43
-1	5	1	506.16	515.71	93.49
0	5	1	842.5	539.53	32.55
-5	6	1	5624.35	5886.65	178.9
-4	6	1	1899.88	1888.31	57.11
-3	6	1	13.56	12.24	1.52
-2	6	1	140.8	175.53	14.55
-1	6	1	3354.15	2641.06	514.03
0	6	1	913.76	776.07	20.05
-6	7	1	1593.18	1631.17	37.96
-5	7	1	3862.22	3843.04	154.01
-4	7	1	182.06	142.54	4.42
-3	7	1	3483.27	3456.45	190.85
-2	7	1	228.96	187.47	9.03
-1	7	1	36.94	48.17	4.73
0	7	1	1637.7	1743.83	76.23
-7	8	1	124.75	130.19	8.84
-6	8	1	2043.37	1845.2	46.09
-5	8	1	583.72	564.24	26.1
-4	8	1	1533.32	1416.77	61.35
-3	8	1	7.36	-1.28	5.01
-2	8	1	43.12	58.62	5.2
-1	8	1	21.33	11.38	3.72
0	8	1	10.63	8.6	2.17
-8	9	1	7.8	4.78	5.98
-7	9	1	1.79	7.12	6.06
-6	9	1	6642.61	6945.38	266.04
-5	9	1	199.07	176.19	13.75
-4	9	1	29.81	29.36	2.18
-3	9	1	0.68	2.59	2.24
-2	9	1	153.75	162	18.19
-1	9	1	2.21	3.28	5.98
0	9	1	657.62	668.28	32.07
-9	10	1	749.93	732.64	23.96
-8	10	1	107.57	99.7	3.05
-7	10	1	825.2	816.14	34.27
-6	10	1	51.2	35.97	2.23
-5	10	1	87.12	74.74	3.44
-4	10	1	20.06	16.8	4.28
-3	10	1	23.67	43.49	5.37
-2	10	1	14.11	15.65	3.06
-1	10	1	21.35	20.62	8.12
0	10	1	122.65	105.22	6.53
-10	11	1	97.28	89.62	3.03
-9	11	1	0.02	4.22	7.07
-8	11	1	2	-3.8	6.68
-7	11	1	123.13	115.49	10.42
-6	11	1	418.62	428.66	29.06
-5	11	1	153.05	114.54	21.7
-4	11	1	0.16	3.84	3.69
-3	11	1	10.57	10.01	3.79
-2	11	1	484.87	474.38	26.83
-1	11	1	0.58	3.84	5.11
0	11	1	70.53	54.9	2.34
-11	12	1	9.44	6.78	4.33
-10	12	1	2.09	4.75	4.74
-9	12	1	162.12	164.16	5.14
-8	12	1	838.43	814.8	39.36
-7	12	1	75.16	81.74	6.23
-6	12	1	60.98	72.35	6.71
-5	12	1	75.33	78.65	6.77
-4	12	1	33.29	43.54	4.71
-3	12	1	21.47	11.59	4.18
-2	12	1	13.91	11.46	5.66
-1	12	1	0.7	-0.35	4.15
0	12	1	3.51	2.45	3.74
-12	13	1	1.5	-1.08	4.18
-11	13	1	157.51	144.39	4.4
-10	13	1	10.69	3.11	7.35
-9	13	1	10.57	14.37	8.7
-8	13	1	389.77	377.5	13.41
-7	13	1	105.59	89.37	8.28
-6	13	1	7.14	4.16	3.06
-5	13	1	3.25	3.54	3.91
-4	13	1	418.05	353.36	29.56

h	k	l	F_c^2	F_o^2	σF_o^2
-3	13	1	122.89	113.81	4.34
-2	13	1	0.12	-0.21	9.16
-1	13	1	36.44	44.03	2.94
0	13	1	4.31	5.06	4.66
-13	14	1	4.72	-2.45	8.37
-12	14	1	17.47	14.49	6.85
-11	14	1	310.86	301.68	17.67
-10	14	1	0.19	-2.76	7.92
-9	14	1	6.92	-2.34	7.74
-8	14	1	15.88	19.74	3.94
-7	14	1	14.93	-6.78	7.99
-6	14	1	74.84	90.93	9.61
-5	14	1	148	106.45	21.35
-4	14	1	9.32	-4.26	5.18
-3	14	1	117.66	106.64	5.42
-2	14	1	13.02	-4.26	12.34
-1	14	1	41.95	26.99	9.89
0	14	1	98.24	101.68	5.76
-14	15	1	0.01	2.49	8.92
-13	15	1	6.92	6.63	8.86
-12	15	1	106.24	88.65	3.73
-11	15	1	5.88	5.92	6.32
-10	15	1	8.2	10.05	8.06
-9	15	1	1.41	-15.04	8.26
-8	15	1	62.88	54.79	6.43
-7	15	1	0.17	-2.14	4.3
-6	15	1	74.74	64.87	20.88
-5	15	1	224.95	159.54	30.09
-4	15	1	0.4	11.05	8.25
-3	15	1	13.48	1.05	8.67
-2	15	1	5.79	-0.5	8.83
-1	15	1	6.21	1.4	9.05
0	15	1	10.73	-10.07	11.26
-15	16	1	28.57	36.12	3.99
-14	16	1	13	12.68	4.09
-13	16	1	83.57	66.64	5.25
-12	16	1	97.87	80.68	4.56
-11	16	1	62.27	61.9	6.8
-10	16	1	92.27	86.56	3.54
-9	16	1	0.02	-8	8.6
-8	16	1	131.71	127.42	23.61
-7	16	1	9.19	11.64	3.2
-6	16	1	1.11	-16.51	8.83
-5	16	1	28.24	31.56	9.18
-4	16	1	0.26	1.14	5.02
-3	16	1	13.61	28.84	6.52
-2	16	1	0.85	-4.95	9.41
-1	16	1	25.44	24.8	7.38
-14	17	1	8.91	-11.37	9.9
-13	17	1	13.96	9.94	3.47
-12	17	1	69.44	77.43	4.3
-11	17	1	19.49	23.74	6.45
-10	17	1	28	22.1	11.36
-9	17	1	21.16	14.55	5.23
-8	17	1	2.16	-3.62	9.29
-7	17	1	64.16	70.53	10.63
-6	17	1	3.68	5.16	9.17
-5	17	1	0.65	5.32	9.15
-4	17	1	0.06	1.4	9.35
-3	17	1	12.38	18.45	7.8
-12	18	1	1.22	3.88	4.13
-11	18	1	51.89	51.91	10.04
-10	18	1	9.28	17.47	4.2
-9	18	1	24.14	18.12	11.6
-8	18	1	1.84	1.75	7.81
-7	18	1	0.03	-5.2	5.4
-6	18	1	4.5	-16.83	12.69
0	0	2	45822.93	43674.58	891.29
0	1	2	407.94	820.92	12.38
-1	2	2	1597.8	1276.47	15.69
0	2	2	7820.02	8015.77	90.54
-2	3	2	5407.14	4876.05	57.24
-1	3	2	22409.36	27102.78	690.04
0	3	2	3902.84	3865.1	39.58
-3	4	2	7784.52	9099.67	117.25
-2	4	2	3833.29	3488.73	41.5
-1	4	2	8734.9	9136.94	446.71
0	4	2	1681.05	2000.34	33.56
-4	5	2	559.65	566.4	8.85
-3	5	2	1733.64	1683.01	25.62
-2	5	2	1934.15	2050.18	38.59
-1	5	2	5.05	3.48	4.32
0	5	2	1.67	-5.09	3.76
-5	6	2	4375.61	4591.16	80.44
-4	6	2	93.16	102.79	3.11
-3	6	2	312.94	386.01	11.65
-2	6	2	530.13	521.68	19.85
-1	6	2	383.24	333.81	22.43
0	6	2	119.49	91.17	3.25
-6	7	2	914.02	988.49	16.05
-5	7	2	379.94	340.63	7.36
-4	7	2	99.42	143.32	18.14
-3	7	2	642.45	761.23	21.25
-2	7	2	389.33	307.65	11.16
-1	7	2	217.29	236.49	17.19
0	7	2	23.37	30.19	1.57
-7	8	2	931.17	868.66	15.09
-6	8	2	1254.44	1380.86	37.89
-5	8	2	345.83	363.17	7.84
-4	8	2	0.4	-2.62	3.72

h	k	l	F_c^2	F_o^2	σF_o^2
-3	8	2	103.61	114.77	3.93
-2	8	2	48.21	61.63	1.96
-1	8	2	573.6	543.71	27.95
0	8	2	37.85	33.2	1.75
-8	9	2	155.92	191.25	6.01
-7	9	2	236.99	238.79	7.02
-6	9	2	266.44	269.15	11.98
-5	9	2	306.45	303.1	11.61
-4	9	2	31.42	41.08	2.05
-3	9	2	107.54	111.86	5.72
-2	9	2	10.99	6.47	2.95
-1	9	2	44.98	40.73	3.18
0	9	2	418.62	416.44	15.37
-9	10	2	262.05	260.21	7.83
-8	10	2	125.86	94.76	2.91
-7	10	2	51.42	47.93	3.76
-6	10	2	59.55	57.52	3.27
-5	10	2	4.49	12.97	3.15
-4	10	2	168.51	171.34	8.92
-3	10	2	5.22	-0.7	6.08
-2	10	2	10.49	18.45	3.13
-1	10	2	16.62	16.05	2.31
0	10	2	72.59	78.73	2.4
-10	11	2	7.82	6.96	2.5
-9	11	2	325.34	314.87	9.12
-8	11	2	415.18	431.08	17.24
-7	11	2	35.02	27.71	2.73
-6	11	2	3.3	2.59	3.44
-5	11	2	120.54	119.46	12.17
-4	11	2	9.05	14.82	4.55
-3	11	2	78.04	75.1	4.76
-2	11	2	79.69	77.63	2.8
-1	11	2	8.48	18.73	2.55
0	11	2	92.89	97.42	7.26
-11	12	2	4.63	-5.55	7.43
-10	12	2	212.14	221.3	6.9
-9	12	2	39.19	41.11	3.54
-8	12	2	0.01	-6.14	7.92
-7	12	2	59.51	67.63	2.75
-6	12	2	0.88	-4.81	6.96
-5	12	2	57.6	51.03	4.9
-4	12	2	7.35	11.42	3.14
-3	12	2	37.76	34.81	2.72
-2	12	2	357.84	380.01	14.03
-1	12	2	8.93	10.53	4.74
0	12	2	80.19	84.84	5.17
-12	13	2	12.96	12.41	2.77
-11	13	2	24.02	18.94	3.32
-10	13	2	44.27	45.94	2.78
-9	13	2	311.39	312.31	9.58
-8	13	2	0.86	-1.75	4.32
-7	13	2	117.64	113.72	4.49
-6	13	2	32.62	21.71	2.64
-5	13	2	78.66	60.69	9.54
-4	13	2	2.35	-1.76	9
-3	13	2	7.81	7.84	4.79
-2	13	2	11.23	14.8	3.86
-1	13	2	77.15	67.41	5.55
0	13	2	1.1	-0.39	4.07
-13	14	2	2.36	-5.1	6
-12	14	2	9.38	7.78	5.88
-11	14	2	7.19	11.19	4.28
-10	14	2	173.55	166.04	5.04
-9	14	2	24.59	29.81	3.07
-8	14	2	42.51	40.64	3.22
-7	14	2	11.2	11.91	4.13
-6	14	2	99.16	94.42	3.12
-5	14	2	88.07	73.69	8.41
-4	14	2	6.09	1.03	7.73
-3	14	2	3.98	2.92	7.92
-2	14	2	4.21	8.34	7.99
-1	14	2	0.24	-2.91	9.99
0	14	2	4.74	-1.09	5.29
-14	15	2	3.37	-8.35	11.38
-13	15	2	18.58	15.1	6.59
-12	15	2	4.21	3.51	8.63
-11	15	2	49.82	51.46	3.06
-10	15	2	12.84	16.86	3.47
-9	15	2	124.94	123.32	3.99
-8	15	2	3.61	-2.28	4.48
-7	15	2	7.17	5.74	7.7
-6	15	2	10.23	6.84	3.38
-5	15	2	27.46	19.21	4.28
-4	15	2	57.52	66.4	3.16
-3	15	2	27.22	22.69	3.76
-2	15	2	23.1	19.34	3.93
-1	15	2	2.62	-19.27	9.26
0	15	2	13.12	9.05	4.97
-15	16	2	2.57	3.57	6.49
-14	16	2	1.42	-5.86	10.74
-13	16	2	21.12	7.59	9.3
-12	16	2	1.57	-3.53	9
-11	16	2	22.26	29.78	3.67
-10	16	2	24.04	18.76	6.26
-9	16	2	3.8	9.32	4.71
-8	16	2	6.23	-1.5	8.72
-7	16	2	0.15	0.17	8.65
-6	16	2	4	-7.91	8.85
-5	16	2	39	32.47	5.84
-4	16	2	0.6	-2.36	12.64

h	k	l	F_c^2	F_o^2	σF_o^2
-3	16	2	10.48	15.93	3.94
-2	16	2	12.42	10.56	4.18
-1	16	2	0.03	-3.33	5.61
-14	17	2	1.69	-3.97	9.59
-13	17	2	5.79	6.24	5.16
-12	17	2	0.33	-4.5	9.18
-11	17	2	32.85	26.21	4.01
-10	17	2	2.58	2.95	7
-9	17	2	0	-2.75	6.43
-8	17	2	0.01	-3.01	4
-7	17	2	10.82	12.61	9.29
-6	17	2	0.33	1.22	9.12
-5	17	2	5.22	-7.74	9.24
-4	17	2	1.65	-3.51	9.24
-3	17	2	14.56	13.75	4.74
-12	18	2	4.55	-13.76	9.89
-11	18	2	1.01	-4.85	9.76
-10	18	2	6.24	2.26	6.1
-9	18	2	3.14	1.33	9.84
-8	18	2	0.39	6.24	5.32
-7	18	2	0.81	7.92	9.61
-6	18	2	0	5.32	11.86
0	1	3	2942.74	2823.98	143.37
-1	2	3	9196.71	8467.76	110.92
0	2	3	21101.94	22118.29	278.61
-2	3	3	10.98	8	2.23
-1	3	3	1047	1275.15	16.11
0	3	3	455.88	348.43	5.6
-3	4	3	17822.92	19640.13	247.95
-2	4	3	268.72	162.79	10.37
-1	4	3	73.89	59.86	9.87
0	4	3	1608.3	1634.67	17.75
-4	5	3	861.59	907.05	12.52
-3	5	3	4610.39	4675.88	55.46
-2	5	3	7.84	-1.53	4.32
-1	5	3	97.98	76.59	2.35
0	5	3	566.85	534.36	7.47
-5	8	3	13.99	15.35	3.83
-4	6	3	239.37	267.01	6.26
-3	6	3	239.59	258.72	6.05
-2	6	3	155.17	215.42	12.84
-1	6	3	90.5	97.38	3.33
0	6	3	166.39	169.37	4.58
-6	7	3	211.67	226.16	7.7
-5	7	3	441.69	534.14	12.74
-4	7	3	110.13	116.22	3.69
-3	7	3	806.15	778.24	22.59
-2	7	3	23.67	31.61	1.73
-1	7	3	309.42	339.46	7.33
0	7	3	1007.67	1104.45	27.08
-7	8	3	144.89	155.09	4.72
-6	8	3	579.12	558.98	9.8
-5	8	3	371.14	398.51	17.59
-4	8	3	1261.35	1327.07	17.95
-3	8	3	445.33	463.89	12.71
-2	8	3	0.3	-2.15	2.76
-1	8	3	280.75	288.79	8.42
0	8	3	3.16	3.87	3.8
-8	9	3	285.61	286.64	16.32
-7	9	3	130.77	106.33	4.09
-6	9	3	568.11	604.4	13.06
-5	9	3	83.51	70.81	2.93
-4	9	3	16.21	23.84	1.96
-3	9	3	105.79	84.94	2.67
-2	9	3	6.88	-1.35	5.73
-1	9	3	139.31	148.02	4.36
0	9	3	35.31	43.69	3.26
-9	10	3	5.95	-1.62	6.54
-8	10	3	1.39	-5.63	3.31
-7	10	3	1.65	-7.75	6.08
-6	10	3	39.64	30.06	6.23
-5	10	3	25.78	24.88	4.15
-4	10	3	16.44	19.74	2.13
-3	10	3	443.97	428.23	14.49
-2	10	3	0.26	3.98	6.3
-1	10	3	24.9	30.93	3.5
0	10	3	65.04	71.87	2.75
-10	11	3	123.74	116.81	4.3
-9	11	3	0.32	3.85	3.54
-8	11	3	58.05	69.64	2.62
-7	11	3	48.07	51.05	2.4
-6	11	3	81.28	78.46	3.65
-5	11	3	154.11	145.54	11.17
-4	11	3	267.42	252.98	7.64
-3	11	3	9.07	7.78	5.35
-2	11	3	91.43	94.09	4.42
-1	11	3	242.14	230.11	15.8
0	11	3	213.01	225.74	10.98
-11	12	3	1.48	5.96	4.12
-10	12	3	20.21	19.68	2.59
-9	12	3	0.83	-14.26	7.1
-8	12	3	10.93	9.11	3.67
-7	12	3	37.39	30.83	6.29
-6	12	3	3.39	10.31	8.32
-5	12	3	504.92	502.46	41.62
-4	12	3	507.07	496.44	16.32
-3	12	3	1.91	3.6	3.16
-2	12	3	184.32	159.36	8.02
-1	12	3	46.14	50.4	2.81
0	12	3	59.68	52.16	2.48

h	k	l	F_c^2	F_o^2	σF_o^2
-12	13	3	5.21	4.3	7.17
-11	13	3	8.03	8.3	4.67
-10	13	3	0.03	-7.56	7.51
-9	13	3	1.69	0.87	5.13
-8	13	3	22.31	15.87	8.73
-7	13	3	31.26	22.7	2.65
-6	13	3	0.11	-4.35	6.59
-5	13	3	44.18	34.23	3.23
-4	13	3	38.47	39.44	2.79
-3	13	3	26.61	18.66	5.62
-2	13	3	105.19	86.24	3.82
-1	13	3	76.06	78.48	3.09
0	13	3	4.32	0.02	7.46
-13	14	3	54.93	56.13	13.57
-12	14	3	2.22	-13.62	8.13
-11	14	3	101.07	103.91	4.32
-10	14	3	9.57	14.29	4.4
-9	14	3	142.34	143.68	4.56
-8	14	3	0.04	-10.03	7.77
-7	14	3	104.71	94.27	4.21
-6	14	3	5.48	2.96	4.24
-5	14	3	2.25	5.25	4.29
-4	14	3	5.99	2.03	4.24
-3	14	3	2.78	1.04	6.36
-2	14	3	2.06	6.26	8.07
-1	14	3	43.5	46.28	4.6
0	14	3	5.09	-0.13	4.52
-14	15	3	0.08	-3.99	6.06
-13	15	3	6.65	2.77	10.2
-12	15	3	24.28	27.98	3.15
-11	15	3	29.7	20.19	2.93
-10	15	3	2.05	2.83	8.08
-9	15	3	5.54	10.04	4.27
-8	15	3	0.27	7.38	4.26
-7	15	3	32.07	29.02	5.55
-6	15	3	1.6	3.49	4.48
-5	15	3	4.45	2.8	8.07
-4	15	3	8.33	7.1	6.45
-3	15	3	18.55	24.01	5.27
-2	15	3	2.6	2.26	4.94
-1	15	3	4.51	3.42	8.91
0	15	3	0.52	2.19	4.84
-15	16	3	0.09	8.04	9.44
-14	16	3	6.02	-1.79	9.31
-13	16	3	9.1	4.75	5
-12	16	3	9.86	-6.33	9.09
-11	16	3	19.11	19.65	3.23
-10	16	3	2.56	3.44	4.91
-9	16	3	6.55	0.32	6.53
-8	16	3	20.03	19.92	5.12
-7	16	3	0.01	1.7	8.46
-6	16	3	70.98	60.59	9.09
-5	16	3	18.6	1.24	8.86
-4	16	3	1.46	1.01	7.68
-3	16	3	18.18	14.9	5.04
-2	16	3	9.07	14.89	5.31
-1	16	3	4.38	-17.24	10.32
-14	17	3	2.42	-4.66	9.57
-13	17	3	0.57	-5.16	7.71
-12	17	3	5.07	2.7	6
-11	17	3	0.9	-2.33	5.24
-10	17	3	1.9	-10	8.91
-9	17	3	3.74	2.68	4.77
-8	17	3	0.02	2.44	5.39
-7	17	3	9.67	8.74	9.13
-6	17	3	8.75	1.47	15.84
-5	17	3	3.97	5.79	9.25
-4	17	3	0.05	-7.61	9.33
-3	17	3	10.95	23.42	14.9
-11	18	3	2.67	-15.16	9.64
-10	18	3	0.18	0.31	9.67
-9	18	3	0.82	-11.94	9.72
-8	18	3	0.78	4.27	5.57
-7	18	3	27.73	27.49	9.25
0	0	4	628.43	827.83	18.94
0	1	4	1374.2	1283.3	113.39
-1	2	4	840.84	1187.67	16.23
0	2	4	270.65	313.06	38.56
-2	3	4	12750.68	13748	177.01
-1	3	4	1971.28	1610.74	20.02
0	3	4	4147.98	3698.51	38.09
-3	4	4	2.5	-5.57	4.35
-2	4	4	357.51	388.63	7.01
-1	4	4	4682.35	4776.88	56.53
0	4	4	1230.45	1154.37	13.14
-4	5	4	118.38	96.74	4.42
-3	5	4	528.64	532.08	8.6
-2	5	4	551.42	498.29	8.63
-1	5	4	3.15	28.26	10.01
0	5	4	956.85	1119.04	13
-5	6	4	60.06	76.96	2.45
-4	6	4	1937.24	2031.38	25.45
-3	6	4	43.57	54.33	1.87
-2	6	4	190.16	252.77	6.27
-1	6	4	403.18	413.96	7.79
0	6	4	454.1	510.8	7.69
-6	7	4	201.94	188.85	5.78
-5	7	4	319.68	322.44	7.18
-4	7	4	4.84	5.78	6.52
-3	7	4	850.85	848.45	12.49
-2	7	4	2016.48	1932.97	31
-1	7	4	332.7	362.73	7.68
0	7	4	969.95	957.96	12.13
-7	8	4	163.31	178.23	5.54
-6	8	4	8.48	8.44	4.48
-5	8	4	71.88	70.54	3.23
-4	8	4	345.72	352.47	9.79
-3	8	4	8.03	4.65	2.83
-2	8	4	363.14	316.79	9.78
-1	8	4	20.39	28.28	2.64
0	8	4	58.16	46.93	1.81
-8	9	4	15.82	4.62	4.93
-7	9	4	12.58	17.1	3.88
-6	9	4	84.86	71.42	2.41
-5	9	4	37.4	49.17	2.07
-4	9	4	22.84	23.14	3.68
-3	9	4	299.13	316.73	11.52
-2	9	4	14.1	17.99	9.93
-1	9	4	574.35	500.94	12.71
0	9	4	7.19	16.3	3.69
-9	10	4	20.2	17.73	3.21
-8	10	4	42.08	41.73	2.28
-7	10	4	97.45	117.07	3.81
-6	10	4	44.24	43.28	2.2
-5	10	4	34.67	33.79	2.19
-4	10	4	76.2	78.95	2.51
-3	10	4	197.46	201.45	7.89
-2	10	4	119.32	109.62	3.94
-1	10	4	93.96	99.13	3.58
0	10	4	1.13	-1.18	4.62
-10	11	4	0.14	-8.9	7.36
-9	11	4	2.88	-2.92	7.62
-8	11	4	2.47	-3.66	6.72
-7	11	4	34.21	41.84	2.44
-6	11	4	51.55	61.48	2.48
-5	11	4	253.72	247.14	9.54
-4	11	4	15.09	5.4	11.66
-3	11	4	42.71	39.02	2.6
-2	11	4	342.63	354.81	14.41
-1	11	4	1.03	7.29	3.97
0	11	4	145.32	146.34	3.78
-11	12	4	1.2	-6.58	4.1
-10	12	4	2.84	-0.01	6.44
-9	12	4	2.39	0.53	4.02
-8	12	4	6.73	-5.5	7.97
-7	12	4	5.1	1.42	7.13
-6	12	4	436.92	428.86	12.72
-5	12	4	1.97	5.83	4.34
-4	12	4	37.38	38.56	2.69
-3	12	4	204.5	216.56	11.91
-2	12	4	17.82	22.66	4.44
-1	12	4	14.81	16.33	5.29
0	12	4	83.79	75.89	2.58
-12	13	4	0.53	8.02	7.76
-11	13	4	64.51	60.75	3.07
-10	13	4	12.72	17.48	6.29
-9	13	4	4.15	1.92	7.71
-8	13	4	18.78	15.11	2.66
-7	13	4	9.07	2.02	7.51
-6	13	4	8.88	12.64	4.06
-5	13	4	32.5	39.17	2.75
-4	13	4	25.8	28.05	2.73
-3	13	4	10.32	9.38	3.27
-2	13	4	13.34	16.05	4.18
-1	13	4	2.08	-4.3	5.14
0	13	4	3.93	-2.26	6.85
-13	14	4	3.16	7.95	2.91
-12	14	4	5.98	6.9	4.31
-11	14	4	7.04	-2.44	8.19
-10	14	4	2.03	1.24	4.71
-9	14	4	36.86	22.75	6.04
-8	14	4	17.51	13.22	4.32
-7	14	4	83.48	83.41	4.11
-6	14	4	54.73	62.61	2.9
-5	14	4	33.14	30.74	3.8
-4	14	4	8.91	-3.66	7.95
-3	14	4	5.66	7.15	4.38
-2	14	4	0.1	12.09	4.55
-1	14	4	56	58.55	3.83
0	14	4	0.54	6.18	4.61
-14	15	4	6.35	-10.33	13.87
-13	15	4	4	3.43	8.78
-12	15	4	13.27	7.49	4.72
-11	15	4	0.01	-5.49	7.91
-10	15	4	19.4	14.65	10.95
-9	15	4	91.9	83.16	3.45
-8	15	4	5.11	-1.83	8.16
-7	15	4	33.59	30.68	2.91
-6	15	4	11.76	8.13	4.35
-5	15	4	0.69	-11.2	8.17
-4	15	4	16.78	24.58	3.85
-3	15	4	18.91	5.91	8.62
-2	15	4	4.57	-11.02	11.69
-1	15	4	1.39	2.69	4.97
0	15	4	24.78	26.57	3.02
-15	16	4	0.11	3.37	9.61
-14	16	4	0.19	-6.7	5.06
-13	16	4	7.75	7.48	8.9
-12	16	4	0.25	-1.07	4.9
-11	16	4	5.81	6.06	5.38
-10	16	4	2.84	2.02	8.67
-9	16	4	0.33	-0.2	8.41
-8	16	4	10.95	0.1	4.86
-7	16	4	3.6	7.14	8.53
-6	16	4	15.49	29.17	8.13
-5	16	4	2.83	-5.03	7.56
-4	16	4	1.24	-9.4	9.03
-3	16	4	10.13	14.73	3.37
-2	16	4	16.1	10.07	5.36
-1	16	4	6.56	3.39	5.44
-14	17	4	0.03	-1.59	11.83
-13	17	4	0.52	-21.53	9.53
-12	17	4	0.92	7.45	6.21
-11	17	4	1.16	-5.86	6.85
-10	17	4	1.09	-12.34	8.9
-9	17	4	0	1.31	9.11
-8	17	4	31.95	35.67	3.43
-7	17	4	0.53	-3.74	9.36
-6	17	4	1	-12.62	9.34
-5	17	4	25.15	30.93	5.4
-4	17	4	5.67	2.8	6.99
-3	17	4	10.37	-1.41	12.04
-11	18	4	0.06	10.09	9.53
-10	18	4	5.86	9.65	7.73
-9	18	4	0.87	-3.02	6.17
-8	18	4	7.21	-1.78	5.88
-7	18	4	14.02	7.18	10.49
0	1	5	2037.68	1338.63	167.28
-1	2	5	109.92	68.99	10.88
0	2	5	1389.78	997.53	315.11
-2	3	5	290.55	322.34	14.7
-1	3	5	5318.52	5506	64.86
0	3	5	262.99	216.86	6.32
-3	4	5	2594.54	2446.12	172.24
-2	4	5	5230.36	5025.44	62.05
-1	4	5	440.44	440.34	7.68
0	4	5	100.58	64.06	1.82
-4	5	5	171.26	201.42	5.66
-3	5	5	759.47	772.4	11.2
-2	5	5	1924.38	1915.45	23.97
-1	5	5	103.66	171.32	9.56
0	5	5	419.75	400.17	6.55
-5	6	5	19.64	25.91	1.7
-4	6	5	95.33	87.37	2.52
-3	6	5	570.65	585.51	9.56
-2	6	5	590.03	655.02	10.22
-1	6	5	2098.63	2234	27.95
0	6	5	12.88	10.7	2.37
-6	7	5	118.23	124.73	3.91
-5	7	5	256.25	253.26	9.69
-4	7	5	1.53	-8.5	4.85
-3	7	5	241.18	284.02	6.9
-2	7	5	160	132.44	3.85
-1	7	5	4.36	12.52	3.73
0	7	5	12.24	17.96	3.29
-7	8	5	46.58	63.78	2.12
-6	8	5	58.6	73.67	2.28
-5	8	5	52.5	69.4	2.06
-4	8	5	70.7	58.13	2.18
-3	8	5	40.06	45.55	2.28
-2	8	5	315.68	340.02	7.92
-1	8	5	62.38	60.93	2.15
0	8	5	44.3	41.81	2.37
-8	9	5	127.15	140.03	4.25
-7	9	5	165.4	148.32	7.23
-6	9	5	48.6	41.46	2.08
-5	9	5	84.85	86.71	3.66
-4	9	5	420.25	428.55	11.23
-3	9	5	82.56	116.29	3.38
-2	9	5	619.11	570.88	10.69
-1	9	5	223.59	253.26	8.89
0	9	5	35.63	42.1	2.03
-9	10	5	80.05	84.89	2.73
-8	10	5	8.17	2.66	6.31
-7	10	5	16.79	16.45	2.99
-6	10	5	198.96	225.98	7.37
-5	10	5	263.66	237.45	7.3
-4	10	5	46.6	43.45	2.34
-3	10	5	59.9	62.35	4.23
-2	10	5	139.58	144.44	4.18
-1	10	5	364.81	381.95	9.8
0	10	5	413.59	462.44	9.26
-10	11	5	178.68	157.65	5.92
-9	11	5	28.74	23.18	2.54
-8	11	5	170.39	171.45	6.78
-7	11	5	27.55	27.05	2.47
-6	11	5	274.28	246.36	7.37
-5	11	5	9.24	14.21	6.63
-4	11	5	0.09	3.12	3.99
-3	11	5	22.13	19.36	4.41
-2	11	5	115.51	109.41	4.72
-1	11	5	1.02	11.27	4.03
0	11	5	1.9	5.88	3.83
-11	12	5	16.05	12.39	2.73
-10	12	5	268.83	301.27	9.23
-9	12	5	11.81	10.62	6.67
-8	12	5	0.33	-3.99	7.36
-7	12	5	3.37	0.42	7.2
-6	12	5	270.1	260.78	11.99
-5	12	5	197.44	220.45	6.91

h	k	l	F_c^2	F_o^2	σF_o^2
-4	12	5	10.23	14.28	3.11
-3	12	5	0.44	-13.14	7.49
-2	12	5	0.49	5.25	2.64
-1	12	5	1.93	4.73	4.21
0	12	5	5.89	8.41	4
-12	13	5	66.44	74.25	3.14
-11	13	5	41.6	44.25	2.95
-10	13	5	18.29	22.03	3.38
-9	13	5	9.3	22.37	2.81
-8	13	5	276.32	298.79	8.94
-7	13	5	166.08	194.68	6.01
-6	13	5	220.89	224.25	6.88
-5	13	5	0.6	9.77	4
-4	13	5	0.05	-18.16	11.12
-3	13	5	92.4	82.08	4.41
-2	13	5	49.16	61.46	2.94
-1	13	5	0.06	-10.86	7.94
0	13	5	0.02	0.55	4
-13	14	5	30.61	30.82	3.14
-12	14	5	0.44	-2.97	11.77
-11	14	5	50.64	53.22	3.04
-10	14	5	1.06	7.06	8.13
-9	14	5	2.2	10.54	8.01
-8	14	5	6.96	13.45	5.1
-7	14	5	7.01	2.7	4.17
-6	14	5	2.76	3.12	4.13
-5	14	5	0.31	-1.02	3.26
-4	14	5	19.2	11.45	11.43
-3	14	5	0.56	-4.36	5.68
-2	14	5	108.37	107.65	4.2
-1	14	5	10.02	11.53	4.69
0	14	5	0.59	0.56	5.61
-14	15	5	4.37	-0.93	10.94
-13	15	5	8.31	2.97	3.75
-12	15	5	4.25	10.38	3.68
-11	15	5	40.12	23.26	4.95
-10	15	5	3.69	-2.19	8.11
-9	15	5	13.2	16.6	3.38
-8	15	5	3.01	2.16	6.74
-7	15	5	0.11	-3.21	4.39
-6	15	5	37.41	41.54	9
-5	15	5	13.9	1.03	8.41
-4	15	5	1.38	5.24	5.21
-3	15	5	6.79	6.92	4.73
-2	15	5	1.13	1.14	10.38
-1	15	5	1.06	6.69	5.11
0	15	5	3.71	-0.28	8.12
-15	16	5	0.16	-1.31	4.52
-14	16	5	7.86	7.17	5.34
-13	16	5	1.86	-2.85	5
-12	16	5	25.2	23.98	3.31
-11	16	5	5.81	0.53	4.78
-10	16	5	14.52	15.28	5.01
-9	16	5	0.78	-1.61	8.57
-8	16	5	30.72	34.02	3.21
-7	16	5	57.59	47.81	4.17
-6	16	5	0.01	-3.41	8.78
-5	16	5	16.38	18.8	3.71
-4	16	5	4.31	2.8	8.96
-3	16	5	0.11	-5.37	7.57
-2	16	5	4.06	4.27	4.25
-1	16	5	2.5	-2.66	9.8
-13	17	5	4.36	7.79	5.2
-12	17	5	0.03	-0.21	4.95
-11	17	5	1.29	0	9.19
-10	17	5	1.28	-5.49	10.58
-9	17	5	0.02	4.99	5.11
-8	17	5	23.03	28.25	3.44
-7	17	5	8.25	15.03	11.3
-6	17	5	1.64	-2.51	5.18
-5	17	5	8.44	2.1	9.65
-4	17	5	4.85	4.22	4.2
-10	18	5	1.6	13.76	5.96
-9	18	5	26.58	25.7	31.06
-8	18	5	2.7	1.1	17.05
0	0	6	4.86	13.9	2.58
0	1	6	1011.65	774.7	69.74
-1	2	6	33.68	37.53	8.86
0	2	6	3492.81	1717.48	914.48
-2	3	6	1305.63	1053.67	154.56
-1	3	6	227.34	313.5	6.47
0	3	6	13.29	13.75	3.88
-3	4	6	6080.58	4664.49	1170.54
-2	4	6	1107.41	937.3	33.48
-1	4	6	1800.17	1890.21	23.65
0	4	6	8391.75	7220.08	1159.99
-4	5	6	5.76	26.06	11.88
-3	5	6	5246.38	5508.66	65.36
-2	5	6	1679.53	1931.87	24.28
-1	5	6	329.65	401.94	7.73
0	5	6	1187.52	1317.32	15.18
-5	6	6	1161.68	1121.47	19.4
-4	6	6	1154.26	1193.69	16.26
-3	6	6	1747.45	1679.02	21.66
-2	6	6	535.34	536.89	9.17
-1	6	6	0.21	-1.3	4.01
0	6	6	5.46	-4.87	4.35
-6	7	6	667.87	727.22	11.6
-5	7	6	79.04	53.14	1.94
-4	7	6	625.51	614.54	10.25
-3	7	6	269.65	358.05	7.71
-2	7	6	1780.45	2025.46	25.91
-1	7	6	163.7	186.74	5.74
0	7	6	22.49	20.67	1.66
-7	8	6	81.1	89.91	2.92
-6	8	6	0.87	1.08	5.43
-5	8	6	267.36	317.36	7.68
-4	8	6	147.96	147.62	4.53
-3	8	6	316.22	313.09	7.65
-2	8	6	51.75	59.77	2.16
-1	8	6	29.1	32.67	2.11
0	8	6	216.89	211.41	5.79
-8	9	6	6.55	4.59	6.25
-7	9	6	7.22	8.75	5.46
-6	9	6	1.76	-4.31	5.88
-5	9	6	19.34	21.22	2.05
-4	9	6	0.96	-1.52	3.17
-3	9	6	306.6	312.37	13.51
-2	9	6	167.08	186.27	6.89
-1	9	6	42.1	41.92	2.56
0	9	6	2.45	-0.36	5.7
-9	10	6	118.71	122.07	3.95
-8	10	6	238.63	274.18	8.18
-7	10	6	330.42	345.77	11.22
-6	10	6	247.33	247.33	7.45
-5	10	6	88.88	97.64	3.05
-4	10	6	118.43	115.08	6.8
-3	10	6	520.44	497.62	10.83
-2	10	6	437.31	403.8	16.86
-1	10	6	5.79	-1.56	7.27
0	10	6	43.45	44.28	2.36
-10	11	6	122.03	142.76	4.36
-9	11	6	31.58	30.03	2.69
-8	11	6	187.51	173.51	5.36
-7	11	6	10.62	7.23	3.85
-6	11	6	400.49	396.57	12.24
-5	11	6	93.26	101.27	3.21
-4	11	6	1015.76	1121	17.52
-3	11	6	674.45	672.42	13.02
-2	11	6	349.27	353.39	17.16
-1	11	6	0.24	6.82	4.07
0	11	6	166	158.6	5.3
-11	12	6	13.99	8.77	3.38
-10	12	6	26.27	32.19	2.96
-9	12	6	136.32	130.56	3.66
-8	12	6	2.81	1.5	7.48
-7	12	6	92.01	74.29	2.92
-6	12	6	14.8	16.95	3.13
-5	12	6	104.46	98.55	3.05
-4	12	6	0.17	-1.36	4.78
-3	12	6	136.71	130.14	6.84
-2	12	6	9.67	11.58	3.21
-1	12	6	0.01	6.24	4.21
0	12	6	2.77	4.06	4.03
-12	13	6	3.15	-5.11	4.51
-11	13	6	21.09	23.75	6.73
-10	13	6	326.25	339.49	11.58
-9	13	6	428.11	436.64	11.48
-8	13	6	198.83	187.82	5.87
-7	13	6	357.39	378.2	12.51
-6	13	6	16.29	18.38	6.64
-5	13	6	19	10.35	5.78
-4	13	6	32.69	27.9	2.78
-3	13	6	24.1	25.27	2.81
-2	13	6	75.38	80.23	3.09
-1	13	6	21.88	26.85	10.3
0	13	6	80.75	84.8	2.77
-13	14	6	12.15	17.86	3.19
-12	14	6	0	-2.97	8.07
-11	14	6	0.05	-4.41	8.36
-10	14	6	32.85	35.31	3.02
-9	14	6	55.38	67.45	3.12
-8	14	6	83.95	86.47	5.12
-7	14	6	2.74	6.87	4.61
-6	14	6	0.78	2.04	8.31
-5	14	6	51.45	49.14	12.54
-4	14	6	76.48	88	3.16
-3	14	6	25.27	27.41	2.9
-2	14	6	63.9	65.65	3.21
-1	14	6	172.16	182.96	5.93
0	14	6	1.25	-4.31	7.6
-14	15	6	0.66	0.59	9.02
-13	15	6	0.1	-3.86	8.76
-12	15	6	0.31	-16.25	8.59
-11	15	6	5.04	2.29	5.14
-10	15	6	8.84	4.41	4.69
-9	15	6	20.32	20.38	4.41
-8	15	6	9.01	7.41	5.75
-7	15	6	1.63	-0.97	8.05
-6	15	6	51.61	46.92	7.38
-5	15	6	33.28	31.99	4.95
-4	15	6	68.92	81.79	3.75
-3	15	6	2.11	-8.03	8.73
-2	15	6	22.09	14.53	3.98
-1	15	6	71.51	60.48	7.28
0	15	6	18.77	10.62	6.33
-14	16	6	3.46	-5.29	5.41
-13	16	6	7.77	7.54	8.85
-12	16	6	3.21	6.58	8.73
-11	16	6	24.62	26.07	3.28
-10	16	6	7.76	7.82	3.81
-9	16	6	30.32	21.42	8.11
-8	16	6	19.6	12.81	4.6
-7	16	6	1.8	-10.68	9.21
-6	16	6	21.91	15.81	5.08
-5	16	6	16.07	4.74	7.89
-4	16	6	8.86	8.36	6.9
-3	16	6	15.2	14.53	5.43
-2	16	6	6.81	7.93	9.74
-13	17	6	0.13	-4.15	9.62
-12	17	6	1.24	-2.15	9.28
-11	17	6	8.62	3.09	9.28
-10	17	6	0.86	2.61	9.24
-9	17	6	3.72	4.14	9.32
-8	17	6	18.66	25.69	4.86
-7	17	6	40.12	43.89	5.73
-6	17	6	0.15	-7.48	9.63
-5	17	6	58.87	61.06	8.08
-4	17	6	0.82	2.82	5.01
0	1	7	623.55	569.71	40.89
-1	2	7	3471.69	1972.45	1002.37
0	2	7	405.14	318.96	66.05
-2	3	7	852.37	757.87	218.1
-1	3	7	2838.73	2761.15	168.41
0	3	7	189.66	114.13	36.85
-3	4	7	2522.53	1532.25	737.03
-2	4	7	189.48	254.09	36.17
-1	4	7	76.07	80.98	2.42
0	4	7	1313.3	1033.8	218.74
-4	5	7	1820.81	1964.8	24.9
-3	5	7	153.8	169.61	5.27
-2	5	7	164.78	199.2	5.93
-1	5	7	1479.74	1597.27	20.74
0	5	7	1297.93	1234.4	49.76
-5	6	7	687.59	734.06	11.52
-4	6	7	155.27	246.05	6.67
-3	6	7	2089.41	2112.76	26.72
-2	6	7	361.28	272.06	6.89
-1	6	7	80.12	71.41	3.14
0	6	7	161.46	160.01	4.18
-6	7	7	2.96	-2.27	5.35
-5	7	7	335.54	387.06	13.28
-4	7	7	109.24	152.12	4.61
-3	7	7	175.52	154.22	4.76
-2	7	7	27.61	33.52	1.99
-1	7	7	183.06	212.79	6.45
0	7	7	436.04	510.26	9.81
-7	8	7	0.16	-5.16	5.83
-6	8	7	278.39	282.62	13.82
-5	8	7	123.46	119.26	3.42
-4	8	7	484.22	487.73	9.74
-3	8	7	45.72	38.7	2.27
-2	8	7	34.86	31.56	2.14
-1	8	7	563.24	599.94	10.99
0	8	7	29.38	17.09	3.36
-8	9	7	48.59	47.66	2.36
-7	9	7	240.24	198.8	7.35
-6	9	7	43.05	53.05	2.27
-5	9	7	0.53	-0.39	3.27
-4	9	7	819.81	931.27	14.5
-3	9	7	157.9	156.49	6.99
-2	9	7	1792.11	1922.25	25.78
-1	9	7	382.78	376.21	14
0	9	7	3.65	2.27	5.8
-9	10	7	11.23	1.72	7.26
-8	10	7	99.34	109.66	3.11
-7	10	7	4.97	6.26	3.72
-6	10	7	169.77	194.48	6.04
-5	10	7	3.12	3.22	6.49
-4	10	7	183.6	168.03	5.14
-3	10	7	1323.85	1251.78	18.86
-2	10	7	829.12	891.66	15.13
-1	10	7	156.29	131.45	3.79
0	10	7	753.23	812.13	12.49
-10	11	7	175.45	182.62	6.01
-9	11	7	27.26	48.68	2.88
-8	11	7	987.47	1083.05	17.28
-7	11	7	29.3	27.88	4.27
-6	11	7	733.23	686.15	12.91
-5	11	7	10.4	12.7	3.06
-4	11	7	9.39	8.74	3.19
-3	11	7	16.49	0.41	8.05
-2	11	7	9.46	12.66	3.4
-1	11	7	115.44	110.8	3.48
0	11	7	110.51	109.35	3.02
-11	12	7	101.76	93.68	4.42
-10	12	7	1456.9	1461.11	22.19
-9	12	7	4.81	9.92	2.95
-8	12	7	1.01	1.72	4.33
-7	12	7	55.83	68.43	2.98
-6	12	7	20.2	14.23	7.68
-5	12	7	93.67	80.75	2.96
-4	12	7	25.62	35.23	4.22
-3	12	7	22.93	22.79	5.82
-2	12	7	168.63	152.41	4.88
-1	12	7	49.8	42.5	2.85
0	12	7	21.6	27.43	2.47
-12	13	7	120.13	113.28	3.68
-11	13	7	17.08	5.17	5.47
-10	13	7	74.92	72.46	4.64

h	k	l	F_c^2	F_o^2	σF_o^2
-9	13	7	16.62	30.04	4.39
-8	13	7	11.12	31.78	3.03
-7	13	7	767.26	802.03	23.45
-6	13	7	187.19	178.23	5.84
-5	13	7	3.84	0.44	7.72
-4	13	7	83.85	92.65	3.27
-3	13	7	32.42	24.72	3.41
-2	13	7	21.07	33.15	5.91
-1	13	7	132.31	126.06	5.09
0	13	7	21.39	23	8.21
-13	14	7	11	7.74	9.51
-12	14	7	6.27	12.17	4.78
-11	14	7	7.15	-3.35	8.24
-10	14	7	8.1	1.9	10.13
-9	14	7	13.57	4.51	7.81
-8	14	7	0.09	-7.48	8.17
-7	14	7	21.51	24.48	6.15
-6	14	7	57.75	67.89	3.02
-5	14	7	16.56	16.67	2.83
-4	14	7	0.64	-6.37	9.53
-3	14	7	1.74	-2.38	3.36
-2	14	7	90.8	100.68	3.55
-1	14	7	2.34	1.18	8.89
0	14	7	0.34	0.71	4.76
-14	15	7	1.69	4.52	5.06
-13	15	7	8.74	11.72	5.12
-12	15	7	0.2	2.41	8.73
-11	15	7	7.4	1.36	8.66
-10	15	7	10.22	12.43	4.74
-9	15	7	5.44	-3.98	8.53
-8	15	7	9.47	16.72	10.47
-7	15	7	30.85	40.5	3.19
-6	15	7	74.79	77.82	10.01
-5	15	7	12.24	8.02	8.66
-4	15	7	9.69	21.47	4.86
-3	15	7	12.87	12.18	3.79
-2	15	7	0.07	-8.91	8.97
-1	15	7	0.1	-6.34	9.39
0	15	7	4.22	0.98	8.34
-14	16	7	7.33	10.32	7.68
-13	16	7	0.76	-21.71	10.03
-12	16	7	0.71	6.23	5
-11	16	7	0	-4.03	6.11
-10	16	7	5.4	4.16	5.05
-9	16	7	23.32	27.26	3.31
-8	16	7	23.58	17.67	6.21
-7	16	7	50.56	51.37	3.46
-6	16	7	35.63	32.81	9.1
-5	16	7	37.5	45.31	3.46
-4	16	7	6.13	2.04	6.09
-3	16	7	23.35	32.47	6.06
-2	16	7	23.47	15.6	7.11
-12	17	7	19.19	21.08	4.21
-11	17	7	0.01	-4	9.35
-10	17	7	0.05	2.49	9.26
-9	17	7	0.06	8.49	5.15
-8	17	7	0.01	10.45	4.25
-7	17	7	6.47	9.53	5.37
-6	17	7	4.12	10.6	5.53
-5	17	7	0	-17.85	9.95
0	0	8	5122.74	4728.73	97.42
0	1	8	70.11	45.46	5.8
-1	2	8	23.77	23.41	8.99
0	2	8	121.42	104.54	20.06
-2	3	8	695.26	534.5	143.24
-1	3	8	255.1	269.68	10.3
0	3	8	4.72	2.15	1.96
-3	4	8	2578.42	1450.59	830.67
-2	4	8	68.5	72.24	11.3
-1	4	8	3302.2	3495.82	42.38
0	4	8	10.88	0.66	4.24
-4	5	8	563.72	524.64	14.45
-3	5	8	189.79	187.98	5.76
-2	5	8	37.77	35.52	1.85
-1	5	8	426.71	438.78	8.53
0	5	8	303.8	222.33	23.81
-5	6	8	58.4	53.4	2.04
-4	6	8	647.71	694.57	11.12
-3	6	8	7.01	4.07	2.79
-2	6	8	2.07	5.12	2.49
-1	6	8	1078.55	1249.33	17.37
0	6	8	65.5	58.45	1.98
-6	7	8	0.74	-4.4	5.7
-5	7	8	280.91	322.8	8.96
-4	7	8	662.78	701.17	11.46
-3	7	8	39.65	51.4	3.38
-2	7	8	1798.27	2115.68	27.29
-1	7	8	286.51	310.4	8.11
0	7	8	1.71	-0.31	4.8
-7	8	8	105.37	102.97	3.12
-6	8	8	242.26	272.4	11.28
-5	8	8	190.73	211.09	7.92
-4	8	8	52.07	52.54	2.21
-3	8	8	290.31	278.5	7.93
-2	8	8	2.02	3.8	3.3
-1	8	8	156.25	165.81	7.07
0	8	8	48.45	51.57	2.06
-8	9	8	4.04	11.52	3.66
-7	9	8	262.73	245.95	7.66
-6	9	8	126.94	137.68	4.12
-5	9	8	45.6	41.81	2.46
-4	9	8	125.79	115.6	5.03
-3	9	8	206.82	219.06	10.71
-2	9	8	3.62	8.96	4.17
-1	9	8	129.92	150.69	4.57
0	9	8	5.43	-8.59	8.51
-9	10	8	448.95	496.19	15.73
-8	10	8	120.53	135.49	5.49
-7	10	8	619.99	615.12	12.08
-6	10	8	250.82	253.75	7.64
-5	10	8	529.78	627.23	18
-4	10	8	5.62	11.89	4.83
-3	10	8	0.02	-5.3	7.5
-2	10	8	114.84	100.35	3.12
-1	10	8	116.66	117.19	3.71
0	10	8	23.61	11.31	5.7
-10	11	8	56.5	82.2	3.2
-9	11	8	3.18	-9.48	8.09
-8	11	8	12.2	5.14	5.5
-7	11	8	405.06	377.07	10.35
-6	11	8	171	160.42	8.21
-5	11	8	0.24	-16.53	8.57
-4	11	8	87.35	119.66	3.63
-3	11	8	946.56	1008.16	16.68
-2	11	8	23.47	19.62	2.75
-1	11	8	19.73	20.23	11.22
0	11	8	59.25	57.34	2.52
-11	12	8	30.92	44.43	2.97
-10	12	8	9.68	3.06	7.32
-9	12	8	56.46	73.88	3.16
-8	12	8	3.85	6.51	4.53
-7	12	8	120.79	112.89	5.85
-6	12	8	6.7	8.18	4.25
-5	12	8	45.43	43.55	2.82
-4	12	8	115.94	150.62	6.42
-3	12	8	8.36	8.77	4.37
-2	12	8	3.17	-5	7.6
-1	12	8	5.34	5.17	4.23
0	12	8	4.75	5.67	4.18
-12	13	8	12.16	4.79	5.85
-11	13	8	7.01	-9.19	8.3
-10	13	8	236.1	239.88	7.37
-9	13	8	536.31	580.09	13.19
-8	13	8	10.19	7.26	8.59
-7	13	8	133.54	152.13	4.82
-6	13	8	10.71	9.05	4.26
-5	13	8	17.29	16.88	3.27
-4	13	8	13.57	15.84	3.94
-3	13	8	35.47	35.29	2.84
-2	13	8	5.61	1.28	4.4
-1	13	8	21.94	30.98	2.96
0	13	8	81.42	86.6	3.03
-13	14	8	65.4	76.52	3.54
-12	14	8	12.68	3.31	8
-11	14	8	92.21	99.25	3.5
-10	14	8	5.62	-8.12	8.81
-9	14	8	1.6	2.42	5
-8	14	8	159.32	154.84	4.76
-7	14	8	0.57	-1.43	7.99
-6	14	8	28.8	32.41	5.66
-5	14	8	0.05	4.79	7.9
-4	14	8	26.68	33.26	2.93
-3	14	8	6.9	6.72	4.69
-2	14	8	60.65	60.11	3.41
-1	14	8	81.9	87.03	4.17
0	14	8	12.44	4.55	5.38
-14	15	8	0.01	-0.81	9.27
-13	15	8	14.83	15.81	7.33
-12	15	8	16.78	21.65	4.53
-11	15	8	16.14	19.22	3.23
-10	15	8	19.07	26.05	3.2
-9	15	8	71.52	90.05	5.98
-8	15	8	0.09	2.66	8.74
-7	15	8	15.93	15.93	5.66
-6	15	8	60.26	66.76	5.78
-5	15	8	24.53	23.14	6.25
-4	15	8	80.73	82.85	3.55
-3	15	8	31.39	26.94	3.42
-2	15	8	38.39	35.82	3.52
-1	15	8	18.88	21.89	4.91
0	15	8	8.43	4.54	5.52
-13	16	8	0.07	3.88	8.1
-12	16	8	0.79	6.08	5.08
-11	16	8	3.15	10.34	3.85
-10	16	8	26.22	14.25	12.05
-9	16	8	18.93	13.48	7.89
-8	16	8	25.18	30.97	3.39
-7	16	8	1.46	2.82	5.22
-6	16	8	1.86	-3.85	5.98
-5	16	8	0.07	-9.15	9.97
-4	16	8	17.54	25.56	9.43
-3	16	8	13.06	1.03	9.86
-11	17	8	16.98	4.32	7.28
-10	17	8	0.02	1.64	7.95
-9	17	8	16.05	16.17	4.21
-8	17	8	10.02	0.02	9.86
-7	17	8	62.21	71.78	3.85
-6	17	8	15.17	10.47	12.24
0	1	9	35.3	48.81	4.25
-1	2	9	383.57	196.45	116.17
0	2	9	0	-5.3	4.15
-2	3	9	602.34	389.67	149.2
-1	3	9	172.26	148.61	19.85
0	3	9	1095.97	759.42	310.76
-3	4	9	2017.59	1277	710.9
			F_c^2	F_o^2	σF_o^2
-2	4	9	534.25	412.73	141.02
-1	4	9	3.63	5.05	2.74
0	4	9	77.47	89.13	15.22
-4	5	9	773.45	792.17	12.24
-3	5	9	1068.59	1126.11	15.82
-2	5	9	688.96	649.43	10.69
-1	5	9	18.87	24	5.14
0	5	9	255.48	224.43	39.56
-5	6	9	2044.87	2011.38	36.76
-4	6	9	10.7	3.85	2.28
-3	6	9	66.68	73.4	2.63
-2	6	9	154.11	132.44	4.3
-1	6	9	4.57	13.85	6.26
0	6	9	162.07	176.83	9.17
-6	7	9	58.88	55.34	2.21
-5	7	9	251.01	257.48	7.58
-4	7	9	190.09	226.26	6.79
-3	7	9	588.89	622.58	11.41
-2	7	9	8.73	2.94	6.01
-1	7	9	527.51	560.8	10.66
0	7	9	17.02	17.34	2.09
-7	8	9	77.42	81.66	6.72
-6	8	9	140.38	136.21	3.91
-5	8	9	30.7	28.72	2.16
-4	8	9	104	96.55	3.28
-3	8	9	239.75	236.57	7.18
-2	8	9	56.68	54.86	2.35
-1	8	9	62.61	57.66	2.49
0	8	9	318.24	305.08	7.63
-8	9	9	59.07	54.73	2.65
-7	9	9	23.97	8.95	3.81
-6	9	9	255.88	273.95	8.33
-5	9	9	96.73	86.27	4.82
-4	9	9	2.9	-0.21	6.59
-3	9	9	21.77	30.59	2.39
-2	9	9	42.23	59.32	2.97
-1	9	9	0.23	-0.96	8.59
0	9	9	196.3	177.24	5.81
-9	10	9	14.01	8.15	8.79
-8	10	9	460.45	539.72	11.65
-7	10	9	11.71	20.58	2.61
-6	10	9	187.02	211.09	6.83
-5	10	9	0	0.87	3.89
-4	10	9	7.03	14.73	5.82
-3	10	9	0.83	7.52	8.24
-2	10	9	15.74	23.81	2.65
-1	10	9	8.25	14.22	4.14
0	10	9	664.74	733.69	12.09
-10	11	9	271.15	286.5	8.95
-9	11	9	3.24	6.37	7.86
-8	11	9	496.3	522.58	11.9
-7	11	9	0.89	-5.36	7.63
-6	11	9	174.22	191.59	5.9
-5	11	9	37.06	34.25	2.74
-4	11	9	66.16	63.07	2.87
-3	11	9	13.19	2.81	7.65
-2	11	9	58.57	53.06	2.86
-1	11	9	29.95	25.86	2.74
0	11	9	2.46	-1.9	6.67
-11	12	9	10.33	4.54	3.36
-10	12	9	240.02	246.77	7.27
-9	12	9	46.38	42.3	3.29
-8	12	9	133.27	137.25	4.57
-7	12	9	107.6	142	4.58
-6	12	9	45.29	58.55	2.89
-5	12	9	78.52	82.38	3.01
-4	12	9	4.14	6.37	4.74
-3	12	9	80.49	87.74	3.03
-2	12	9	25.14	19.22	4.98
-1	12	9	18.48	17.5	2.78
0	12	9	60.33	69.39	2.67
-12	13	9	0.88	-15.51	8.48
-11	13	9	79.88	74.18	4.71
-10	13	9	35.23	29.37	2.96
-9	13	9	96.13	85.68	3.25
-8	13	9	50.31	42.86	3.02
-7	13	9	102.23	104.42	3.34
-6	13	9	21.11	16.29	2.77
-5	13	9	16.49	19.59	5.65
-4	13	9	75.33	69.4	3.01
-3	13	9	22.13	14.59	3.36
-2	13	9	0.01	-0.61	7.82
-1	13	9	88.53	104.19	3.67
0	13	9	37.21	29.3	7.17
-13	14	9	19.33	20.34	7.44
-12	14	9	0.12	0.99	6.25
-11	14	9	10.24	11.15	5.03
-10	14	9	18.1	15.93	3.13
-9	14	9	138.27	148.06	6.87
-8	14	9	2.95	-2.24	11.42
-7	14	9	46.06	61.43	3.64
-6	14	9	0.01	0.56	7.99
-5	14	9	5.18	3.33	6.72
-4	14	9	1.14	-4.38	8.34

h	k	l	F_c^2	F_o^2	σF_o^2
-3	14	9	39.65	48.77	3.5
-2	14	9	27.86	29.26	9.11
-1	14	9	16.14	18.09	7.05
0	14	9	1.51	3.04	9.55
-14	15	9	13.13	12.57	4.21
-13	15	9	5.55	-1.66	9.15
-12	15	9	10.16	8.3	9.14
-11	15	9	24.01	21.49	8.06
-10	15	9	4.67	10.87	3.74
-9	15	9	5.23	4.06	5
-8	15	9	6.96	4.13	8.75
-7	15	9	15.45	10.81	8.97
-6	15	9	16.1	-2.82	8.98
-5	15	9	0.03	-11.37	8.74
-4	15	9	4.43	2.65	4.98
-3	15	9	0.25	-9.33	9.13
-2	15	9	2.08	4.76	5.27
-1	15	9	0.07	2.97	4.26
-13	16	9	8.44	15.12	5.35
-12	16	9	0	-15.44	9.43
-11	16	9	6.44	0.06	8.31
-10	16	9	0.77	0.37	9.11
-9	16	9	24.21	26.18	10.08
-8	16	9	3.86	3.88	6.56
-7	16	9	11.16	17.95	4.19
-6	16	9	40.8	44.08	10.57
-5	16	9	26.31	29.99	8.86
-4	16	9	6.81	3.39	9.63
-3	16	9	7.31	3.14	9.98
-9	17	9	0	-1.22	6.93
-8	17	9	19.26	10.66	13.19
0	0	10	1073.61	1057.05	25.57
0	1	10	69.88	45.98	2.22
-1	2	10	78.42	104.62	25.45
0	2	10	3.19	-1.94	5.55
-2	3	10	96.23	119.45	30.46
-1	3	10	323.87	267.17	64.86
0	3	10	726.7	472.03	187.89
-3	4	10	55.07	64.27	15.82
-2	4	10	408.72	243.47	115.76
-1	4	10	187.99	217.51	24.99
0	4	10	53.76	62.9	8.76
-4	5	10	10.28	14.8	1.93
-3	5	10	58.66	69.12	2.3
-2	5	10	100.33	102.39	5.48
-1	5	10	89.16	84.21	2.41
0	5	10	11.55	9.38	1.97
-5	6	10	26.57	26.27	2.1
-4	6	10	502.2	513.41	9.9
-3	6	10	428.07	414.2	8.92
-2	6	10	29.64	16.8	7.11
-1	6	10	126.8	139.65	4.39
0	6	10	93.82	119.99	3.19
-6	7	10	18.36	11.01	4.14
-5	7	10	344.04	326.73	10.14
-4	7	10	323.4	342.8	8.57
-3	7	10	86.37	84.91	2.62
-2	7	10	318.29	349.34	10.56
-1	7	10	2.76	-0.83	5.3
0	7	10	427.27	420.42	8.37
-7	8	10	1.13	0.51	3.72
-6	8	10	21.5	21.31	2.39
-5	8	10	170.09	163.56	5.51
-4	8	10	227.57	227.06	6.99
-3	8	10	6.04	5.52	2.61
-2	8	10	267.27	306.8	8.69
-1	8	10	9.96	3.51	6.91
0	8	10	74.19	81.91	2.82
-8	9	10	16.79	20.58	2.57
-7	9	10	41.33	50.03	2.64
-6	9	10	30.99	26.56	2.52
-5	9	10	244.15	257.93	8.13
-4	9	10	16.44	8.76	7.03
-3	9	10	32.39	22.62	6.58
-2	9	10	6.84	3.37	4.51
-1	9	10	112.44	110.3	3.14
0	9	10	44.03	57.65	2.42
-9	10	10	259.83	248.17	7.89
-8	10	10	2.52	1.54	7.45
-7	10	10	45.25	54.01	3.3
-6	10	10	14.97	20.55	3.31
-5	10	10	607.83	640.33	12.59
-4	10	10	129.57	145.69	4.33
-3	10	10	3.34	3.17	7.23
-2	10	10	27.88	24.16	2.63
-1	10	10	18.86	26.04	2.69
0	10	10	25.84	30.9	5.42
-10	11	10	0.15	-0.04	7.64
-9	11	10	2.48	0.55	3.22
-8	11	10	36.98	34.32	2.77
-7	11	10	127.61	134.65	3.8
-6	11	10	154.4	153.81	4.95
-5	11	10	18.34	22.05	6.6
-4	11	10	15.64	5.01	7.61
-3	11	10	21.37	33.96	2.71
-2	11	10	164	154.96	4.85
-1	11	10	5.13	7.25	4.14
0	11	10	1.98	-1.4	3.08
-11	12	10	0.95	-1.98	9.23
-10	12	10	27.96	30.16	2.85
-9	12	10	42.84	45.09	2.88
-8	12	10	65.33	73.25	3.15
-7	12	10	2.95	8.85	7.73
-6	12	10	1.37	-2.61	7.45
-5	12	10	32.98	34.87	2.76
-4	12	10	70.14	71.92	2.93
-3	12	10	103.25	105.3	3.85
-2	12	10	12.53	10.03	4.63
-1	12	10	3.37	2.14	8
0	12	10	5.69	4.59	4.18
-12	13	10	7.73	5.76	4.89
-11	13	10	0.03	3.95	8.5
-10	13	10	2.86	-2.23	7.8
-9	13	10	2.06	-2.16	8.08
-8	13	10	7.45	11.44	8.11
-7	13	10	6.82	7.23	3.85
-6	13	10	7.56	9.85	4.26
-5	13	10	16.01	30.59	3.53
-4	13	10	3.12	5.26	4.25
-3	13	10	0.68	4.51	4.33
-2	13	10	1.07	2.82	4.65
-1	13	10	3.24	-1.51	8.5
0	13	10	23.51	16.99	6.75
-13	14	10	0.07	-0.64	6.02
-12	14	10	33.06	40.14	3.37
-11	14	10	85.58	88.98	3.57
-10	14	10	1.79	-2.44	8.73
-9	14	10	22.21	25.21	3.18
-8	14	10	33.2	36.08	3.17
-7	14	10	0.47	-3.58	8.31
-6	14	10	16.77	11.16	3.1
-5	14	10	2.48	0.71	9.44
-4	14	10	10.55	12	3.1
-3	14	10	8.61	17.27	4.85
-2	14	10	3	-0.59	8.83
-1	14	10	29.92	37.63	12.73
0	14	10	7.52	6.3	8.14
-14	15	10	0	-12.73	16.67
-13	15	10	2.56	-11.8	9.85
-12	15	10	0.09	1.5	6.22
-11	15	10	43.48	55.84	5.65
-10	15	10	0.51	-0.07	8.72
-9	15	10	33.38	23.76	4.74
-8	15	10	3.41	1.32	8.87
-7	15	10	0.13	-7.48	8.75
-6	15	10	0.05	2.63	4.92
-5	15	10	0.03	-5.06	5.84
-4	15	10	1.72	2.41	5.02
-3	15	10	2.18	3.45	9.26
-2	15	10	0.72	-4.88	10.46
-12	16	10	1.43	-3.41	9.56
-11	16	10	3.86	-3.95	9.61
-10	16	10	18.63	16.48	6.67
-9	16	10	6.38	6.97	3.41
-8	16	10	8.39	15.68	5.33
-7	16	10	0.5	1.58	9.35
-6	16	10	0.71	10.89	9.31
-5	16	10	0.02	9.9	9.56
-4	16	10	4.44	6.9	5.49
0	1	11	263.39	261.43	14.85
-1	2	11	284.64	142.97	74.97
0	2	11	251.07	226.64	48.82
-2	3	11	452.4	262.55	159.73
-1	3	11	98.63	80.45	16.31
0	3	11	7.47	8.78	2.25
-3	4	11	351.69	229.79	110.9
-2	4	11	70.65	66.9	15.05
-1	4	11	6.21	3.36	2.94
0	4	11	6.07	0.32	3.14
-4	5	11	3.13	4.45	5.65
-3	5	11	0.19	-12.16	5.73
-2	5	11	4.64	3.69	4.65
-1	5	11	24.38	35.72	2.06
0	5	11	113.11	119.65	22.85
-5	6	11	13.07	6.18	6.81
-4	6	11	143.24	167.68	8.2
-3	6	11	280.23	271.16	7.81
-2	6	11	18.2	24.02	2.08
-1	6	11	4.37	5.57	3.31
0	6	11	0.85	-3.52	5.48
-6	7	11	748.65	767.01	13.17
-5	7	11	260.01	232.93	8.71
-4	7	11	58.63	60.77	3.92
-3	7	11	53.49	53.22	2.31
-2	7	11	51.16	43.67	2.3
-1	7	11	6.83	7.91	2.67
0	7	11	22.82	33.18	2.16
-7	8	11	11.2	5.38	3.9
-6	8	11	440.47	532.94	14.55
-5	8	11	230.75	245.96	17.17
-4	8	11	164.72	178.37	9.81
-3	8	11	173.84	178.68	5.56
-2	8	11	54.67	69.1	3.05
-1	8	11	2.37	-7.64	7.11
0	8	11	70.07	57.04	2.37
-8	9	11	68.24	83	4.25
-7	9	11	140.97	130.79	4.11
-6	9	11	458.27	479.73	10.98
-5	9	11	169.95	169.85	5.22
-4	9	11	0.14	4.9	6.94
-3	9	11	154.9	142.31	4.4
-2	9	11	198.34	193.75	6.14
-1	9	11	17.63	9.84	3.73
0	9	11	0.32	3.34	4.72
-9	10	11	46.99	54.59	3.21
-8	10	11	0.63	6.19	7.26
-7	10	11	0.54	0.76	4.02
-6	10	11	20.93	22.73	2.6
-5	10	11	162.34	177.08	5.45
-4	10	11	58.69	60.43	3.29
-3	10	11	1.61	7.34	2.99
-2	10	11	0.18	-1.8	4
-1	10	11	0.02	-6.26	7.33
0	10	11	42.71	48.05	2.43
-10	11	11	38.21	31.5	2.96
-9	11	11	18.06	22.51	3.6
-8	11	11	3.87	6.61	7.38
-7	11	11	27.31	26.07	3.92
-6	11	11	13.75	17.45	7.63
-5	11	11	46.17	44.26	2.73
-4	11	11	4.84	-0.09	6.57
-3	11	11	7.44	4.5	4.97
-2	11	11	0.62	-3.24	4.08
-1	11	11	3	0.24	4.16
0	11	11	2.58	3.95	6.64
-11	12	11	37.21	33.14	2.9
-10	12	11	1.29	-1.24	4.35
-9	12	11	1.71	-11.26	7.88
-8	12	11	2.31	1.06	7.57
-7	12	11	29.66	25.95	2.72
-6	12	11	0.39	3.41	4.13
-5	12	11	1.21	5.17	4.05
-4	12	11	47.75	51.76	2.85
-3	12	11	1.07	-7.45	7.74
-2	12	11	9.68	10.1	4.5
-1	12	11	3.44	-0.56	7.96
0	12	11	11.6	0.29	7.33
-12	13	11	24.49	32.03	3.28
-11	13	11	17.3	21.07	3.18
-10	13	11	19.71	13.57	8.57
-9	13	11	54.01	60.74	3.41
-8	13	11	7.05	-14.13	8.02
-7	13	11	2.7	6.21	5.01
-6	13	11	0.15	-4.12	7.87
-5	13	11	1.13	5.35	7.28
-4	13	11	7.11	7.56	7.96
-3	13	11	17.97	14.27	4.66
-2	13	11	1.06	6.07	8.4
-1	13	11	5.95	-6.93	8.8
0	13	11	30.18	28.46	2.89
-13	14	11	0.31	-15.54	10.02
-12	14	11	11.5	18.88	10.92
-11	14	11	38.43	33.82	6.48
-10	14	11	0.72	-3.62	8.79
-9	14	11	33.31	45.22	5.09
-8	14	11	0.39	-8.66	8.42
-7	14	11	1.22	-5.21	9.21
-6	14	11	11.31	-4.15	8.56
-5	14	11	5.94	0.18	8.64
-4	14	11	0.07	-9.08	8.62
-3	14	11	0.87	1.65	8.69
-2	14	11	0.8	5.23	8.63
-1	14	11	0.32	-3.47	9.34
0	14	11	5.62	4.8	4.83
-13	15	11	9.04	10.73	5.46
-12	15	11	0.42	-11.58	8.51
-11	15	11	0.15	8.4	9.19
-10	15	11	1.03	-1.89	9.2
-9	15	11	4.41	8.85	5.98
-6	15	11	0.27	-6.89	8.9
-7	15	11	1.61	4.83	8.79
-8	15	11	0.44	7.3	3.86
-5	15	11	0.41	-0.98	6.96
-4	15	11	0	-2.6	13.41
-3	15	11	0.33	2.16	9.35
-2	15	11	1.45	-3.55	9.63
-11	16	11	3.57	2.26	16.22
-10	16	11	3.85	7.61	4.18
-9	16	11	3.95	5.24	9.51
-8	16	11	11.77	13.07	4.12
-7	16	11	20.99	28.46	4.14
-6	16	11	1.32	-10.34	9.51
0	0	12	5235.17	4322.3	91.21
0	1	12	2.98	0.5	5.23
-1	2	12	78.43	82.19	21.04
0	2	12	45.6	23.61	7.39
-2	3	12	1.55	3.36	5.71
-1	3	12	7.76	11	3.17
0	3	12	7.68	3.24	2.29
-3	4	12	103.7	83.1	21.76
-2	4	12	27.96	33.19	7.67
-1	4	12	20.27	27.08	5.9
0	4	12	12.51	4.16	5.74
-4	5	12	26.24	22.43	5.7
-3	5	12	94.76	95.01	3.04
-2	5	12	45.73	33.89	2.13
-1	5	12	43.27	31.81	2.16
0	5	12	15.45	16.8	4.62
-5	6	12	25.51	20.37	2.38
-4	6	12	32.92	30.18	2.22

h	k	l	F_c^2	F_o^2	σF_o^2
-3	6	12	106.6	102.55	3.77
-2	6	12	48.48	43.1	2.25
-1	6	12	8.3	5.81	3.4
0	6	12	89.28	83.72	2.75
-6	7	12	141.41	181.92	5.54
-5	7	12	521.95	519.95	11.08
-4	7	12	0.19	1.39	7.41
-3	7	12	6.61	11.67	3.63
-2	7	12	25.71	25.69	2.4
-1	7	12	0.26	5.78	3.7
0	7	12	34.85	37.41	2.29
-7	8	12	450.85	458.12	16.83
-6	8	12	97.03	113.63	3.37
-5	8	12	31.39	40.57	2.7
-4	8	12	367.9	374.85	14.35
-3	8	12	57.6	67.36	3.07
-2	8	12	15.3	12.85	4.23
-1	8	12	180.45	191.35	6.26
0	8	12	9.24	-4.5	7.7
-8	9	12	39.28	43.09	2.71
-7	9	12	183.1	169.99	8.94
-6	9	12	113.52	121.19	4.16
-5	9	12	9.03	-0.65	7.34
-4	9	12	52.8	47.13	3.77
-3	9	12	23.26	18.43	3.47
-2	9	12	4.85	5.64	7.05
-1	9	12	2.28	6.82	7.23
0	9	12	0.03	3.15	6.29
-9	10	12	3.92	-9.35	7.32
-8	10	12	52.57	45.18	2.73
-7	10	12	109.81	103.81	3.15
-6	10	12	3.87	4.82	4.01
-5	10	12	1.27	-2.03	7.24
-4	10	12	32.99	34.39	2.62
-3	10	12	2.19	-0.82	6.22
-2	10	12	0.13	1.69	3.91
-1	10	12	5.67	-1.35	7.43
0	10	12	0.73	0.9	6.51
-10	11	12	33.86	20.06	9.83
-9	11	12	16.82	14.69	4.15
-8	11	12	46.43	39.18	2.77
-7	11	12	0.7	-5.98	7.46
-6	11	12	101.17	104.98	3.29
-5	11	12	0	-2.15	6.89
-4	11	12	9.14	-5.42	7.52
-3	11	12	29.6	37.14	2.74
-2	11	12	1.79	-0.58	7.5
-1	11	12	1.79	6.03	7.77
0	11	12	3.37	-0.66	4.06
-11	12	12	0.38	-4.28	11.13
-10	12	12	15.81	-3.12	8.01
-9	12	12	63.88	66.4	5.11
-8	12	12	3.79	-3.97	7.81
-7	12	12	11.16	1.28	10.62
-6	12	12	0.33	-6.53	7.74
-5	12	12	1.57	-3.7	7.71
-4	12	12	3.51	10.68	3.26
-3	12	12	0.01	-3.09	8.9
-2	12	12	6.7	2.65	6.8
-1	12	12	22.87	22.71	3.71
0	12	12	0.1	-5.66	7.36
-12	13	12	27.1	31.7	3.31
-11	13	12	17.25	15.14	4.87
-10	13	12	0.67	-6.93	11.99
-9	13	12	1.75	4.06	4.7
-8	13	12	20.68	24.98	5.7
-7	13	12	10.55	8.13	8.33
-6	13	12	0	0.18	4.54
-5	13	12	1.22	1.46	3.54
-4	13	12	2.19	-3.27	8.43
-3	13	12	22.91	21.29	6.5
-2	13	12	1.59	-2.58	8.65
-1	13	12	11.16	5.9	5.11
0	13	12	3.57	0.23	6.03
-13	14	12	0.01	9.15	5.19
-12	14	12	0.15	-2.08	5.07
-11	14	12	11.89	15.54	12.13
-10	14	12	5.51	7.7	8.96
-9	14	12	13.27	1.31	8.86
-8	14	12	7.42	1.99	4.93
-7	14	12	2.46	3.24	8.55
-6	14	12	1.61	-2.91	4.85
-5	14	12	3.33	-0.29	8.67
-4	14	12	1.38	-18.25	8.96
-3	14	12	10.51	10.88	11.69
-2	14	12	15.32	12.04	4.01
-1	14	12	13.51	21.13	4.15
-12	15	12	5.03	8.1	5.96
-11	15	12	0.44	1.23	9.34
-10	15	12	0	-8.45	9.61
-9	15	12	0.1	-9.93	8.68
-8	15	12	35.7	38.59	3.47
-7	15	12	0.73	-1.79	9.16
-6	15	12	4.68	10.62	5.78
-5	15	12	0.25	-10.16	6.16
-4	15	12	10.18	12.17	5.27
-3	15	12	4.43	-0.04	5.45
0	1	13	357.28	374.3	15.3
-1	2	13	194.81	171.92	56.95
0	2	13	390.02	259.74	69.22
-2	3	13	246.4	158.49	64.66
-1	3	13	0.1	5.19	6.07
0	3	13	139.76	102.72	20.31
-3	4	13	125.34	116.21	27.79
-2	4	13	12.99	4.02	6.12
-1	4	13	8.91	5.81	4.29
0	4	13	22.51	12.25	4.78
-4	5	13	11.46	14.79	2.18
-3	5	13	7.44	14.49	3.4
-2	5	13	0.99	-1.32	3.31
-1	5	13	1.12	4.64	2.6
0	5	13	18.71	5.34	3.72
-5	6	13	68.48	69.83	2.67
-4	6	13	16.29	3.43	3.46
-3	6	13	12.87	5.78	3.77
-2	6	13	13.25	14.97	7.91
-1	6	13	12.29	10.64	4.06
0	6	13	93.9	112.25	2.76
-6	7	13	239.26	252.04	7.83
-5	7	13	189.51	171.68	5.56
-4	7	13	30.64	30.97	2.59
-3	7	13	102.64	93.65	3.23
-2	7	13	1.46	3.71	3.73
-1	7	13	0	-11.37	11.08
0	7	13	86.03	77.24	2.57
-7	8	13	0.06	-4.64	4
-6	8	13	1.83	1.16	4.49
-5	8	13	0.65	3.96	4.1
-4	8	13	11.83	17.49	2.58
-3	8	13	4	1.79	3.79
-2	8	13	8.39	13.84	2.92
-1	8	13	8.24	-8.2	7.17
0	8	13	0.17	-6.45	6.36
-8	9	13	9.07	4.84	7.39
-7	9	13	20.52	39	2.7
-6	9	13	19.26	17.51	3.01
-5	9	13	46.51	54.89	2.77
-4	9	13	29.85	24.87	6.36
-3	9	13	0.23	-2.07	7.13
-2	9	13	16	21.8	2.54
-1	9	13	4.89	7.08	7.35
0	9	13	0.14	0.6	6.52
-9	10	13	23.57	34.83	2.81
-8	10	13	7.59	5.88	7.51
-7	10	13	90.83	103.55	3.36
-6	10	13	3.81	1.24	4.37
-5	10	13	0.79	-2.75	4.01
-4	10	13	16.29	9.41	5.19
-3	10	13	2.43	7.98	4.35
-2	10	13	21.77	15.24	4.18
-1	10	13	0.21	-16.84	7.66
0	10	13	1.42	-2.08	6.71
-10	11	13	24.97	18.74	5.87
-9	11	13	3.69	4.82	4.29
-8	11	13	22.26	16.2	2.76
-7	11	13	1.54	2.79	6.07
-6	11	13	1.89	2.71	4.1
-5	11	13	18.56	9.75	4.23
-4	11	13	0.11	9.83	4.17
-3	11	13	0.21	4.19	7.77
-2	11	13	49.93	45.09	8.05
-1	11	13	3.37	2.66	6.57
0	11	13	0.12	-14.59	7.19
-11	12	13	0.75	-13.44	11.36
-10	12	13	2.23	0.36	5.81
-9	12	13	16.4	17.4	4.74
-8	12	13	111.46	108.22	3.36
-7	12	13	30.02	29.43	2.92
-6	12	13	0.96	-8.41	4.93
-5	12	13	5.67	1.86	4.36
-4	12	13	6.68	0.12	4.36
-3	12	13	9.35	9.42	4.62
-2	12	13	0.84	-6.42	3.62
-1	12	13	0.1	-1.01	4.82
0	12	13	2.84	2.23	7.58
-12	13	13	0.01	-1.01	9
-11	13	13	47.96	43.38	11.59
-10	13	13	0	-9.62	17.56
-9	13	13	0.62	-0.41	8.56
-8	13	13	7.72	-12.12	8.62
-7	13	13	7.11	2.34	8.38
-6	13	13	1.51	1.06	4.65
-5	13	13	6.6	17.15	6.46
-4	13	13	21.28	24.83	3.18
-3	13	13	4.45	-1.06	8.75
-2	13	13	8.24	5.16	5.06
-1	13	13	8.6	3.94	9.12
0	13	13	0.21	-1.74	5.08
-12	14	13	4.11	11.27	8.43
-11	14	13	23.96	38.29	7.79
-10	14	13	0	-0.84	5.18
-9	14	13	3.88	-14.42	9.47
-8	14	13	0.01	-8.43	8.9
-7	14	13	0.09	-2.55	8.84
-6	14	13	4.21	7.23	8.77
-5	14	13	14.92	26.02	3.35
-4	14	13	2.01	-2.22	8.88
-3	14	13	7.56	7.17	4.06
-2	14	13	7.45	6.42	9.43
-10	15	13	0	-5.19	9.62
-9	15	13	4.25	6.57	9.69
-8	15	13	0.86	-20.08	9.63
-7	15	13	0.11	2.42	5.22
-6	15	13	27.43	20.85	11.95
-5	15	13	20.05	15.88	8.17
0	0	14	4476.24	4203.92	90.07
0	1	14	55.68	41.92	3.88
-1	2	14	11.46	2.54	7.03
0	2	14	368.56	218.29	59.35
-2	3	14	158.1	117.68	31.91
-1	3	14	190.88	127.26	44.79
0	3	14	11.11	6.59	3.44
-3	4	14	15.11	10.65	9.74
-2	4	14	28.18	21.11	6.67
-1	4	14	49.2	37.1	6.99
0	4	14	24.99	22.89	8.05
-4	5	14	17.55	15.78	2.99
-3	5	14	6.68	-1.08	7.01
-2	5	14	31.6	28.53	2.47
-1	5	14	11.28	13.91	2.46
0	5	14	129.07	123.46	21.77
-5	6	14	114.82	105.06	3.54
-4	6	14	46.6	56.59	2.79
-3	6	14	86.82	76.81	2.85
-2	6	14	4.09	-3.36	6.93
-1	6	14	6.14	9.56	2.98
0	6	14	82.68	83.72	3.7
-6	7	14	444.63	474.35	20.87
-5	7	14	584.34	643.29	12.95
-4	7	14	0.04	-7.83	7.55
-3	7	14	2.41	4.94	4
-2	7	14	29.44	52.19	4.49
-1	7	14	87.35	75.25	2.82
0	7	14	108.94	107.51	3.24
-7	8	14	14.77	25.61	2.68
-6	8	14	96.87	113.54	8.4
-5	8	14	206.73	210.59	8.03
-4	8	14	141.54	136.56	3.99
-3	8	14	0.52	-4.44	3.95
-2	8	14	0.51	-13.32	7.26
-1	8	14	28.89	18.84	2.74
0	8	14	20.12	25.9	2.33
-8	9	14	10.84	2.76	3.19
-7	9	14	29.92	37.39	4.07
-6	9	14	117.81	98.71	5.08
-5	9	14	0	-6.42	7.5
-4	9	14	30.47	44.74	2.77
-3	9	14	56.89	63.33	2.97
-2	9	14	29.02	27.24	5.47
-1	9	14	149.07	152.13	4.59
0	9	14	3.69	3.28	4.02
-9	10	14	170.61	166.57	7.59
-8	10	14	39.71	44.96	3.17
-7	10	14	14.2	17.91	4.78
-6	10	14	0.27	-5.88	5.94
-5	10	14	17.19	7.82	6.3
-4	10	14	0.88	-8.42	7.56
-3	10	14	5.07	2.12	7.66
-2	10	14	2.91	-5.1	9.83
-1	10	14	0	3.65	4.28
0	10	14	82.78	65.69	2.66
-10	11	14	1.34	-1.97	8.31
-9	11	14	4.52	-4.23	8.35
-8	11	14	129.85	134.27	4.13
-7	11	14	8.93	9.36	3.57
-6	11	14	0.87	6.59	4.22
-5	11	14	7.18	0.39	7.81
-4	11	14	16.46	16.7	3.31
-3	11	14	36.96	25.81	2.89
-2	11	14	1.67	4.45	8.28
-1	11	14	0.08	-0.1	8.3
0	11	14	0.33	-18.25	7.48
-11	12	14	6.01	5.09	11.94
-10	12	14	70.76	82.48	3.49
-9	12	14	21.78	27.42	3.23
-8	12	14	21.92	17.74	5.72
-7	12	14	8.49	7.87	7.41
-6	12	14	15.39	4.11	8.31
-5	12	14	2.57	-2.22	8.35
-4	12	14	20.01	20.6	7.05
-3	12	14	14.99	13.77	4.86
-2	12	14	2.81	-0.14	6.71
-1	12	14	0.01	-5.31	8.92
0	12	14	6.95	10.94	3.27
-12	13	14	0.02	-1.06	9.4
-11	13	14	36.54	49.77	3.61
-10	13	14	0.23	-9.75	9.23
-9	13	14	83.15	104.51	3.85
-8	13	14	4.05	-21.43	8.94
-7	13	14	1.55	-7.03	14.19
-6	13	14	8.62	9.93	3.75
-5	13	14	0.03	-12.38	6.03
-4	13	14	0.12	4.55	3.83
-3	13	14	5.74	10.62	8.56
-2	13	14	1.67	3.87	5.22
-1	13	14	0.82	5.18	5.31
0	13	14	1.75	14.21	16
-11	14	14	0	2.78	9.81
-10	14	14	3.79	-2.78	9.92
-9	14	14	2.04	5.99	5.36

h	k	l	F_c^2	F_o^2	σF_o^2
-8	14	14	3.35	5.74	5.26
-7	14	14	3.42	6.1	5.23
-6	14	14	1.66	0.11	5.93
-5	14	14	2.41	9.23	8.12
-4	14	14	12.64	18.72	4.14
-3	14	14	0.21	6.13	9.36
0	1	15	1.13	2.44	3.91
-1	2	15	30.54	23.39	11.02
0	2	15	48.39	30.17	6.49
-2	3	15	194.91	181.37	47.42
-1	3	15	16.53	25.47	15.88
0	3	15	241.56	185.41	44.45
-3	4	15	335.39	214.8	101.96
-2	4	15	220.57	181.3	58.14
-1	4	15	6.08	12.28	2.54
0	4	15	73.18	80.03	13.4
-4	5	15	295.27	314.34	9.47
-3	5	15	86.41	76.61	2.95
-2	5	15	10.7	4.49	3.07
-1	5	15	125.67	140.94	5.54
0	5	15	548.51	367.87	130.37
-5	6	15	86.46	95	4.41
-4	6	15	79.6	99.56	4.67
-3	6	15	378.74	346.78	10.34
-2	6	15	44.77	40.16	2.7
-1	6	15	32.16	36.79	2.75
0	8	15	3.43	4.99	3.98
-6	7	15	158.88	151.7	7.23
-5	7	15	0.97	2.48	7.86
-4	7	15	199.28	244.88	7.6
-3	7	15	62.86	51.01	3.07
-2	7	15	37.01	37.09	2.68
-1	7	15	30.99	36.92	2.75
0	7	15	15	7.38	4.58
-7	8	15	9.49	5.82	5.33
-6	8	15	15.87	13.08	3.25
-5	8	15	0.4	4.36	9.33
-4	8	15	44.67	33.58	2.79
-3	8	15	0.46	-8.84	7.5
-2	8	15	21.34	27.57	4.19
-1	8	15	17.48	23.17	3.35
0	8	15	6.34	3.31	3.98
-8	9	15	84.34	102.78	4.37
-7	9	15	42.9	55.4	2.92
-6	9	15	19.3	6.69	6.99
-5	9	15	49.34	55.16	2.94
-4	9	15	10.74	3.16	4.24
-3	9	15	73.94	81.42	3.03
-2	9	15	36.16	36.91	2.82
-1	9	15	21.84	21.89	4.34
0	9	15	24.99	23.52	6.94
-9	10	15	2.24	0.04	8.24
-8	10	15	15.49	20.4	3.42
-7	10	15	6.4	-0.93	8.02
-6	10	15	0.2	-1.92	5.6
-5	10	15	11.8	6.03	9.49
-4	10	15	1.9	-11.97	4.28
-3	10	15	1.16	-4.78	7.83
-2	10	15	30.77	32.25	2.91
-1	10	15	4.1	2.99	4.7
0	10	15	3.84	-4.31	4.55
-10	11	15	4.47	-4.23	8.73
-9	11	15	15.11	0.94	11.3
-8	11	15	1.73	-8.63	7.37
-7	11	15	92.56	102.74	3.64
-6	11	15	6.63	3.83	8.34
-5	11	15	5.41	7.53	4.55
-4	11	15	1.01	-5.57	8.25
-3	11	15	0.79	-3.03	8.42
-2	11	15	16.3	20.72	3.14
-1	11	15	2.19	-8.12	8.74
0	11	15	3.18	7.49	3.68
-11	12	15	0.5	7.76	3.94
-10	12	15	31.52	39.29	3.59
-9	12	15	6.25	5.78	9.05
-8	12	15	0.63	-7.17	8.87
-7	12	15	6.7	15.89	3.79
-6	12	15	0.85	-1.17	6.6
-5	12	15	1.02	7.14	8.44
-4	12	15	18.13	12.43	5
-3	12	15	8.69	-2.89	5.07
-2	12	15	6.35	9.34	5.09
-1	12	15	0.44	2.34	3.99
0	12	15	7.24	13.43	4.32
-11	13	15	1.74	-1.86	9.84
-10	13	15	4.99	1.72	4.71
-9	13	15	4.06	4.13	5.38
-8	13	15	29.47	28.17	3.45
-7	13	15	0.41	-20.53	11.72
-6	13	15	0	-6.39	10.96
-5	13	15	41.38	58.68	3.54
-4	13	15	3.22	13.55	5.18
-3	13	15	16.19	17.76	4.15
-2	13	15	22.28	28.47	8.1
-9	14	15	0	-9.26	5.57
-8	14	15	0.22	-6.45	15.07
-7	14	15	28.66	34.04	3.54
-6	14	15	0.06	0.19	9.52
-5	14	15	0.06	2.3	8.69
0	0	16	691.55	531.61	20.45
0	1	16	109.9	132.44	5.89
-1	2	16	46.03	70.42	16.58
0	2	16	273.43	150.78	49.02
-2	3	16	33.51	15.47	7.49
-1	3	16	236.74	169.59	63.55
0	3	16	93.54	66.1	11.68
-3	4	16	248.04	192.55	79.75
-2	4	16	54.1	70.32	16.23
-1	4	16	19.97	18.76	5.65
0	4	16	46.73	35.94	6.07
-4	5	16	6.07	-3.81	7.88
-3	5	16	15.25	23.93	5.79
-2	5	16	94.48	88.65	3.01
-1	5	16	1.06	-5.71	7.49
0	5	16	45.96	41.12	5.91
-5	6	16	86.72	76.85	3.04
-4	6	16	0.33	-4.49	7.76
-3	6	16	68.26	87.87	3.09
-2	6	16	11.48	7.77	4.07
-1	6	16	33.76	26.39	6.45
0	6	16	8.46	-1.28	6.65
-6	7	16	1.06	-4.23	4.93
-5	7	16	42.3	47.99	2.88
-4	7	16	69.84	73.75	3
-3	7	16	13.83	0.19	7.59
-2	7	16	0.05	-14.94	14.06
-1	7	16	1.84	2.47	7.54
0	7	16	75.19	75.34	4.66
-7	8	16	61.85	74.11	3.88
-6	8	16	1.47	6.87	3.23
-5	8	16	3.9	4.18	7.87
-4	8	16	23.46	13.64	4.32
-3	8	16	28.28	34.4	2.81
-2	8	16	69.58	62.42	2.96
-1	8	16	0.96	3.32	7.83
0	8	16	43.2	49.79	2.57
-8	9	16	63.52	64.35	3.08
-7	9	16	0.18	4.41	6.92
-6	9	16	12.49	19.97	2.82
-5	9	16	5.5	3.38	4.4
-4	9	16	13.44	17.65	2.8
-3	9	16	12.1	4.44	5.82
-2	9	16	0.91	-8.06	10.44
-1	9	16	0.87	-23.45	8.19
0	9	16	0.24	-10.39	7.28
-9	10	16	33.61	15.44	4.97
-8	10	16	0.36	-21.5	8.46
-7	10	16	54.07	64.45	4.81
-6	10	16	47.79	48.9	3.14
-5	10	16	9.86	6.03	4.42
-4	10	16	8.86	17.11	3.47
-3	10	16	1.59	10.15	5.35
-2	10	16	1.1	-1.8	15.6
-1	10	16	36.54	32	3.48
0	10	16	14.49	18.16	3.68
-10	11	16	15.46	17.34	3.94
-9	11	16	78.66	91.82	4.38
-8	11	16	37.56	49.94	11.46
-7	11	16	20.52	10.24	4.92
-6	11	16	0.12	-4.04	8.56
-5	11	16	6.4	-9.97	8.09
-4	11	16	13.58	16.63	3.11
-3	11	16	12.35	4.03	8.79
-2	11	16	0.13	-6.94	10.99
-1	11	16	2.66	-0.14	8.13
0	11	16	0.01	-2.37	5.33
-11	12	16	2.82	-7.77	9.55
-10	12	16	8.46	9.85	7.63
-9	12	16	0.02	-2.98	9.33
-8	12	16	21.49	21.38	3.44
-7	12	16	0.99	4.04	8.82
-6	12	16	14.39	20.51	8.68
-5	12	16	4.84	6.46	5.53
-4	12	16	5.07	4.24	9.13
-3	12	16	5.87	9.65	4.01
-2	12	16	28.19	30.16	4.51
-1	12	16	0.59	1.45	9.65
-10	13	16	33.73	44.87	4.86
-9	13	16	26.16	32.05	3.69
-8	13	16	1.36	10.6	9.41
-7	13	16	2.84	12.13	3.99
-6	13	16	1.15	7.73	5.56
-5	13	16	8.52	7.19	5.34
-4	13	16	5.3	-0.85	5.4
-3	13	16	1.66	4.29	7.3
0	1	17	30.37	21.95	2.41
-1	2	17	31.98	19.16	3.46
0	2	17	4.02	0.85	3.69
-2	3	17	198.97	133.66	42.85
-1	3	17	10.08	17.84	4.68
0	3	17	20.52	2.76	8.03
-3	4	17	141.31	119.53	31.51
-2	4	17	10.28	2.95	5.15
-1	4	17	1.3	-5.31	11.49
0	4	17	45.63	56.24	14.14
-4	5	17	6.92	8.57	7.67
-3	5	17	56.45	35.51	3.17
-2	5	17	0.14	-1.47	7.49
-1	5	17	10.86	5.76	7.58
0	5	17	14.09	0.67	4.75
-5	6	17	0.65	0.81	4.2
-4	6	17	7.76	-8.66	7.73
-3	6	17	14.12	6.25	4.24
-2	6	17	43.94	51.43	3.25
-1	6	17	13.98	10.41	3.3
0	6	17	20.46	17.69	2.75
-6	7	17	42.27	44.05	2.89
-5	7	17	25.51	35.06	2.81
-4	7	17	1.63	0	5.39
-3	7	17	40.89	47.71	2.91
-2	7	17	0.05	-4.18	7.88
-1	7	17	29.61	28.65	2.86
0	7	17	107.01	107.25	2.88
-7	8	17	16.6	11.05	6.97
-6	8	17	30.77	39.83	4.39
-5	8	17	0.2	1.91	8.68
-4	8	17	38.79	7.79	8.21
-3	8	17	2.09	-6.87	7.92
-2	8	17	20.96	29.69	2.9
-1	8	17	5.06	6.53	4.36
0	8	17	15.24	15.2	3.18
-8	9	17	0.86	2.2	8.47
-7	9	17	0.07	0.72	3.57
-6	9	17	32.99	22.62	5.91
-5	9	17	0.02	2.47	9.25
-4	9	17	10.22	5.74	8.55
-3	9	17	2.58	-10.36	8.73
-2	9	17	2.4	4.35	9.05
-1	9	17	6.58	10.08	4.68
0	9	17	21.64	31.06	2.8
-9	10	17	4.46	-6.76	8.85
-8	10	17	18.8	19.21	4.44
-7	10	17	0.53	0.45	8.55
-6	10	17	9.38	2.71	8.53
-5	10	17	0.63	0.34	8.37
-4	10	17	0.2	-3.81	8.49
-3	10	17	2.52	1.94	5.31
-2	10	17	0.5	-1.1	8.38
-1	10	17	12.19	7.34	4.99
0	10	17	1.81	5.43	4.85
-10	11	17	0	-1	5.19
-9	11	17	5.04	8.18	5.13
-8	11	17	14.3	18.61	6.69
-7	11	17	0.2	-2.19	8.86
-6	11	17	6.7	-6.94	8.82
-5	11	17	0.54	-2.15	4.94
-4	11	17	0.86	9.58	4.96
-3	11	17	6.01	8.87	15.43
-2	11	17	0.04	6.19	3.69
-1	11	17	1.31	-7.39	9.37
0	11	17	1.52	-4.02	6.19
-10	12	17	0.37	0.81	5.33
-9	12	17	0.24	-17.81	9.6
-8	12	17	0.56	-1.16	11.85
-7	12	17	0.08	-1.34	5.11
-6	12	17	2.35	-1.82	9.17
-5	12	17	30.61	45.04	4.55
-4	12	17	0.74	-0.58	9.22
-3	12	17	2.17	-1.52	8.81
-2	12	17	3.31	-6.55	9.63
0	0	18	519.26	471.5	20.54
0	1	18	37.76	40.69	2.47
-1	2	18	8.11	7.45	7.62
0	2	18	4.86	0.62	5.76
-2	3	18	3.39	2.44	7.65
-1	3	18	0.67	1.66	4.21
0	3	18	4.04	-1.81	6.68
-3	4	18	17.11	7.13	11.64
-2	4	18	1.09	5.8	4.2
-1	4	18	5.86	-4.37	4.57
0	4	18	105.9	94.19	14.68
-4	5	18	74.84	78.64	3.09
-3	5	18	66.2	66.77	2.99
-2	5	18	4.52	12.56	4.28
-1	5	18	3.16	5.8	7.22
0	5	18	73.41	75.97	2.71
-5	6	18	21.76	16.38	6.42
-4	6	18	49.45	60.69	3.02
-3	6	18	34	34.3	3.57
-2	6	18	35.45	31.3	2.91
-1	6	18	43.63	50.19	3.18
0	6	18	120.05	124.29	4.37
-6	7	18	0.35	1.09	7.21
-5	7	18	4.28	-6.29	4.43
-4	7	18	1.18	-9.22	8.08
-3	7	18	23.83	29.47	2.91
-2	7	18	12.81	18.36	5.13
-1	7	18	11.05	21.21	2.9
0	7	18	0.37	-6.52	5.29
-7	8	18	24.88	19.95	4.8
-6	8	18	18.94	11.96	8.44
-5	8	18	43.43	50.62	3.22
-4	8	18	13.27	12.35	3.71
-3	8	18	0.21	-0.01	4.62
-2	8	18	7.11	2.94	4.69
-1	8	18	2.35	1.68	4.62
0	8	18	0.5	-7.29	4.52
-8	9	18	0.08	-9.57	8.59
-7	9	18	4.39	2.98	4.78
-6	9	18	1.49	-11.17	8.57

h	k	l	F_c^2	F_o^2	σF_o^2
-5	9	18	12.14	27.69	13.61
-4	9	18	0.98	-12.08	8.53
-3	9	18	0.38	4.03	8.51
-2	9	18	1.12	4.01	5.98
-1	9	18	0.98	1.16	6.01
0	9	18	7.66	5.77	5.4
-9	10	18	11.09	-3.16	9.21
-8	10	18	20.53	20.37	16.2
-7	10	18	19.71	23.17	3.9
-6	10	18	4.16	4.02	8.8
-5	10	18	0.13	-1.34	4.78
-4	10	18	15.5	14.29	5.66
-3	10	18	0.2	-0.58	4.91
-2	10	18	2.89	4.91	8.94
-1	10	18	0	-0.84	9.22
0	10	18	0.12	-5.53	10.09
-10	11	18	0.8	-4.44	16.12
-9	11	18	0.75	-12.62	12.38
-8	11	18	5.39	-3.85	11.3
-7	11	18	2.58	4.94	9.07
-6	11	18	6.48	9.7	5.52
-5	11	18	0.7	-5.02	9.11
-4	11	18	3.44	-1.63	5.19
-3	11	18	13.19	7.99	11.51
-2	11	18	1.75	-5.32	9.34
-7	12	18	0.94	-6.25	7.2
-6	12	18	0.6	6.18	9.24
-5	12	18	1.38	-0.84	9.35
0	1	19	0.64	6.82	3.17
-1	2	19	0.52	-4.3	7.75
0	2	19	4.27	-0.83	4.12
-2	3	19	19.03	-0.78	7.86
-1	3	19	0.9	-0.43	7.71
0	3	19	0.4	-3.78	4.07
-3	4	19	14.12	1.29	4.31
-2	4	19	2.23	-1.67	6.82
-1	4	19	9.39	3.72	8.66
0	4	19	0.02	-8.12	6.96
-4	5	19	0.36	3.92	7.99
-3	5	19	1.38	-9.53	7.95
-2	5	19	59.68	58.9	3.03
-1	5	19	5	5.6	4.39
0	5	19	7.05	-0.12	8.48
-5	6	19	0.29	-3.01	11.18
-4	6	19	0.12	-1.49	4.37
-3	6	19	33.63	21.53	4.86
-2	6	19	4.17	-1.37	11.44
-1	6	19	0.05	-9.28	8.25
0	6	19	9.93	5.2	4.53
-6	7	19	1.23	0.5	4.76
-5	7	19	26.68	28.58	3.17
-4	7	19	0.42	-14.98	8.43
-3	7	19	1.55	-0.09	8.27
-2	7	19	2.75	-6.63	9.97
-1	7	19	0.34	-0.14	8.43
0	7	19	0.77	5.18	4.66
-7	8	19	0.3	2.03	5.35
-6	8	19	1.56	-2.59	8.53
-5	8	19	0.8	4.98	3.66
-4	8	19	19	15.29	7.07
-3	8	19	7.05	-0.88	9.94
-2	8	19	0.26	0.57	6.16
-1	8	19	9.48	2.78	9.36
0	8	19	3.81	-6.04	7.97
-8	9	19	0.92	0.61	9.02
-7	9	19	6.47	7.18	3.55
-6	9	19	7.44	3.24	4.92
-5	9	19	0	-12.31	8.78
-4	9	19	4.56	-6.53	8.92
-3	9	19	0	-13.63	8.95
-2	9	19	0.01	3.48	4.53
-1	9	19	0.04	-5.14	10.07
0	9	19	0.71	0.01	7.94
-9	10	19	0.1	-0.66	9.29
-8	10	19	0.37	-10.78	9.19
-7	10	19	2.87	-10.26	10.85
-6	10	19	0	-14.97	9.11
-5	10	19	1.78	11.75	5.05
-4	10	19	0.71	-0.19	9.08
-3	10	19	0	0.2	10.06
-2	10	19	2.77	-2.51	9.27
-1	10	19	2.95	-0.17	5.26
-7	11	19	0.04	-4.75	9.5
-6	11	19	3.02	3.43	5.21
-5	11	19	2.54	3.98	5.15
-4	11	19	0.07	1.58	9.65
h	k	l	F_c^2	F_o^2	σF_o^2
0	0	20	1.69	-4.82	13.94
0	1	20	0.16	-6.96	9.08
-1	2	20	2.61	-0.99	5.72
0	2	20	4.45	1.34	6.9
-2	3	20	12.26	0.21	8.13
-1	3	20	14.23	9.06	8.06
0	3	20	12.08	-4.29	7.12
-3	4	20	50.67	41.57	12.22
-2	4	20	0.12	-4.03	8.23
-1	4	20	3.63	5.27	4.75
0	4	20	12.97	15.95	4.41
-4	5	20	1.51	-0.36	4.8
-3	5	20	0.34	-16.38	8.41
-2	5	20	8.67	1.15	4.75
-1	5	20	0.38	1.44	5.5
0	5	20	7.99	10.81	3.58
-5	6	20	3.21	0.69	10.3
-4	6	20	8.85	1.88	9.43
-3	6	20	26.6	19.92	5.72
-2	6	20	9.56	-1.08	6.27
-1	6	20	18.05	16.19	7.45
0	6	20	16.64	23.73	2.85
-6	7	20	1.16	0.26	8.2
-5	7	20	0.62	-5.35	8.76
-4	7	20	3.88	4.67	3.76
-3	7	20	11.08	10.53	3.86
-2	7	20	30.39	33.33	3.34
-1	7	20	4.4	6.78	7.98
0	7	20	9.32	10.34	3.73
-7	8	20	8.77	6.72	5.03
-6	8	20	2.31	-2.07	10.99
-5	8	20	11.78	16.72	4.7
-4	8	20	4.93	6.53	9
-3	8	20	10.9	21.97	3.93
-2	8	20	0.92	1.91	9.01
-1	8	20	4.28	1.08	9.08
0	8	20	0.11	-11.56	8.09
-8	9	20	0.01	-21.01	9.13
-7	9	20	0.85	-16.6	11
-6	9	20	0.23	12.12	5.05
-5	9	20	2.26	9.85	5.14
-4	9	20	0.64	-29.45	9.17
-3	9	20	0.58	-3.2	5.13
-2	9	20	1.71	-21	9.34
-1	9	20	0.07	-3.58	9.4
-6	10	20	3.07	-6.8	9.27
-5	10	20	0	-2.62	9.27
-4	10	20	1.28	2.32	11.13
0	1	21	16.44	3.31	5.01
-1	2	21	2.2	5.58	6.99
0	2	21	0.13	1.7	3.64
-2	3	21	15.24	19.3	6.35
-1	3	21	1.14	7.17	9.13
0	3	21	5.75	2.41	7.73
-3	4	21	10.77	1.15	7.12
-2	4	21	16.3	9.5	4.9
-1	4	21	1	6.68	4.95
0	4	21	6.21	-0.06	5.78
-4	5	21	0.83	-0.11	9
-3	5	21	10.87	1.28	5.27
-2	5	21	9.62	16.43	3.68
-1	5	21	7.38	6.58	9.18
0	5	21	35.98	32.9	5.43
-5	6	21	0.16	9.71	8.89
-4	6	21	2.74	-14.32	9.17
-3	6	21	45.13	51.83	3.49
-2	6	21	10.67	8.11	9.32
-1	6	21	1.81	-2.84	9.44
0	6	21	2.49	-1.98	8.12
-6	7	21	5.03	5.24	5.28
-5	7	21	9.98	4.02	5.28
-4	7	21	18.59	25.14	8.38
-3	7	21	1.43	0.95	9.44
-2	7	21	0.94	-10.4	9.45
-1	7	21	16.38	19.06	6.6
0	7	21	0.38	4.61	7.97
-7	8	21	0.01	0.94	9.33
-6	8	21	8.62	1.75	8.05
-5	8	21	4.33	5.02	9.31
-4	8	21	8.59	4.39	9.55
-3	8	21	0.42	1.85	5.27
-2	8	21	7.77	-3.26	9.73
-1	8	21	0.09	-15.59	9.81
0	0	22	10.97	1.07	5.72
0	1	22	0	-8.62	7.84
-1	2	22	0.43	3.73	5.03
0	2	22	0.07	-7.94	7.83
-2	3	22	6.53	1.57	8.99
-1	3	22	0.01	-7.53	16.17
0	3	22	8.19	2.7	7.97
-3	4	22	0.16	-8.97	13.2
-2	4	22	4.27	9.61	7.79
-1	4	22	5.17	-1.15	5.22
0	4	22	5.29	7.58	8.16
-4	5	22	3.64	-6.38	9.6
-3	5	22	4.2	1.67	6.02
-2	5	22	6.87	11.23	4.09
-1	5	22	0.7	0.21	6.41
0	5	22	1.22	-14.28	8.38
-5	6	22	0.05	0.82	7.5
-4	6	22	0.54	0.82	9.54
-3	6	22	36.83	48.17	3.67
-2	6	22	0.12	-8.87	16.19
-1	6	22	18.85	19.46	4.3
0	6	22	15.73	10.45	5.28
-5	7	22	17.22	8.88	5.87
-4	7	22	17.88	24.59	4.56
-3	7	22	0.25	6.4	9.57
h	k	l	F_c^2	F_o^2	σF_o^2
-2	7	22	5.57	4.63	6.79
0	1	23	0	-5.08	9.38
-1	2	23	13.54	-4.56	21.05
0	2	23	5.95	-3.34	5.06
-2	3	23	2.76	1.01	5.31
-1	3	23	7.91	17.6	4.8
0	3	23	5.93	7.07	10.28
-3	4	23	2.62	13.08	8.77
-2	4	23	12.32	9.23	4.2
-1	4	23	0.14	-1.86	9.56
0	4	23	2.35	0.32	5.16
-3	5	23	11.26	15.7	5.54
-2	5	23	0.23	-4.98	7.68

A3.2 ALTAR

h	k	l	F_c^2	F_o^2	σF_o^2
1	0	0	370.41	351.65	3.32
2	0	0	1720.82	1766.07	25.41
3	0	0	27.4	25.08	1.44
4	0	0	40.53	36.85	2.54
5	0	0	20.49	21.01	0.82
-5	1	0	0.21	0.52	0.58
-4	1	0	367.32	352.06	3.51
-3	1	0	20.14	19.79	0.84
-2	1	0	1044.76	1049.66	22.34
-1	1	0	147.89	132.6	3.09
0	1	0	137.22	116.23	5.41
1	1	0	2.62	3.3	0.18
2	1	0	0.15	-0.01	0.43
3	1	0	5.7	5.84	0.3
4	1	0	5.53	5.37	0.6
5	1	0	8.15	8.28	0.66
6	1	0	0.25	-0.15	0.37
-5	2	0	0.75	0.82	0.4
-4	2	0	123.45	125.87	2.11
-3	2	0	96.98	96.03	3.29
-2	2	0	24.55	24.52	0.85
-1	2	0	19.56	23.67	1.1
0	2	0	42.46	39.38	4.61
1	2	0	364.46	325.74	42.97
2	2	0	180.76	184.14	24.83
3	2	0	0.08	0.09	0.61
4	2	0	37.85	41.09	3.86
5	2	0	127.23	127.47	14.56
6	2	0	10.68	10.06	2.06
-4	3	0	0.03	-0.19	0.61
-3	3	0	6.93	5.94	0.59
-2	3	0	14.68	14.48	0.53
-1	3	0	16.29	16.91	0.59
0	3	0	2.47	2.88	0.71
1	3	0	693.72	645.61	128.94
2	3	0	0.07	0.05	0.56
3	3	0	552.51	514.26	94.47
4	3	0	1.36	-0.09	0.97
5	3	0	41.01	37.02	5.42
6	3	0	1.57	1.44	0.18
-4	4	0	13.08	13.74	0.49
-3	4	0	246.69	250.79	14.97
-2	4	0	119.44	119.55	11.6
-1	4	0	323.19	326.57	34.03
0	4	0	25.27	20.03	2.71
1	4	0	182.21	166.76	44.26
2	4	0	1.97	2.33	0.92
3	4	0	8.12	5.84	1.87
4	4	0	64.18	60.07	13.66
5	4	0	13.76	14	5.39
-3	5	0	25.54	24.08	1.65
-2	5	0	0.19	-1.3	0.74
-1	5	0	0.89	1.9	0.35
0	5	0	47.48	36.4	9.83
1	5	0	0.19	0.24	1.44
2	5	0	92.83	84.02	35.24
3	5	0	8.99	8.83	3.78
4	5	0	4.45	4.38	1.75
5	5	0	12.32	10.48	3.97
-2	6	0	2.16	1.77	0.82
-1	6	0	51.44	44.61	11.24
0	6	0	12.77	11.93	4.13
1	6	0	119.76	110.41	44.45
2	6	0	59.64	45.29	24.83
3	6	0	1.13	1.24	0.38
4	6	0	1.64	1.79	0.82
-1	7	0	8.2	7.39	2.36
0	7	0	1.33	0.64	0.96
1	7	0	0.04	-1.16	0.58
2	7	0	5.34	5.35	1.89
3	7	0	0.73	-0.02	0.5
4	7	0	9.62	8.4	5.8
-3	-7	1	1.36	2.04	0.34
-2	-7	1	9.97	11.76	0.59
-1	-7	1	29.59	36.55	1.51
0	-7	1	1.7	1.76	0.38
1	-7	1	4.5	4.31	0.31
-4	-6	1	9.96	11.9	0.6
-3	-6	1	0.5	1.42	0.46
-2	-6	1	49.26	56.39	2.16
-1	-6	1	0.53	0.38	1.1
0	-6	1	14.54	16.27	0.82
1	-6	1	3.38	3.44	0.49
2	-6	1	5.77	6.53	0.41
-5	-5	1	8.16	9.62	0.49
-4	-5	1	32.15	35.9	1.77
-3	-5	1	1.69	-0.13	1.17
-2	-5	1	7.42	9.49	0.63
-1	-5	1	11.61	13.05	0.71
0	-5	1	42.95	47.55	2.15
1	-5	1	105.19	117.56	3.06
2	-5	1	51.32	53.83	2.08
3	-5	1	8.49	8.42	0.45
-5	-4	1	0.62	0	0.9
-4	-4	1	0.2	-0.89	1.15
-3	-4	1	9.5	10.41	0.64
-2	-4	1	21.59	26.87	1.29
-1	-4	1	234.58	251.54	3.6
0	-4	1	119.99	140.82	2.75
1	-4	1	96.9	101.04	2.59
2	-4	1	8.02	8.58	0.63
3	-4	1	0.64	0.69	0.96
4	-4	1	6.77	6.92	0.38
-5	-3	1	18.87	22	1.09
-4	-3	1	204.49	239.02	4.2
-3	-3	1	3.44	2.94	0.49
-2	-3	1	433.82	535.86	4.77
-1	-3	1	0.16	0.69	0.35
0	-3	1	76.82	88.56	1.85
1	-3	1	81.53	85.02	2.02
2	-3	1	11.65	14.59	0.68
3	-3	1	43.01	44.57	1.98
4	-3	1	36.35	38.47	1.68
-6	-2	1	9.77	11.91	0.59
-5	-2	1	63.62	78.53	2.41
-4	-2	1	10.55	11.96	0.7
-3	-2	1	271.19	296.13	3.77
-2	-2	1	0.77	0.42	0.74
-1	-2	1	60.8	72.88	1.38
0	-2	1	52.14	54.46	1.21
1	-2	1	18.11	20.26	0.97
2	-2	1	118.98	123.96	2.42
3	-2	1	6.88	6.51	0.58
4	-2	1	0.82	0.13	1.03
5	-2	1	0.17	-0.52	0.63
-6	-1	1	2.13	2.6	0.28
-5	-1	1	41.05	48.8	1.97
-4	-1	1	63.76	65.45	2.32
-3	-1	1	19.26	20.66	1.09
-2	-1	1	691.91	740.13	4.51
-1	-1	1	458.95	474.37	2.73
0	-1	1	2775.77	3270.66	25.95
1	-1	1	526.91	518.75	3.18
2	-1	1	170.35	191.85	2.55
3	-1	1	52.53	50.58	1.95
4	-1	1	44.13	45.34	2.07
5	-1	1	0.03	-0.59	0.85
-5	0	1	0.04	-0.21	0.9
-4	0	1	69.45	66.66	2.31
-3	0	1	0.11	-0.56	0.87
-2	0	1	3.18	4.29	0.3
-1	0	1	34.08	30.5	0.78
0	0	1	82.91	74.83	0.72
1	0	1	10.32	11.07	0.53
2	0	1	6.81	7.43	0.34
3	0	1	216.59	213.3	3.2
4	0	1	2.45	2.08	0.56
5	0	1	51.94	52.62	1.98
-5	1	1	12.46	11.83	0.68
-4	1	1	101.18	95.63	2.66
-3	1	1	65.95	63.82	1.93
-2	1	1	227.49	222.37	2.56
-1	1	1	81.87	72.1	1.16
0	1	1	7.99	5.73	0.3
1	1	1	1700.91	1420.75	4.79
2	1	1	0.69	-0.57	0.63
3	1	1	1.58	2.69	0.38
4	1	1	6.28	5.82	0.55
5	1	1	134.21	128.18	2.98
6	1	1	14.85	14.28	0.69
-5	2	1	5.29	4.33	0.38
-4	2	1	28.84	28.9	1.43
-3	2	1	16.62	14.34	0.65
-2	2	1	6.13	6.88	0.39
-1	2	1	549.24	506.25	3.43
0	2	1	291.24	239.87	2.07
1	2	1	2426.08	2100.13	7.16
2	2	1	16.21	15.24	0.77
3	2	1	248.54	225.47	3.27
4	2	1	4.65	3.36	0.54
5	2	1	0.07	0.67	0.41
6	2	1	0.01	-0.41	0.5
-5	3	1	67.7	68.2	1.23
-4	3	1	1.73	1.88	0.45
-3	3	1	1005.99	1004.49	8.39
-2	3	1	155.13	143.3	2.74
-1	3	1	610.35	594.95	4.57
0	3	1	2.61	4.25	0.31
1	3	1	0.02	-0.02	0.68
2	3	1	21.34	14.43	0.69
3	3	1	9.86	11.54	0.64
4	3	1	4.62	4.91	0.54
5	3	1	35.87	34.99	1.71
6	3	1	96.37	82.16	1.45
-4	4	1	10.35	9.64	0.49
-3	4	1	3.32	2.85	0.48
-2	4	1	19.73	19.7	0.97
-1	4	1	1.93	1.93	0.42
0	4	1	22.67	19.88	0.92
1	4	1	7.2	5.53	0.41
2	4	1	54.39	36.93	1.54
3	4	1	4.61	3.23	0.49
4	4	1	36.93	31.72	1.48
5	4	1	2.93	1.85	0.42
-3	5	1	1.3	0.5	0.82
-2	5	1	4.21	4.34	0.55
-1	5	1	52.14	43.88	1.98
0	5	1	3.02	0.28	1.09
1	5	1	9.85	6.46	0.51
2	5	1	259.98	177.9	3.56
3	5	1	95.89	66.63	2.42
4	5	1	27.47	20.31	1.05
5	5	1	4.52	3.21	0.37
-2	6	1	47.31	42.01	1.51
-1	6	1	2.31	2.52	0.47
0	6	1	182.63	128.48	3.04
1	6	1	2.2	1.84	0.5
2	6	1	56.43	35.27	1.69
3	6	1	1.66	1.32	0.45
4	6	1	4.06	2.7	0.4
5	6	1	1.33	0.87	0.25
-1	7	1	16.53	10.41	0.48
0	7	1	6.88	4.97	0.42
1	7	1	0.23	0.05	0.83
2	7	1	6.97	4.43	0.44
3	7	1	9.87	6.66	0.43
4	7	1	9.48	5.71	0.33
1	8	1	0.32	-0.13	0.48
2	8	1	4.5	2.9	0.27
-3	-7	2	5.12	8.28	0.42
-2	-7	2	3.77	4.48	0.38
-1	-7	2	0.37	0.59	0.34
0	-7	2	6.27	6.74	0.38
-4	-6	2	2.85	3.08	0.37
-3	-6	2	2.22	4.01	0.44
-2	-6	2	2.54	2.27	0.49
-1	-6	2	94.53	110.36	2.84
0	-6	2	5.24	5.24	0.54
1	-6	2	145.6	170.41	3
2	-6	2	21.72	18.98	0.94
-5	-5	2	23.66	26.43	0.99
-4	-5	2	0.81	1.72	0.43
-3	-5	2	118.98	147.15	3.26
-2	-5	2	0	-1.29	1.17
-1	-5	2	141.84	166.71	3.56
0	-5	2	0.01	-0.66	1.11
1	-5	2	24.53	26.01	1.26
2	-5	2	19.64	19.85	1.05
3	-5	2	0.5	0.45	0.63
-5	-4	2	2.28	2.6	0.38
-4	-4	2	53.95	59.49	2.22
-3	-4	2	4.18	3.93	0.59
-2	-4	2	24.02	31.39	1.62
-1	-4	2	40.65	54.77	1.97
0	-4	2	53.02	67.51	2.18
1	-4	2	0.72	-0.79	1.23
2	-4	2	9.25	9.78	0.6
3	-4	2	16.2	14.93	0.75
4	-4	2	19.72	20.99	0.86
-5	-3	2	21.65	27.06	1.34
-4	-3	2	0.26	0.63	1.12
-3	-3	2	8.31	11.08	0.57
-2	-3	2	0.02	0.67	0.92
-1	-3	2	4.05	5.35	0.42
0	-3	2	21.67	21.9	1.11
1	-3	2	65.95	74.33	2.1
2	-3	2	178.98	190.65	3.6
3	-3	2	4.78	3.46	0.56
4	-3	2	165.44	159.66	2.88
-5	-2	2	2.91	3.71	0.48
-4	-2	2	12.24	12.23	0.67
-3	-2	2	15.61	14.59	0.66
-2	-2	2	656.85	754.28	5.32
-1	-2	2	394.61	436.11	3.49
0	-2	2	1054.66	1210.69	5.86
1	-2	2	430.71	477.74	4.05
2	-2	2	843.26	918.45	6.85
3	-2	2	19.74	20.13	0.85
4	-2	2	66.22	65.66	2.28
5	-2	2	2.67	2.66	0.33
-5	-1	2	2.54	4	0.47
-4	-1	2	257.28	267.16	4.25
-3	-1	2	63.6	70.03	1.92
-2	-1	2	1089.21	1206.05	6.1
-1	-1	2	126.64	125.62	1.67
0	-1	2	87.65	99.04	1.39
1	-1	2	27.12	25.64	0.98
2	-1	2	1.39	1.29	0.37
3	-1	2	37.75	37.89	1.79
4	-1	2	2.34	0.73	1.21
5	-1	2	0.48	0.45	0.36
-5	0	2	66.35	69.84	2.04
-4	0	2	18.38	16.7	0.79
-3	0	2	72.81	73.75	2
-2	0	2	468.54	503.67	3.71
-1	0	2	85.83	84.65	1.33
0	0	2	4.34	3.43	0.25
1	0	2	601.41	537.16	3.14
2	0	2	177.85	181.54	2.33
3	0	2	0.68	0.82	0.91
4	0	2	116.95	114.43	2.94

h	k	l	F_c^2	F_o^2	σF_o^2
5	0	2	10.94	12.59	0.64
-5	1	2	0.09	0.3	0.36
-4	1	2	27.47	31.33	1.58
-3	1	2	0.45	0.01	0.44
-2	1	2	3.18	3.02	0.31
-1	1	2	1.43	1.05	0.27
0	1	2	4.88	5	0.27
1	1	2	574.88	485.48	2.89
2	1	2	3.52	3.33	0.32
3	1	2	531.94	513.92	4.92
4	1	2	1.51	1.86	0.5
5	1	2	94.25	87.1	2.42
-5	2	2	6.03	7.33	0.4
-4	2	2	6.47	4.59	0.56
-3	2	2	54.64	52.37	1.98
-2	2	2	269.41	246.11	3.06
-1	2	2	1523.41	1575.33	6.65
0	2	2	166.3	146.41	1.79
1	2	2	2614.46	2338.43	7.89
2	2	2	46.24	42.17	1.28
3	2	2	82.33	82.83	2.14
4	2	2	65.99	66.93	2.34
5	2	2	60.33	57.35	2.03
6	2	2	112.82	110.35	1.61
-5	3	2	13.78	14.31	0.68
-4	3	2	0.06	-0.1	0.89
-3	3	2	64.41	67.26	2.3
-2	3	2	2.08	2.23	0.42
-1	3	2	0.43	0.23	0.7
0	3	2	203.9	192.62	2.4
1	3	2	27.02	25.01	1.04
2	3	2	297.54	252.38	3.08
3	3	2	30.48	25.81	1.37
4	3	2	27.2	29.19	1.48
5	3	2	5.16	4.72	0.52
6	3	2	0.39	0.35	0.25
-4	4	2	0.11	-1.11	0.71
-3	4	2	33.03	33.18	1.63
-2	4	2	81.36	76.6	2.38
-1	4	2	18.36	19.85	1.02
0	4	2	0.18	0.93	0.37
1	4	2	8.49	5.39	0.43
2	4	2	269.57	221.51	3.42
3	4	2	157.56	135.43	2.99
4	4	2	2.82	3.5	0.5
5	4	2	5.37	4.37	0.45
-3	5	2	16.1	14.44	0.75
-2	5	2	50.97	49.19	2
-1	5	2	14.74	16.52	0.96
0	5	2	35.85	30.34	1.47
1	5	2	4.66	4.57	0.5
2	5	2	32.89	25.74	1.34
3	5	2	3.69	3.57	0.5
4	5	2	12.2	9.92	0.57
5	5	2	5.81	5.26	0.38
-3	6	2	0.67	0.78	0.24
-2	6	2	28.4	25.03	1.24
-1	6	2	58.61	46.26	1.89
0	6	2	8.78	7.98	0.56
1	6	2	30.35	21.48	1.1
2	6	2	21.38	15.89	0.71
3	6	2	158.15	118.81	2.98
4	6	2	7.92	5.69	0.45
5	6	2	20.44	15.36	0.76
-1	7	2	7.7	6	0.41
0	7	2	1.06	-0.19	0.83
1	7	2	33.14	25.96	1.27
2	7	2	3.19	2.98	0.44
3	7	2	1.36	0.8	0.38
4	7	2	10.67	8.35	0.38
1	8	2	0.63	0.74	0.27
2	8	2	7.09	5.19	0.33
-2	-7	3	7.44	8.77	0.42
-1	-7	3	21.37	24.31	0.89
-4	-6	3	4.57	4.87	0.31
-3	-6	3	0.95	1.17	0.34
-2	-6	3	13.26	14.45	0.89
-1	-6	3	8.99	11.64	0.59
0	-6	3	30.24	37.84	1.56
1	-6	3	3.38	3.28	0.39
-4	-5	3	0.39	0.53	0.76
-3	-5	3	2.48	0.51	1.01
-2	-5	3	4.17	4.82	0.56
-1	-5	3	132.82	154.62	3.44
0	-5	3	14.53	16.83	0.86
1	-5	3	20.46	21.3	1.09
2	-5	3	10.09	11.19	0.52
-5	-4	3	22.1	23.09	1.04
-4	-4	3	2.78	3.48	0.49
-3	-4	3	90.41	101.38	2.8
-2	-4	3	1.32	1.44	0.56
-1	-4	3	55.19	55.54	2.19
0	-4	3	40.47	43.36	1.97
1	-4	3	2.31	2.54	0.56
2	-4	3	55.1	57.62	2.23
3	-4	3	9.82	11.7	0.57
-5	-3	3	4.42	5	0.43
-4	-3	3	44.88	51.61	2.03
-3	-3	3	4.13	4.99	0.59
-2	-3	3	372.62	445.25	4.98
-1	-3	3	101.38	130.25	2.6
0	-3	3	1.71	-0.13	1.07
1	-3	3	72.12	90.14	2.44
2	-3	3	1.72	2.85	0.56
3	-3	3	0.78	-0.43	1.1
4	-3	3	0.49	0.67	0.73
-5	-2	3	1.38	1.23	0.4
-4	-2	3	108.18	125.09	3.05
-3	-2	3	4	4.96	0.52
-2	-2	3	53.09	62.74	1.84
-1	-2	3	103.65	124.71	2.22
0	-2	3	8.35	8.13	0.41
1	-2	3	22.14	27.33	1.32
2	-2	3	4.56	4.32	0.5
3	-2	3	20.59	20.1	0.96
4	-2	3	1.67	2.73	0.48
-5	-1	3	3.35	3.46	0.43
-4	-1	3	65.72	65.22	2.25
-3	-1	3	240.08	260.33	3.72
-2	-1	3	0.87	0.35	0.36
-1	-1	3	2.25	3.09	0.32
0	-1	3	124.35	131.93	1.82
1	-1	3	20.75	21.85	1.03
2	-1	3	230.87	270.63	3.47
3	-1	3	30.61	23.79	1.23
4	-1	3	109.89	103.05	2.94
5	-1	3	0.04	0.2	0.66
-5	0	3	4.65	4.22	0.45
-4	0	3	21.88	22.38	1.19
-3	0	3	26.83	26.4	1.28
-2	0	3	2.81	4.52	0.37
-1	0	3	666.43	726.31	4.18
0	0	3	210.17	174.84	1.86
1	0	3	2571.06	2700.45	8.98
2	0	3	1.3	2.4	0.34
3	0	3	443.01	428.43	4.89
4	0	3	0.12	0.2	1.06
5	0	3	20.17	18.54	0.87
-5	1	3	73.58	72.19	1.93
-4	1	3	26.65	21.8	1.11
-3	1	3	360.04	346.54	4.33
-2	1	3	382.47	385.95	3.69
-1	1	3	4158.76	4745.76	44.66
0	1	3	235.7	229.11	2.12
1	1	3	1497.96	1386.32	5.83
2	1	3	32.37	30.04	1.19
3	1	3	9.55	10.54	0.56
4	1	3	0.28	0.07	0.49
5	1	3	31.25	25.65	1.28
-5	2	3	100.79	104.77	1.94
-4	2	3	19.35	23.68	1.23
-3	2	3	39.98	35.31	1.68
-2	2	3	2.51	2.7	0.38
-1	2	3	7.46	9.32	0.5
0	2	3	15.07	14.85	0.75
1	2	3	8.83	7.18	0.39
2	2	3	40.19	39.28	1.32
3	2	3	1.51	0.82	1.1
4	2	3	23.5	25.94	1.25
5	2	3	10.21	10.73	0.56
-4	3	3	2.21	2.51	0.42
-3	3	3	13.97	12.8	0.87
-2	3	3	40.86	37.59	1.63
-1	3	3	35.75	33.24	1.41
0	3	3	1.24	1.24	0.33
1	3	3	271.79	247.31	2.9
2	3	3	23.23	24.92	1.17
3	3	3	15.24	16.24	0.86
4	3	3	126.57	124.11	3.13
5	3	3	0	-0.89	0.85
-4	4	3	9.35	9.64	0.47
-3	4	3	0.4	0.14	0.44
-2	4	3	133.62	126.31	2.98
-1	4	3	5.28	4.36	0.47
0	4	3	731.57	699.3	5.8
1	4	3	0.71	1.28	0.38
2	4	3	596.4	547.52	5.5
3	4	3	3.66	4.01	0.54
4	4	3	22.82	19.43	1.1
5	4	3	8.52	8.53	0.47
-3	5	3	1.47	1.37	0.38
-2	5	3	390.53	371.56	4.99
-1	5	3	23.68	22.42	1.02
0	5	3	40.37	38.91	1.91
1	5	3	21.75	18.24	0.94
2	5	3	16.47	14.62	0.75
3	5	3	141.86	132.98	3.21
4	5	3	19.36	17.15	0.78
5	5	3	0.33	-0.79	0.67
-3	6	3	1.36	1.63	0.24
-2	6	3	6.8	7.48	0.47
-1	6	3	16.39	15.43	0.88
0	6	3	3.21	2.67	0.5
1	6	3	21.16	16.12	0.86
2	6	3	5.7	6.14	0.56
3	6	3	0.01	-0.25	1.03
4	6	3	3.9	3.08	0.42
5	6	3	0.49	0.47	0.48
-1	7	3	19.27	18.59	0.82
0	7	3	86.99	83.43	2.17
1	7	3	24.58	20.93	1.04
2	7	3	5.48	4.83	0.5
3	7	3	28.02	26.88	1.3
4	7	3	0.15	-0.27	0.56
0	8	3	2.72	2.62	0.28
1	8	3	8.04	8.12	0.42
2	8	3	1.99	2.49	0.3
-3	-6	4	0.01	0	0.3
-2	-6	4	13.74	18	0.89
-1	-6	4	36.24	41.05	1.5
0	-6	4	0	0.13	0.67
1	-6	4	0.54	0.04	0.53
-4	-5	4	0.05	0.25	0.3
-3	-5	4	18.34	18.27	0.92
-2	-5	4	0.03	-1.16	0.99
-1	-5	4	20.9	21.9	0.89
0	-5	4	2.54	4.32	0.52
1	-5	4	9.84	10.37	0.54
2	-5	4	22.21	25.61	1.12
-5	-4	4	0.08	-0.21	0.45
-4	-4	4	1.06	0.52	0.85
-3	-4	4	0.97	0.58	1.07
-2	-4	4	27	25.19	1.21
-1	-4	4	43.16	49.8	2.2
0	-4	4	687.81	776	7.47
1	-4	4	6.79	8.35	0.61
2	-4	4	129.6	127.51	2.91
3	-4	4	0.1	-0.02	0.34
-5	-3	4	10.22	11.46	0.57
-4	-3	4	71.47	79.73	2.48
-3	-3	4	37.94	41.12	2
-2	-3	4	151.17	162.73	3.35
-1	-3	4	105.56	109.02	2.72
0	-3	4	24.21	25.44	1.34
1	-3	4	2.35	2.19	0.56
2	-3	4	0.57	-0.79	1.21
3	-3	4	19.01	19	0.99
4	-3	4	1.32	1.16	0.31
-5	-2	4	6.13	7.99	0.44
-4	-2	4	170.14	185.61	3.58
-3	-2	4	143.46	162.41	3.31
-2	-2	4	109.21	114.35	2.63
-1	-2	4	24.17	26.16	1.3
0	-2	4	167.12	174.3	2.83
1	-2	4	48.81	50.98	1.85
2	-2	4	12.86	17.33	0.91
3	-2	4	10.41	6.99	0.61
4	-2	4	6.98	6.11	0.47
-5	-1	4	0.02	0.2	0.72
-4	-1	4	79.62	82.65	2.56
-3	-1	4	5.4	5.56	0.53
-2	-1	4	5.64	4.89	0.48
-1	-1	4	39.61	40.35	1.32
0	-1	4	34.69	36.04	1.29
1	-1	4	2.66	2.16	0.38
2	-1	4	11.5	12.99	0.67
3	-1	4	98.75	95.23	2.74
4	-1	4	0.58	-1.2	1.08
5	-1	4	32.42	31.23	1.04
-5	0	4	23.19	21.17	0.99
-4	0	4	28.4	29.08	1.45
-3	0	4	49.05	49.98	1.94
-2	0	4	185.58	195.83	2.94
-1	0	4	52.78	58.61	1.44
0	0	4	3.41	2.13	0.31
1	0	4	121.3	131.82	2.12
2	0	4	28.98	25.37	1.23
3	0	4	25.58	23.25	1.21
4	0	4	58.21	49.9	2.12
5	0	4	4.67	4.16	0.39
-5	1	4	0.35	-0.34	0.66
-4	1	4	7.71	9.13	0.59
-3	1	4	36.29	32.78	1.61
-2	1	4	25.62	24.11	1.21
-1	1	4	0.1	0.09	0.67
0	1	4	111.74	120.02	1.79
1	1	4	22.77	21.9	1.04
2	1	4	342.51	332.29	3.73
3	1	4	10.29	11.76	0.66
4	1	4	17.73	19.79	0.92
5	1	4	7.98	7.16	0.49
-5	2	4	5.28	5.76	0.36
-4	2	4	0.21	-0.2	0.42
-3	2	4	52.3	57.24	2.1
-2	2	4	4.82	4	0.45
-1	2	4	62.67	60.63	1.61
0	2	4	12.92	12.37	0.6
1	2	4	529.22	504.01	3.96
2	2	4	32.15	34.4	1.42
3	2	4	39.71	44.99	1.85
4	2	4	27.43	32.77	1.61
5	2	4	0.4	0.38	0.86
-4	3	4	26.11	25.67	1.26
-3	3	4	14.83	11.22	0.6
-2	3	4	338.65	328.86	4.41
-1	3	4	26.61	23.61	1.22
0	3	4	446.42	447.49	4.15
1	3	4	0.55	0.56	0.34
2	3	4	17.86	16.76	0.8
3	3	4	1.7	1.99	0.49

h	k	l	F_c^2	F_o^2	σF_o^2
4	3	4	12.26	13.19	0.64
5	3	4	1.57	2.38	0.41
-4	4	4	215.01	218.3	2.69
-3	4	4	14.64	14.1	0.67
-2	4	4	171.16	159.49	3.37
-1	4	4	19.12	18.54	0.79
0	4	4	24.76	23.21	1.19
1	4	4	14.39	12.24	0.6
2	4	4	0.44	-1.04	1.07
3	4	4	1.55	1.36	0.52
4	4	4	50.51	56.47	2.11
5	4	4	46.37	47.35	1.61
-3	5	4	1.3	1.73	0.36
-2	5	4	2.91	0.71	1.14
-1	5	4	33.22	34.74	1.73
0	5	4	3.73	3.72	0.56
1	5	4	49.35	58.25	2.14
2	5	4	13.53	14.22	0.67
3	5	4	12.49	11.98	0.63
4	5	4	6.14	7.08	0.5
5	5	4	0.43	0.95	0.31
-2	6	4	4.91	4.45	0.41
-1	6	4	12.01	11.75	0.6
0	6	4	18.83	18.16	0.88
1	6	4	140.6	138.27	3.35
2	6	4	1.81	0.96	1.07
3	6	4	54.79	57.87	2.2
4	6	4	0.57	0.42	0.7
-1	7	4	84.23	94.34	1.94
0	7	4	0.26	-0.54	0.86
1	7	4	5.73	6.87	0.52
2	7	4	0.04	0.41	0.41
3	7	4	1.31	0.91	0.38
4	7	4	0.22	0.51	0.52
1	8	4	16.47	15.73	0.77
2	8	4	5.65	6	0.35
-2	-6	5	0.07	0.69	0.27
-1	-6	5	1.1	1.61	0.29
0	-6	5	0.79	0.11	0.49
-3	-5	5	5.24	4.81	0.38
-2	-5	5	61.93	61.51	1.94
-1	-5	5	29.95	33.27	1.6
0	-5	5	263.85	280.96	3.9
1	-5	5	25.24	26.86	1.2
-4	-4	5	78.42	83.77	1.91
-3	-4	5	5.45	6.73	0.54
-2	-4	5	23.55	25.06	1.18
-1	-4	5	13.99	15.39	0.74
0	-4	5	5.05	6.39	0.59
1	-4	5	37.47	40.61	1.83
2	-4	5	0.37	0.52	0.4
3	-4	5	0.01	0.31	0.49
-5	-3	5	14.7	13.97	0.68
-4	-3	5	71.1	73.06	2.05
-3	-3	5	8.34	7.45	0.6
-2	-3	5	4.01	3.03	0.59
-1	-3	5	0.74	1.17	0.58
0	-3	5	4.59	4.8	0.61
1	-3	5	67.49	69.99	2.57
2	-3	5	1.33	0.81	1.13
3	-3	5	2.32	4.47	0.45
-5	-2	5	2.02	2.54	0.33
-4	-2	5	0.26	-0.32	0.86
-3	-2	5	0.03	0.81	0.55
-2	-2	5	1.46	0.34	1.25
-1	-2	5	133.12	131.79	2.82
0	-2	5	36.69	42.2	1.71
1	-2	5	521.5	519.08	5.71
2	-2	5	0.8	1.02	0.52
3	-2	5	190.28	183.8	3.57
4	-2	5	1.01	-0.2	0.73
-5	-1	5	36.59	38.45	1.28
-4	-1	5	12.1	13.52	0.64
-3	-1	5	1093.86	1195.11	9.27
-2	-1	5	109.11	110.4	2.63
-1	-1	5	979.03	1047.71	7.04
0	-1	5	0.21	0	0.88
1	-1	5	108.67	116.28	2.53
2	-1	5	0.01	0.34	1.07
3	-1	5	8.32	6.97	0.57
4	-1	5	22.09	22.15	1.11
-5	0	5	89.74	84.85	1.83
-4	0	5	29.44	31.79	1.57
-3	0	5	61.36	62.76	2.21
-2	0	5	0.02	0.34	1.07
-1	0	5	10.75	10.5	0.57
0	0	5	70.99	78.11	1.81
1	0	5	15.04	15.61	0.83
2	0	5	2.83	3.55	0.5
3	0	5	2.82	2.87	0.54
4	0	5	6.42	5.24	0.51
5	0	5	6.98	8.26	0.45
-5	1	5	2.15	1.56	0.3
-4	1	5	5.76	9.29	0.54
-3	1	5	46.44	48.25	2.03
-2	1	5	2.43	-0.2	1.12
-1	1	5	20.36	19.78	1.03
0	1	5	8.04	5.28	0.39
1	1	5	7.52	8.77	0.44
2	1	5	415.76	422.12	4.67
3	1	5	170.58	191.33	3.7
4	1	5	51.03	54.04	2.15
5	1	5	3.28	2.5	0.38
-5	2	5	0.44	0.27	0.23
-4	2	5	1.58	2	0.42
-3	2	5	0	0.06	1.07
-2	2	5	82.13	83.41	2.32
-1	2	5	6.1	5.19	0.47
0	2	5	880.58	883.69	6
1	2	5	0.65	2.44	0.38
2	2	5	604.05	587.59	5.47
3	2	5	2.65	2.18	0.56
4	2	5	69.1	66.25	2.43
5	2	5	10.8	12.82	0.71
-4	3	5	16.44	12.93	0.6
-3	3	5	0.09	0.57	0.49
-2	3	5	107.69	115.5	2.86
-1	3	5	138.68	148.72	2.98
0	3	5	298.4	299.04	3.76
1	3	5	51.71	43.53	1.65
2	3	5	1.24	1.64	0.43
3	3	5	5.36	4.89	0.56
4	3	5	49.93	50.36	2.09
5	3	5	13.28	13.9	0.7
-4	4	5	2.61	2.49	0.31
-3	4	5	1.52	1.83	0.44
-2	4	5	12.99	12.25	0.63
-1	4	5	131.25	135.96	3.09
0	4	5	6.04	6.85	0.53
1	4	5	61.71	69.02	2.24
2	4	5	9.9	9.78	0.59
3	4	5	1.72	2.37	0.52
4	4	5	0.07	-0.53	0.97
5	4	5	0	-0.49	0.7
-3	5	5	18.33	19.51	0.9
-2	5	5	26.12	25.76	1.3
-1	5	5	54.75	57.66	2.17
0	5	5	31.44	34.4	1.65
1	5	5	20.74	18.83	0.97
2	5	5	0.16	0.13	1.08
3	5	5	2.25	1.49	0.52
4	5	5	0.06	-1.86	0.86
5	5	5	2.78	3.24	0.31
-2	6	5	0.11	0.18	0.75
-1	6	5	2.1	2.52	0.46
0	6	5	0.35	0.63	1.14
1	6	5	47.23	48.73	2.14
2	6	5	4.3	4.5	0.56
3	6	5	16.12	17.46	0.84
4	6	5	19.39	20.24	1
-1	7	5	4.91	5.16	0.36
0	7	5	6.06	6.24	0.45
1	7	5	24.41	25.87	1.37
2	7	5	70.9	74.62	2.09
3	7	5	9.68	12.46	0.66
4	7	5	50.28	56.44	1.16
1	8	5	4.09	4.28	0.31
2	8	5	0.01	-0.04	0.46
-3	-5	6	35.11	33.65	1.03
-2	-5	6	17.82	20.1	0.94
-1	-5	6	27.56	27.69	1.22
0	-5	6	0	0.23	0.32
1	-5	6	4.78	4.13	0.31
-4	-4	6	9.89	10.45	0.52
-3	-4	6	4.59	4.27	0.45
-2	-4	6	68.1	70.3	2.19
-1	-4	6	3.1	3.18	0.53
0	-4	6	6.11	5.63	0.56
1	-4	6	27.71	29.65	1.48
2	-4	6	28.25	29.32	1.16
-4	-3	6	27.15	24.2	1.16
-3	-3	6	0.24	0.27	0.45
-2	-3	6	20.76	19.84	0.91
-1	-3	6	42.28	45.41	2.11
0	-3	6	7.11	7.89	0.8
1	-3	6	13.76	14.85	0.84
2	-3	6	5.89	5.96	0.53
3	-3	6	5.57	5.7	0.4
-4	-2	6	4.73	4.55	0.45
-3	-2	6	288.54	304.91	4.65
-2	-2	6	139.92	141.13	3.27
-1	-2	6	6.38	3.78	0.63
0	-2	6	93.19	93.35	2.62
1	-2	6	119.75	115.53	2.99
2	-2	6	6.65	7.28	0.61
3	-2	6	9.11	8.15	0.52
4	-2	6	0.34	0.23	0.47
-5	-1	6	3.87	3.37	0.29
-4	-1	6	15.36	17.78	0.86
-3	-1	6	0.92	1.64	0.5
-2	-1	6	75.81	77.03	2.49
-1	-1	6	0.05	0.75	1.08
0	-1	6	0.02	-1.42	1.15
1	-1	6	4.65	5.49	0.58
2	-1	6	51.37	52.98	2.2
3	-1	6	6.22	6.9	0.56
4	-1	6	5.5	4.1	0.41
-5	0	6	31.8	29.35	0.99
-4	0	6	6.72	8.06	0.54
-3	0	6	46.51	47.85	2.19
-2	0	6	34.34	33.96	1.73
-1	0	6	63.99	64.2	1.98
0	0	6	4.81	3.46	0.46
1	0	6	7.11	6.75	0.54
2	0	6	473.11	495.05	5.85
3	0	6	61.9	59.58	2.38
4	0	6	19.47	19.06	0.87
-5	1	6	7.8	5.92	0.31
-4	1	6	30.72	31.01	1.52
-3	1	6	7.7	7.31	0.6
-2	1	6	436.48	467.39	5.52
-1	1	6	9.38	9.35	0.54
0	1	6	723.51	730.48	5.92
1	1	6	4.69	3.94	0.49
2	1	6	88.71	92.08	2.54
3	1	6	0.04	0.29	0.53
4	1	6	0.43	0.34	0.45
5	1	6	0.22	0.18	0.51
-4	2	6	106.85	94.53	2.21
-3	2	6	0.24	2.94	0.53
-2	2	6	20.27	24.42	1.33
-1	2	6	93.66	103.03	2.51
0	2	6	22.09	21.34	0.99
1	2	6	2.86	2.07	0.43
2	2	6	27.01	26.41	1.34
3	2	6	113.85	122.62	3.09
4	2	6	15.13	15.19	0.77
5	2	6	16.57	17.26	0.85
-4	3	6	2.24	2.14	0.34
-3	3	6	1.12	0.99	1
-2	3	6	6.52	7.55	0.6
-1	3	6	0.48	0.18	1.16
0	3	6	4.17	3.72	0.5
1	3	6	52.67	54.74	1.96
2	3	6	14.69	13.97	0.78
3	3	6	4.79	5.14	0.56
4	3	6	14.66	17.37	0.88
5	3	6	1.39	2.5	0.33
-3	4	6	9.14	12.46	0.6
-2	4	6	4.01	2.88	0.56
-1	4	6	226.59	254.98	4.42
0	4	6	255.41	261.36	4.2
1	4	6	70.79	71.26	2.41
2	4	6	21.85	27.51	1.37
3	4	6	50.4	54.14	2.18
4	4	6	0.12	-0.68	0.93
5	4	6	2.11	3.24	0.3
-3	5	6	127.12	138.54	2.13
-2	5	6	2.04	1.39	0.45
-1	5	6	241.74	270.47	4.41
0	5	6	6.02	6.24	0.58
1	5	6	109.8	120.91	3.06
2	5	6	1.23	1.39	0.5
3	5	6	4.73	4.35	0.53
4	5	6	5.37	5.81	0.47
-2	6	6	0	0.42	0.63
-1	6	6	0.04	-0.39	0.92
0	6	6	0	0.51	0.46
1	6	6	16.78	17.69	0.81
2	6	6	15.25	15.32	0.8
3	6	6	4.14	5.59	0.48
4	6	6	9.45	11.72	0.64
-1	7	6	1.16	0.97	0.3
0	7	6	1.04	-0.04	0.8
1	7	6	0.77	1.46	0.37
2	7	6	0.29	0.39	0.74
3	7	6	0.13	0.04	0.32
-3	-4	7	0.9	0.07	0.56
-2	-4	7	11.44	10.8	0.49
-1	-4	7	4.86	4.36	0.43
0	-4	7	5.49	5.46	0.47
1	-4	7	75.34	74.18	1.68
-4	-3	7	5.28	3.9	0.33
-3	-3	7	4.82	4.04	0.43
-2	-3	7	106.72	97.96	2.64
-1	-3	7	301.48	289.65	4.42
0	-3	7	56.56	51.55	2.09
1	-3	7	165.65	156.27	3.07
2	-3	7	4.48	3.21	0.41
-4	-2	7	22.56	20.92	1.03
-3	-2	7	14.96	13.62	0.6
-2	-2	7	9.67	7.97	0.61
-1	-2	7	3.07	3.89	0.59
0	-2	7	18.25	16.38	0.89
1	-2	7	3.5	2.62	0.56
2	-2	7	8.87	8.36	0.56
3	-2	7	1.29	1.79	0.34
-4	-1	7	1.05	2.14	0.36
-3	-1	7	93.16	89.31	2.62
-2	-1	7	32.86	33.78	1.76
-1	-1	7	112.02	105.47	2.83
0	-1	7	4.66	5.14	0.6
1	-1	7	127.68	140.21	3.31
2	-1	7	66.99	69.4	2.4
3	-1	7	4.23	4.47	0.45
4	-1	7	31.67	30.78	0.96
-4	0	7	1.36	0.92	0.39
-3	0	7	1.62	1.82	0.52
-2	0	7	1.65	1.94	0.58
-1	0	7	7.22	8.65	0.61

h	k	l	F_c^2	F_o^2	σF_o^2
0	0	7	169.97	151.9	3.21
1	0	7	0	-0.63	1.18
2	0	7	196.98	200.59	3.92
3	0	7	1.19	1.96	0.5
4	0	7	32.4	30.59	1.24
-4	1	7	84.33	89.28	2.1
-3	1	7	26.96	23.9	1.23
-2	1	7	480.9	459.03	5.82
-1	1	7	6.43	6.69	0.61
0	1	7	63.61	68.22	2.29
1	1	7	6.93	8.42	0.59
2	1	7	37.51	37.99	1.75
3	1	7	201.59	208.43	3.88
4	1	7	7.45	7.38	0.49
-4	2	7	1.45	1.21	0.34
-3	2	7	0.98	0.88	0.49
-2	2	7	22.74	21.62	0.99
-1	2	7	86.34	87.65	2.65
0	2	7	5.79	5.74	0.58
1	2	7	81.81	87.03	2.55
2	2	7	1.94	1.99	0.53
3	2	7	0.01	0.45	0.99
4	2	7	0.14	-0.38	0.84
-4	3	7	27.93	27.41	0.98
-3	3	7	0.44	0.2	0.83
-2	3	7	3.45	1.33	0.58
-1	3	7	199.45	197.01	3.79
0	3	7	202.41	205.26	3.85
1	3	7	0.07	0.91	1.09
2	3	7	1.34	2.12	0.52
3	3	7	13.14	13.3	0.71
4	3	7	0.13	-1.05	0.81
-3	4	7	67.48	66.65	1.8
-2	4	7	0.28	0	0.98
-1	4	7	4.24	4.32	0.56
0	4	7	2.4	1.71	0.58
1	4	7	14.83	16.91	0.73
2	4	7	0.92	0.85	1.06
3	4	7	9.92	10.23	0.6
4	4	7	8.61	10.65	0.6
-3	5	7	5.86	6.65	0.38
-2	5	7	0.47	-0.39	0.83
-1	5	7	7.98	8.78	0.6
0	5	7	62.28	72.81	2.45
1	5	7	14.09	16.46	0.84
2	5	7	33.15	44.59	1.98
3	5	7	0.4	0.94	0.45
4	5	7	0.07	-0.59	0.67
-2	6	7	18.63	19.99	0.88
-1	6	7	0.02	-0.75	0.81
0	6	7	12.13	14.99	0.69
1	6	7	8.25	9.63	0.58
2	6	7	0.21	-0.73	0.98
3	6	7	4.75	5.7	0.42
4	6	7	0.1	0.13	0.25
0	7	7	7.59	9.18	0.5
1	7	7	3.88	4.36	0.39
2	7	7	5.11	7.88	0.4
3	7	7	0.15	-0.23	0.27
-1	-4	8	31.24	23.95	0.94
0	-4	8	0.14	0.24	0.49
-3	-3	8	0.1	0.3	0.54
-2	-3	8	28.69	26.25	1.26
-1	-3	8	0.56	0.13	0.92
0	-3	8	8.6	8.44	0.48
1	-3	8	0.67	0.34	0.67
-3	-2	8	0.14	-0.25	0.69
-2	-2	8	0.77	0.86	0.93
-1	-2	8	17.18	15.59	0.85
0	-2	8	0.22	0.05	0.92
1	-2	8	58.29	55.5	1.91
2	-2	8	2.6	2.63	0.38
-4	-1	8	5.97	4.55	0.37
-3	-1	8	3.25	2.81	0.45
-2	-1	8	155.74	146.69	3.17
-1	-1	8	0.89	1.71	0.52
0	-1	8	317.31	305.09	4.8
1	-1	8	2	2.55	0.52
h	k	l	F_c^2	F_o^2	σF_o^2
2	-1	8	65.88	62.5	2.12
3	-1	8	0.1	0	0.66
-4	0	8	340.52	337.22	3.26
-3	0	8	15.9	17.51	0.96
-2	0	8	425.26	419.55	5.45
-1	0	8	46.07	40.46	1.88
0	0	8	3.09	4.23	0.55
1	0	8	17.8	16.78	0.86
2	0	8	8.48	7.78	0.62
3	0	8	43.98	42.13	1.63
-4	1	8	1.13	1.1	0.29
-3	1	8	5.71	5.68	0.53
-2	1	8	16.47	14.84	0.72
-1	1	8	14.91	15.62	0.77
0	1	8	7.03	6.51	0.59
1	1	8	4.62	3.75	0.56
2	1	8	13.92	14.22	0.76
3	1	8	1.47	2.04	0.49
4	1	8	10.43	11.31	0.56
-4	2	8	11.56	10.28	0.5
-3	2	8	0.01	0.24	0.93
-2	2	8	30.68	28.64	1.4
-1	2	8	35.42	36.72	1.86
0	2	8	33.32	35.21	1.73
1	2	8	256.02	233.87	4.15
2	2	8	0.62	0.99	0.52
3	2	8	156.31	166.7	3.28
4	2	8	0.16	0.23	0.67
-3	3	8	109.46	118.56	2.31
-2	3	8	0.24	-2.31	1.14
-1	3	8	361.88	371.12	5.26
0	3	8	1.58	1.23	0.54
1	3	8	139.16	143.87	3.34
2	3	8	0.82	0.13	1.05
3	3	8	11.01	8.77	0.58
4	3	8	7.18	7.89	0.42
-3	4	8	6.71	6.19	0.34
-2	4	8	2.02	2.46	0.47
-1	4	8	1.9	2.48	0.52
0	4	8	82.85	95.85	2.77
1	4	8	34.54	37.07	1.85
2	4	8	4.7	5.31	0.56
3	4	8	6.13	7.99	0.53
4	4	8	21.18	25.53	1.1
-2	5	8	31.71	35.24	1.27
-1	5	8	0.31	-1.07	0.94
0	5	8	4.63	4.9	0.55
1	5	8	0.11	0.55	1
2	5	8	0.03	-0.18	0.83
3	5	8	0.09	-0.28	0.76
4	5	8	3.89	4.96	0.32
-1	6	8	0.06	-0.25	0.65
0	6	8	45.32	56.47	1.77
1	6	8	9.46	12.4	0.53
2	6	8	19.8	22.28	1.17
3	6	8	0.95	-0.38	0.63
0	7	8	9.63	10.33	0.51
1	7	8	2.34	3.09	0.31
2	7	8	4.48	5.56	0.32
-1	-3	9	0.21	0.09	0.54
0	-3	9	0.01	-0.32	0.5
-2	-2	9	5.65	4.5	0.39
-1	-2	9	3.25	2.29	0.42
0	-2	9	4.19	4.72	0.42
1	-2	9	1.15	1.08	0.33
-3	-1	9	4.72	3.9	0.34
-2	-1	9	3.68	3.88	0.42
-1	-1	9	149.05	132.04	2.85
0	-1	9	38.34	35.91	1.68
1	-1	9	2.9	2.25	0.45
2	-1	9	0.24	-0.13	0.87
-3	0	9	10.19	10.16	0.5
-2	0	9	11.35	9.43	0.59
-1	0	9	13.19	14.01	0.6
0	0	9	3.1	3.81	0.52
1	0	9	24.49	20.85	1.09
2	0	9	0.6	0.7	0.44
3	0	9	0.47	0.2	0.59
-3	1	9	9.8	10.08	0.57
-2	1	9	6.97	6.38	0.55
h	k	l	F_c^2	F_o^2	σF_o^2
-1	1	9	17.2	15.66	0.78
0	1	9	83.33	78.3	2.49
1	1	9	145.8	140.52	3.21
2	1	9	8.15	7.85	0.56
3	1	9	21.06	22.58	1.11
-3	2	9	124.3	121.91	2.19
-2	2	9	0.03	-1.14	0.94
-1	2	9	60.41	66.95	2.37
0	2	9	0.01	-1.83	0.99
1	2	9	0.68	0.22	0.52
2	2	9	0.51	-1.38	1.04
3	2	9	4.99	5.51	0.44
-3	3	9	16.87	17.71	0.88
-2	3	9	0.05	0.31	0.4
-1	3	9	5.25	5.83	0.56
0	3	9	5.53	4.54	0.55
1	3	9	47	48.72	2.03
2	3	9	64.02	65.38	2.14
3	3	9	21.56	24.1	1.21
-2	4	9	2.75	3.42	0.4
-1	4	9	1.22	1.32	0.43
0	4	9	8.65	9.19	0.6
1	4	9	9.48	10.05	0.58
2	4	9	2.17	2.5	0.45
3	4	9	2.01	1.79	0.38
-2	5	9	129.5	144.44	1.9
-1	5	9	5.82	6.72	0.45
0	5	9	181.89	209.82	3.28
1	5	9	12.22	14.61	0.71
2	5	9	22.22	25.14	1.22
3	5	9	0.5	0.18	0.56
0	6	9	1.85	1.5	0.32
1	6	9	0.07	0.25	0.34
2	6	9	0.03	-0.59	0.59
-1	-1	10	11.7	9.59	0.51
0	-1	10	5.66	4.1	0.38
1	-1	10	0.33	-0.02	0.63
-2	0	10	1.4	1.35	0.34
-1	0	10	69.64	60.7	1.83
0	0	10	161.55	135.74	2.69
1	0	10	2.23	2.92	0.4
2	0	10	9.53	8.85	0.46
-2	1	10	-0.2	-1.23	0.7
-1	1	10	159.86	147.56	2.79
1	1	10	93.18	85.37	2.17
2	1	10	0.02	-1.02	0.68
-2	2	10	1.89	1.25	0.36
-1	2	10	3.02	2.52	0.45
0	2	10	2.58	1.92	0.44
1	2	10	25	23.01	1.18
2	2	10	56.19	51.09	1.59
3	2	10	7.98	8.22	0.43
-2	3	10	27.43	25.82	1.06
-1	3	10	2.95	3.06	0.42
0	3	10	3.88	3.49	0.47
1	3	10	0.61	0.76	0.4
2	3	10	1.21	0.87	0.76
3	3	10	2.47	2.28	0.31
-1	4	10	0.01	-0.2	0.65
0	4	10	12.75	14.09	0.73
1	4	10	7.86	8.92	0.47
2	4	10	17.29	18.68	0.87
-1	5	10	0.13	0.18	0.45
0	5	10	18.66	22.01	1.07
1	5	10	7.21	9.44	0.46
2	5	10	1.75	1.88	0.3
0	0	11	0	-0.78	0.49
-1	1	11	0.65	-0.13	0.55
0	1	11	0.01	0.11	0.31
1	1	11	10.27	7.74	0.4
-1	2	11	4.6	3.14	0.34
0	2	11	4.05	3.49	0.34
1	2	11	9.58	8.26	0.4
0	3	11	33.65	27.98	1.13
1	3	11	13.9	11.26	0.58
0	4	11	14.24	13.58	0.72
1	4	11	5.64	5.4	0.32

A3.3 ALTXL

h	k	l	F_c^2	F_o^2	σF_o^2
2	0	0	826.51	874.88	19.53
4	0	0	30.59	33	1.91
6	0	0	2731.47	2793	61.23
8	0	0	132.74	115.23	6.25
1	1	0	1054.45	976.67	14.71
2	1	0	35.47	39.56	4.01
3	1	0	3446.86	3527.29	51.64
4	1	0	239.22	201.29	6.03
5	1	0	30.19	28.2	1.63
6	1	0	12.11	10.34	1.7
7	1	0	23.19	22.39	1.96
8	1	0	0.58	-2.26	5.91
9	1	0	7.45	3.21	6.82
0	2	0	7360.74	7035.47	114.25
1	2	0	1.34	-6.38	5.81
2	2	0	1005.42	987.33	15.69
3	2	0	18.65	19.37	1.56
4	2	0	17.42	18.3	1.42
5	2	0	516.48	485.55	10.58
6	2	0	136.17	138.83	5.27
7	2	0	0.66	3.46	5.57
8	2	0	4.85	1.32	6.02
9	2	0	75.77	76.26	3.1
1	3	0	2530.61	2524.83	37.27
2	3	0	10.62	9.74	3.17
3	3	0	1493.81	1525.13	23.91
4	3	0	79.09	76.28	2.96
5	3	0	653.09	652.78	13.12
6	3	0	47.22	45.07	3.11
7	3	0	50.98	58.76	5.04
8	3	0	0.12	0.29	6.26
0	4	0	7179.02	7141.72	109.77
1	4	0	2543.78	2540.75	37.95
2	4	0	406.85	400.25	8.56
3	4	0	57.83	59.59	2.25
4	4	0	232.73	231.57	7.41
5	4	0	1340.19	1330.22	22.86
6	4	0	304.28	310.92	9.59
7	4	0	99.15	110.03	7.2
8	4	0	147.89	151.46	5.66
1	5	0	1198.2	1268.62	24.19
2	5	0	1262.48	1390.49	23.85
3	5	0	0.99	2.1	4.83
4	5	0	12.01	11.14	1.79
5	5	0	177.93	185.01	7.09
6	5	0	217.21	224.88	8.43
7	5	0	0.07	1.16	6.35
8	5	0	187.67	204.58	8.3
0	6	0	1200.69	1236.38	20.98
1	6	0	279.64	279.35	10.77
2	6	0	192.92	210.5	7.37
3	6	0	14.75	15.7	5.69
4	6	0	53.44	52.33	2.37
5	6	0	34.41	32.67	3.66
6	6	0	91.26	92.84	4.64
7	6	0	3.95	9.21	3.18
1	7	0	13.26	11.71	2.38
2	7	0	38.68	31.28	1.98
3	7	0	1048.89	996.18	18.68
4	7	0	273.42	275.38	9.29
5	7	0	6.41	-2.25	6.23
6	7	0	50.46	52.86	2.56
7	7	0	19.7	25.67	3.24
0	8	0	10.71	-0.11	5.91
1	8	0	1000.51	1000.26	19.06
2	8	0	83.38	78.03	2.9
3	8	0	17.05	13.18	2.1
4	8	0	96.63	91.75	3.53
5	8	0	2.87	0.8	6.72
6	8	0	93.93	97	3.6
1	9	0	80.19	76.8	2.83
2	9	0	44.3	43.46	2.9
3	9	0	229.95	230.93	8.67
4	9	0	0.61	3.55	3.21
5	9	0	8.81	7.31	5.41
0	10	0	8.6	12.68	2.33
1	10	0	5.34	0.43	7.45
2	10	0	7.6	11.13	3.23
3	10	0	0.01	0.97	7.56
1	11	0	0.1	8.83	4.2
1	0	1	19.58	24.5	1.24
2	0	1	336.45	299.21	8.81
3	0	1	260.42	261.57	8.68
4	0	1	378.29	383.75	11.61
5	0	1	51.82	50.17	2.75
6	0	1	363.93	360.36	13.95
7	0	1	19.77	13.32	2.75
8	0	1	33.54	35.89	3.1
9	0	1	37.74	37.01	3.67
-9	1	1	101.09	93.26	5.54
-8	1	1	3.55	3.67	2.84
-7	1	1	58.56	48.65	3.03
-6	1	1	112.36	120.19	5.87
-5	1	1	169.71	161.86	8.71
-4	1	1	336.63	323.03	10.61
-3	1	1	8508.75	8825.21	179.03
-2	1	1	109.58	123.73	6.04
-1	1	1	151.02	142.37	5.51
0	1	1	110.14	97.64	3.03
1	1	1	152.51	142.73	5.7
2	1	1	109.25	116.74	5.92
3	1	1	8517.24	8625.17	175.01
4	1	1	337.18	309.21	10.49
5	1	1	170.12	161.15	8.61
6	1	1	112.53	117.14	6.23
7	1	1	58.33	48.77	3.03
7	1	1	58.33	48.77	3.03
8	1	1	3.55	9.28	2.81
9	1	1	101.36	104.78	5.08
-9	2	1	4.21	3.51	9.74
-8	2	1	63.01	65.2	4.05
-7	2	1	15.73	2.51	7.8
-6	2	1	62.17	62.68	2.91
-5	2	1	46.52	48.2	2.57
-4	2	1	390.1	398.1	12.3
-3	2	1	134.84	145.4	6.85
-2	2	1	379.75	393.34	10.75
-1	2	1	563.37	534.42	13.01
0	2	1	2036.41	2026.24	29.77
1	2	1	561.87	532.74	13.13
2	2	1	377.92	392.03	10.89
3	2	1	134.04	152.7	7.27
4	2	1	392.88	377.21	11.89
5	2	1	46.89	50.49	2.79
6	2	1	61.98	61.96	3.55
7	2	1	15.88	11.9	2.82
8	2	1	62.43	63.54	4.05
9	2	1	4.31	-2.1	10.19
-8	3	1	116.31	107.15	6.39
-7	3	1	62.02	55.45	3.29
-6	3	1	325.07	302.15	12.71
-5	3	1	288.51	291.35	11.88
-4	3	1	60.25	61.2	2.94
-3	3	1	1112.07	1172.7	26.83
-2	3	1	1888.08	1988.95	42.48
-1	3	1	2146.31	2088.9	44.09
0	3	1	136.18	114.84	5.39
1	3	1	2148.91	1930.27	40.94
2	3	1	1891.35	1939.24	41.5
3	3	1	1113.3	1172.39	26.98
4	3	1	59.86	61.82	3.67
5	3	1	290.38	308.02	12.16
6	3	1	323.61	321.62	12.97
7	3	1	61.94	58.29	3.37
8	3	1	116.58	121.75	6.66
-8	4	1	125.22	137.44	8.11
-7	4	1	42.98	44.17	3.1
-6	4	1	373.43	393.37	14.83
-5	4	1	828.15	842.26	22.73
-4	4	1	442.74	422.48	13.99
-3	4	1	98.67	104.8	5.85
-2	4	1	538.86	565.04	15.06
-1	4	1	155.72	154.24	7.11
0	4	1	0.17	-5.91	4.9
1	4	1	154	150.07	7.37
2	4	1	538.33	535.68	14.61
3	4	1	100.09	104.11	5.72
4	4	1	444.28	434.64	14.33
5	4	1	827.82	814.13	22.25
6	4	1	374.24	360.32	14.76
7	4	1	42.79	40.01	3.25
8	4	1	124.74	138.39	7.61
-8	5	1	72.52	77.06	4.24
-7	5	1	6.39	2.98	9.24
-6	5	1	30.61	25.01	3
-5	5	1	478.23	472.3	16.05
-4	5	1	220.94	229.92	10.8
-3	5	1	161.69	183.43	9.3
-2	5	1	78.51	77.15	4.32
-1	5	1	463.62	457.68	13.39
0	5	1	11.79	12.26	5
1	5	1	461.88	465.5	13.75
2	5	1	78.49	75.1	4.36
3	5	1	162.31	164.68	8.56
4	5	1	220.42	221.24	10.93
5	5	1	481.27	492.21	16.83
6	5	1	30.77	29.47	3.08
7	5	1	6.27	1.19	9.3
8	5	1	73.05	76.45	4.29
-7	6	1	1.85	-1.93	9.95
-6	6	1	87.97	92.81	5.11
-5	6	1	208.12	214.51	10.99
-4	6	1	66.16	73.51	3.34
-3	6	1	27.18	29.92	2.57
-2	6	1	51.88	54.11	2.72
h	k	l	F_c^2	F_o^2	σF_o^2
-1	6	1	94.55	97.34	5.44
0	6	1	33.71	23.76	2.98
1	6	1	93.76	106.4	6.01
2	6	1	52.01	47.88	2.86
3	6	1	26.54	26.44	2.75
4	6	1	66.33	61.53	3.37
5	6	1	207.63	202.27	10.76
6	6	1	88.15	88.11	4.39
7	6	1	1.92	-19.56	10.24
-7	7	1	62.05	68.12	4.15
-6	7	1	36.49	36.07	3.44
-5	7	1	129.98	128.92	6.2
-4	7	1	149.43	150.93	7.71
-3	7	1	244.06	257.41	12.19
-2	7	1	41.81	40.83	2.77
-1	7	1	192.16	198.65	10.33
0	7	1	54.63	49.32	2.18
1	7	1	192.29	180.94	9.5
2	7	1	41.69	36.84	2.96
3	7	1	244.58	229.93	12.28
4	7	1	149.42	149.03	8.07
5	7	1	130.45	133.41	7.3
6	7	1	36.41	38.51	3.49
7	7	1	62.11	68.38	4.44
-6	8	1	177.87	178.75	8.92
-5	8	1	125.38	121.98	6.35
-4	8	1	9.95	6.95	8.97
-3	8	1	20.13	21.05	2.98
-2	8	1	20.86	23.09	2.87
-1	8	1	69.7	69.19	3.31
-1	8	1	69.7	69.19	3.31
0	8	1	549.88	551.76	15.48
1	8	1	69.47	68.59	3.6
2	8	1	21.16	21.04	3.12
3	8	1	20.58	25.82	3.13
4	8	1	9.78	8.23	3.17
5	8	1	125.64	122.24	6.8
6	8	1	178.18	187.01	10.38
-5	9	1	44.37	52.88	4.06
-4	9	1	128.99	131.83	6.73
-3	9	1	2.59	1.17	9.12
-2	9	1	13.89	16.04	3.01
-1	9	1	67.21	63.72	3.94
0	9	1	95.4	97.52	3.64
1	9	1	67.87	58.5	3.72
2	9	1	14.13	15.56	3.31
3	9	1	2.66	-6.42	9.98
4	9	1	129.79	119.21	5.78
5	9	1	44.32	48.01	4.15
-3	10	1	2.08	-14.65	10.21
-2	10	1	7.14	8.49	3.36
-1	10	1	5.74	-7.97	9.18
0	10	1	10.97	-0.71	6.8
1	10	1	5.67	9.3	3.49
2	10	1	7.07	-8.23	11.12
3	10	1	2.03	-8.31	11.09
0	11	1	45.81	50.69	3.03
0	0	2	493.66	496.47	11.55
1	0	2	220.84	210.09	6.94
2	0	2	61.86	71.04	4.01
3	0	2	138.26	188.23	7.49
4	0	2	1028.94	1010.54	23.87
5	0	2	87.49	79.8	4.32
6	0	2	224.84	219.38	10.97
7	0	2	69.45	76.3	3.98
8	0	2	2.74	0.29	8.31
9	0	2	10.31	5.43	6.1
-9	1	2	13.8	-6.99	10.16
-8	1	2	26.29	21.35	2.98
-7	1	2	39.85	47.24	3
-6	1	2	71.12	66.21	4.03
-5	1	2	138.94	133.59	6.9
-4	1	2	579.82	617.13	16.22
-3	1	2	872.83	850.16	20.01
-2	1	2	515.36	494.56	12.6
-1	1	2	750.48	794.61	17.8
0	1	2	1910.89	1915.41	28.08
1	1	2	754.68	784.99	17.72
2	1	2	516.29	492.54	12.67
3	1	2	872.69	858.48	20.18
4	1	2	578.53	610.98	16.18
5	1	2	138.59	158.63	8.52
6	1	2	71.49	73.58	3.36
7	1	2	40.16	29.87	3.06
8	1	2	26.21	22.36	3.03
9	1	2	13.5	15.22	3.48
-8	2	2	114.48	115.44	5.77
-7	2	2	34.64	29.18	2.93
-6	2	2	9.84	7.73	2.44
-5	2	2	0.83	4.97	2.19
-4	2	2	170.46	181.1	8.63
-3	2	2	866.7	866.18	20.59
-2	2	2	1269.98	1279.03	28.07
-1	2	2	372.28	393.7	10.65
0	2	2	5281.91	5134.31	73.82

h	k	l	F_c^2	F_o^2	σF_o^2
1	2	2	373.5	384.74	10.72
2	2	2	1273.95	1295.64	28.5
3	2	2	866.95	848.66	20.33
4	2	2	170.58	174.74	8.59
5	2	2	0.79	5.39	7.06
6	2	2	9.94	-5.49	7.87
7	2	2	34.65	36.39	3.01
8	2	2	114.71	113.21	5.7
-8	3	2	214.64	229.77	12.59
-7	3	2	99.03	96.62	4.84
-6	3	2	275.96	264.36	12.14
-5	3	2	146.06	149.88	8.01
-4	3	2	95.19	106.56	5.66
-3	3	2	537.04	549.8	14.89
-2	3	2	151.02	124.52	6.25
-1	3	2	579.58	547.93	13.9
0	3	2	2952.93	3213.16	47.07
1	3	2	579.33	557.22	14.26
2	3	2	149.99	146.15	7.23
3	3	2	537.7	528.57	14.68
4	3	2	94.11	92.9	5.11
5	3	2	146.09	141.07	7.71
6	3	2	276.69	252.86	12.62
7	3	2	98.96	97.36	5.6
8	3	2	215.86	212.09	11.59
-8	4	2	114.69	132.63	7.45
-7	4	2	43.58	40.65	3.12
-6	4	2	205.7	206.24	10.59
-5	4	2	275.14	275.67	11.74
-4	4	2	247.32	250.92	10.69
-3	4	2	527.89	557.01	15.54
-2	4	2	411.27	374.93	11.53
-1	4	2	283.16	263.67	9.11
0	4	2	0.15	-0.97	3.64
1	4	2	282.94	248.65	9.15
2	4	2	412.33	365.76	11.71
3	4	2	528.37	567.85	16.23
4	4	2	248.94	254.66	11.4
5	4	2	274.47	274.81	12.62
6	4	2	206.08	214.71	11.24
7	4	2	43.66	35.82	3.31
8	4	2	115.06	117.16	5.94
-8	5	2	10.22	-11.52	10.33
-7	5	2	20.37	21.79	3.05
-6	5	2	67.01	64.25	3.82
-5	5	2	5.42	-8.06	8.04
-4	5	2	163.25	171.2	9.28
-3	5	2	1.19	-3.7	6.89
-2	5	2	207.44	207.33	9.32
-1	5	2	56.9	59.74	3.29
0	5	2	1.94	16.84	8.21
1	5	2	57.31	57.78	3.49
2	5	2	208.68	195.85	9.61
3	5	2	1.16	0.46	2.43
4	5	2	162.52	151.76	7.94
5	5	2	5.37	5.8	8.57
6	5	2	67.74	68.64	3.8
7	5	2	20.2	8.13	9.81
8	5	2	10.38	6.27	10.98
-7	6	2	4.4	-6.83	9.69
-6	6	2	1.3	-16.8	8.56
-5	6	2	78.72	76.39	3.51
-4	6	2	203.44	200.8	10.43
-3	6	2	22.13	26.06	2.55
-2	6	2	766.18	811.97	21.52
-1	6	2	246.49	277.13	11.16
0	6	2	254.48	268.6	8.62
1	6	2	247.98	251.66	11.31
2	6	2	767.58	744.54	20.61
3	6	2	22.23	27.2	2.77
4	6	2	204.17	190.13	10.66
5	6	2	78.38	73.56	3.96
6	6	2	1.31	-3.98	9.12
7	6	2	4.48	4.23	10.35
-7	7	2	18.26	19.75	3.68
-6	7	2	2.11	6.9	9.33
-5	7	2	35.54	37.43	3.24
-4	7	2	130.4	122.79	6.78
-3	7	2	81.77	80.93	4.11
-2	7	2	184.86	209.08	10.93
-1	7	2	135.17	131.04	7.32
0	7	2	423.66	429.85	10.53
1	7	2	136.03	120.49	6.04
2	7	2	184.35	185.43	9.59
3	7	2	82.37	69.17	3.87
4	7	2	130.02	125.99	6.65
5	7	2	35.51	34.91	3.37
6	7	2	2.2	-8.11	9.74
7	7	2	18.48	13.84	3.89
-6	8	2	24.77	25.79	3.77
-5	8	2	238.69	226.61	12.29
-4	8	2	16.05	20.57	3.08
-3	8	2	147.85	135.77	7.23
-2	8	2	10.18	15.03	2.74
-1	8	2	44.15	41.51	2.98
0	8	2	52.75	49.45	2.38
1	8	2	43.59	44.54	3.31
2	8	2	10.17	8.16	3.05
3	8	2	148.33	142.9	7.25
4	8	2	16.4	10.36	3.25
5	8	2	239.26	229.11	12.55
6	8	2	24.42	11.36	11.72
-5	9	2	0.47	-19.47	10.52
-4	9	2	13.57	15.87	3.55
-3	9	2	6.81	11.03	3
-2	9	2	119.6	124.63	6.9
-1	9	2	46.1	45.43	3.25
0	9	2	2.96	0.58	2.73
1	9	2	45.75	51.7	3.67
2	9	2	119.22	110.01	5.75
3	9	2	6.72	2.84	3.31
4	9	2	13.44	9.95	3.72
5	9	2	0.49	6.59	10.69
-3	10	2	15.71	12.76	3.67
-2	10	2	8.11	-2.26	10.35
-1	10	2	74.04	74.37	3.89
0	10	2	42.44	41.36	3.06
1	10	2	74.83	68.86	4.54
2	10	2	8.01	7.47	3.8
3	10	2	15.84	3.36	11.18
1	0	3	5039.73	4957.56	100.96
2	0	3	3031.5	3112.54	64.54
3	0	3	104.33	86.85	4.89
4	0	3	265.44	262.04	10.06
5	0	3	0.18	-6.37	6.97
6	0	3	47.68	50.25	2.82
7	0	3	95.5	99.13	5.41
8	0	3	128.8	136.53	7.13
9	0	3	60.86	71.2	4.1
-8	1	3	24.21	23.24	3
-7	1	3	50.97	50.66	3.1
-6	1	3	125.46	124.48	6.71
-5	1	3	443.17	434.36	14.19
-4	1	3	25.51	24.76	2.08
-3	1	3	1800.52	1826.02	39.6
-2	1	3	1159.6	1210.74	26.78
-1	1	3	1726.23	1758.11	37.23
0	1	3	1557.5	1563.6	23.5
1	1	3	1722.01	1771.19	37.54
2	1	3	1158.15	1225.83	27.12
3	1	3	1799.43	1832.92	39.74
4	1	3	25.89	27.73	2.17
5	1	3	444.97	450.22	14.66
6	1	3	125.41	113.72	5.84
7	1	3	51.05	59.19	3.34
8	1	3	24.1	22.88	3.08
-8	2	3	82.96	84.27	4.68
-7	2	3	21.76	22.43	2.82
-6	2	3	0.16	-1.55	7.44
-5	2	3	421.03	429.13	14.43
-4	2	3	244.15	239.84	9.75
-3	2	3	600.71	623.32	16.05
-2	2	3	584.29	566.43	14.46
-1	2	3	601.69	587.78	14.5
0	2	3	439.03	470.39	12.16
1	2	3	800.81	565.75	14.28
2	2	3	583.58	570.11	14.6
3	2	3	801.48	610.82	16.13
4	2	3	244.38	235.19	9.92
5	2	3	422.92	428.82	14.37
6	2	3	0.19	-13.17	8.06
7	2	3	21.79	22.22	2.98
8	2	3	83.01	86.84	5.16
-8	3	3	236.39	248.58	13.03
-7	3	3	23.44	30.42	2.96
-6	3	3	211.98	217.82	11.52
-5	3	3	165.89	157.19	8.57
-4	3	3	115.02	123.45	6.4
-3	3	3	36.04	38.24	2.1
-2	3	3	2011.36	2040.83	44.01
-1	3	3	411.01	402.38	11.42
0	3	3	41.1	39.7	1.53
1	3	3	410.01	393.13	11.6
2	3	3	2013.57	2079.52	44.84
3	3	3	35.81	36.62	2.51
4	3	3	115.45	118.63	6.15
5	3	3	165.59	162.82	9.28
6	3	3	211.83	217.77	11.02
7	3	3	23.56	31.19	3.01
8	3	3	236.14	249.87	13.55
-8	4	3	44.62	48.94	3.74
-7	4	3	51.1	52.83	3.31
-6	4	3	139.53	152.75	8.76
-5	4	3	303.35	303.18	12.45
-4	4	3	220.92	208.27	10.19
-3	4	3	1967.92	2062.68	45.47
-2	4	3	754.37	808.52	20.15
-1	4	3	924.08	949.92	22.61
0	4	3	500.53	500.29	9.78
1	4	3	923.07	932.57	22.49
2	4	3	756.25	766.17	19.62
3	4	3	1972	1953.78	43.52
4	4	3	221.02	216.52	10.93
5	4	3	305.51	268.11	12.8
6	4	3	138.51	145.73	7.61
7	4	3	50.92	52.08	3.48
8	4	3	44.69	45.07	3.89
-7	5	3	8.09	10.74	3
-6	5	3	255.61	257.56	12.72
-5	5	3	290.38	285.77	12.85
-4	5	3	327.91	347.02	13.19
-3	5	3	18.55	21.76	2.38
-2	5	3	240.38	267.27	10.69
-1	5	3	545.21	540.91	15.46
0	5	3	553.09	573.67	11.43
1	5	3	544.67	551.51	15.64
2	5	3	239.92	246.15	10.66
3	5	3	18.42	23.64	2.65
4	5	3	330.88	320.89	13.11
5	5	3	290.78	295.36	13.62
6	5	3	255.3	267.64	13.52
7	5	3	8.15	13.72	3.17
-7	6	3	0.05	4.67	9.5
-6	6	3	0.27	3.65	2.91
-5	6	3	66.34	68.26	3.43
-4	6	3	0.08	-10.21	8.13
-3	6	3	154.37	145.03	7.87
-2	6	3	288	295.98	11.87
-1	6	3	25.27	28.22	2.38
0	6	3	215.35	228.26	7.62
1	6	3	25.43	25.37	2.58
2	6	3	287.51	270.56	11.92
3	6	3	154.48	149.42	7.8
4	6	3	0.06	-10.62	8.71
5	6	3	66.66	65.37	3.7
6	6	3	0.34	2.03	9.35
7	6	3	0.05	-11.96	10.66
-6	7	3	0.07	-3.2	9.26
-5	7	3	10.14	13.13	2.98
-4	7	3	14.61	6.92	8.64
-3	7	3	407.09	412.53	15.38
-2	7	3	236.5	226.87	11.33
-1	7	3	48.77	46.52	2.82
0	7	3	60.98	62.12	2.25
1	7	3	48.49	48.19	3.03
2	7	3	237.25	228.05	11.33
3	7	3	407.24	388.58	15.35
4	7	3	14.9	18.78	3.08
5	7	3	10.06	6.82	9.66
6	7	3	0.07	0.88	3.53
-8	8	3	29.72	26.73	3.84
-5	8	3	46.59	43.11	3.68
-4	8	3	48.11	47.69	3.41
-3	8	3	349.77	342.39	14.91
-2	8	3	45.78	50.51	3.13
-1	8	3	58.45	58.81	4.08
0	8	3	1026.02	1032.78	19.66
1	8	3	59.02	60.19	3.46
2	8	3	45.77	44.24	3.36
3	8	3	350.15	337.44	15
4	8	3	48.89	44.62	3.56
5	8	3	46.72	47.46	3.93
6	8	3	29.62	30.49	4.01
-4	9	3	29.51	34.74	3.74
-3	9	3	21.12	24.57	3.22
-2	9	3	16.6	18.56	3.06
-1	9	3	29.42	32.26	3.13
0	9	3	96.31	89.78	3.27
1	9	3	29.11	28.75	3.49
2	9	3	16.54	5.27	3.36
3	9	3	21.05	9.71	10.21
4	9	3	29.82	34.15	3.91
-3	10	3	5.24	10.6	3.62
-2	10	3	23.26	24.34	3.6
-1	10	3	4.96	2.86	9.67
0	10	3	88.12	82.14	3.16
1	10	3	4.98	-2.55	10.85
2	10	3	23.24	10.81	11.57
3	10	3	5.26	7.85	3.84
0	0	4	9445.48	9427.45	190.7
1	0	4	897.35	829.32	19.31
2	0	4	10.66	12.5	1.58
3	0	4	1262.78	1292.96	29.39
4	0	4	118.77	124.93	7.15
5	0	4	126.9	141.03	7.95
6	0	4	717.87	734.27	20.97
7	0	4	54.8	54.33	3.18
8	0	4	86.96	83.67	4.48
-8	1	4	212.77	207.92	11.47
-7	1	4	60.85	60.56	3.27
-6	1	4	173.99	160.39	8.64
-5	1	4	131.49	128.92	6.78
-4	1	4	264.35	263.39	10.18
-3	1	4	424.64	413.44	12.23
-2	1	4	639.65	735.58	17.88
-1	1	4	3184.94	3147.71	65.37
0	1	4	403.47	405.84	9.45
1	1	4	3194.17	3244.82	67.35
2	1	4	641.64	728.57	17.81
3	1	4	425.49	439.71	12.83
4	1	4	264.91	251.16	10.4
5	1	4	130.63	129.13	7.02
6	1	4	173.32	160.4	8.3
7	1	4	61.33	60.68	3.58
8	1	4	213.24	210.09	11.54
-8	2	4	2.13	4.17	9.09
-7	2	4	7.66	-0.28	8.45
-6	2	4	396.4	391.88	14.6
-5	2	4	732.99	732.25	20.35
-4	2	4	651.87	657.09	17.9

h	k	l	F_c^2	F_o^2	σF_o^2
-3	2	4	846.3	890.08	21.67
-2	2	4	427.77	436.82	12.3
-1	2	4	748.08	705.28	17.14
0	2	4	361.04	348.38	7.33
1	2	4	750.7	727.62	17.76
2	2	4	429.63	431.81	12.56
3	2	4	847.52	859.74	21.29
4	2	4	651.01	636.5	17.78
5	2	4	735.32	713.84	20.35
6	2	4	397.23	371.44	14.38
7	2	4	7.82	0.83	8.88
8	2	4	2.06	6.71	3.25
-8	3	4	58.14	59.29	3.79
-7	3	4	42.54	39.28	3.12
-6	3	4	250.3	249.13	12.28
-5	3	4	294.08	286.64	12.11
-4	3	4	229.9	236.95	10.5
-3	3	4	25.8	22.91	2.1
-2	3	4	204.07	221.17	8.82
-1	3	4	523.64	506.43	13.77
0	3	4	1647.52	1599.59	24.86
1	3	4	524.68	523.96	14.46
2	3	4	205.27	216.57	9.26
3	3	4	25.72	22.4	2.32
4	3	4	230.55	234.5	10.9
5	3	4	292.6	301.57	12.88
6	3	4	250.07	269.1	12.81
7	3	4	42.28	47.19	3.29
8	3	4	58.51	56	3.89
-8	4	4	122.03	125.08	6.92
-7	4	4	35.85	35.91	3.17
-6	4	4	115.68	123.91	6.35
-5	4	4	517.22	515.02	16.79
-4	4	4	196.1	195.49	9.76
-3	4	4	393.18	414.8	13.54
-2	4	4	64.2	98.25	4.96
-1	4	4	195.69	203.61	8.59
0	4	4	49.27	55.79	2.04
1	4	4	196.73	180.38	9.28
2	4	4	64.38	59.34	2.75
3	4	4	393.38	411.89	14.07
4	4	4	194.55	189.41	10.09
5	4	4	518.24	528.49	17.55
6	4	4	116.13	105.64	5.72
7	4	4	35.85	35.96	3.39
8	4	4	123.04	123.1	6.97
-7	5	4	7.99	4.48	9.74
-6	5	4	350.36	333.84	15
-5	5	4	55.4	52.83	3.68
-4	5	4	122.41	122.83	5.99
-3	5	4	2.63	0.19	7.2
-2	5	4	323.87	330.31	11.94
-1	5	4	481.97	469.91	14.49
0	5	4	1520.6	1487.59	24.29
1	5	4	483.04	463.05	14.71
2	5	4	323.94	335.22	12.74
3	5	4	2.69	2.24	2.63
4	5	4	123.07	132.42	6.01
5	5	4	55.27	55.67	3.36
6	5	4	352.55	338.66	15.24
7	5	4	8.07	9.59	3.46
-7	6	4	2.39	8.59	9.45
-6	6	4	19.15	20.78	3.06
-5	6	4	61.36	63.96	3.37
-4	6	4	610.45	611.27	19.31
-3	6	4	15.36	7.28	8.14
-2	6	4	280.2	273.4	11.88
-1	6	4	48.21	47.79	2.84
0	6	4	1249.62	1299.58	34.9
1	6	4	48.56	49.67	2.94
2	6	4	281.96	286.93	12.49
3	6	4	15.38	15.39	2.96
4	6	4	608.1	568.29	18.88
5	6	4	61.27	59.31	3.6
6	6	4	19.15	22.14	3.31
7	6	4	2.39	9.24	10.52
-6	7	4	114.04	104.83	5.7
-5	7	4	29.66	28.44	3.17
-4	7	4	26.7	28.68	3.05
-3	7	4	271.03	260.69	12.78
-2	7	4	140.65	131.63	7.61
-1	7	4	202.83	208.76	11.12
0	7	4	801.66	785.51	21.34
1	7	4	203.72	203.44	10.71
2	7	4	140.52	135.4	6.63
3	7	4	271.26	263.67	13.16
4	7	4	26.95	26.77	3.29
5	7	4	29.48	5.01	10.36
6	7	4	114.08	115.42	6.83
-5	8	4	7.32	2.62	9.95
-4	8	4	19.2	25.62	3.17
-3	8	4	15.42	16.23	3
-2	8	4	80.04	82.53	4.18
-1	8	4	17.2	16.75	2.84
0	8	4	182.55	182.6	10.59
1	8	4	17.3	8.99	9.04
2	8	4	79.63	79.92	3.8
3	8	4	15.67	14.39	3.2
4	8	4	19.13	17.63	3.41
5	8	4	7.43	5.89	10.76

h	k	l	F_c^2	F_o^2	σF_o^2
-4	9	4	7.68	4.7	3.55
-3	9	4	162.59	163.48	8.42
-2	9	4	34.36	37.8	3.29
-1	9	4	34.18	33.67	3.2
0	9	4	127.93	118.53	4.21
1	9	4	34.58	30.85	3.53
2	9	4	34.41	35.45	3.46
3	9	4	162.76	153.34	7.9
4	9	4	7.9	8.37	10.95
-2	10	4	14.5	17.56	3.56
-1	10	4	17.27	22.22	3.46
0	10	4	19.65	23.54	14.5
1	10	4	17.06	15.7	3.94
2	10	4	14.6	14.96	3.98
1	0	5	33.12	26.94	1.77
2	0	5	362.07	343.29	10.73
3	0	5	184.33	183.17	8.68
4	0	5	7.38	4.32	6.82
5	0	5	1931.56	1919.08	43.9
6	0	5	28.7	26.22	2.84
7	0	5	37.64	38.11	3.1
8	0	5	56.73	56.85	3.75
-8	1	5	28.31	25.5	3.41
-7	1	5	15.22	15.11	2.87
-6	1	5	191.89	199.77	10.4
-5	1	5	307.25	317.82	12.49
-4	1	5	143.77	136.76	6.89
-3	1	5	660.51	675.54	17.82
-2	1	5	6.83	9	1.65
-1	1	5	824.01	860.34	20.42
0	1	5	280.81	265.97	6.5
1	1	5	821.41	857.42	20.52
2	1	5	6.99	5.7	1.79
3	1	5	660.47	702	18.46
4	1	5	143.5	143.51	7.59
5	1	5	307.88	291.71	12.42
6	1	5	191.8	200.97	10.5
7	1	5	15.02	6.7	8.44
8	1	5	28.5	31.8	3.51
-8	2	5	83.33	84.44	4.36
-7	2	5	19.89	18.56	2.98
-6	2	5	38.09	37.79	2.91
-5	2	5	1558.65	1525.35	36.36
-4	2	5	398.13	383.98	13.26
-3	2	5	201.01	193.55	9.16
-2	2	5	1190.32	1167.69	27.14
-1	2	5	157.46	154.05	7.35
0	2	5	1391.81	1419.41	22.38
1	2	5	159.26	167.07	7.84
2	2	5	1188.97	1182.61	27.6
3	2	5	201.16	212.12	9.45
4	2	5	400.6	415.91	13.87
5	2	5	1561.15	1561.06	37.08
6	2	5	38.35	41.4	3.05
7	2	5	20.14	18.85	3.01
8	2	5	82.75	95.19	5.01
-8	3	5	64.31	73.08	4.05
-7	3	5	0.41	-7.73	8.49
-6	3	5	606.03	621.55	19.55
-5	3	5	97.11	89.25	5.37
-4	3	5	335.53	354.33	12.97
-3	3	5	2.72	9.05	2.08
-2	3	5	276.63	290.58	10.44
-1	3	5	296.11	326.83	10.89
0	3	5	976.16	975.18	16.47
1	3	5	295.5	326.8	11.42
2	3	5	278.61	311.28	11.38
3	3	5	2.74	5.72	7.23
4	3	5	335.92	344.41	13.3
5	3	5	97.53	90.01	4.86
6	3	5	605.28	586.65	19.24
7	3	5	0.45	-5.35	9.23
8	3	5	64.75	67.59	4.17
-7	4	5	36.94	36.74	3.24
-6	4	5	47.18	46.36	3.15
-5	4	5	10.72	-8	8.33
-4	4	5	0.49	4.1	7.42
-3	4	5	85.53	88.13	4.75
-2	4	5	183.93	185.83	9.14
-1	4	5	48.96	51.96	3.03
0	4	5	339.82	347.87	8.41
1	4	5	48.77	48.6	2.88
2	4	5	184.21	194.92	10.23
3	4	5	86.44	88.73	4.37
4	4	5	0.54	-6.33	8.28
5	4	5	10.87	7.97	8.75
6	4	5	46.9	47.36	3.39
7	4	5	36.78	38.65	3.46
-7	5	5	15.4	14.39	3.34
-6	5	5	21.7	6.11	8.8
-5	5	5	346.4	325.61	14.22
-4	5	5	7.2	9.59	2.6
-3	5	5	81.16	70.67	3.99
-2	5	5	12.5	11.16	2.29
-1	5	5	589.13	602.91	17.35
0	5	5	123.05	118.39	9.58
1	5	5	586.67	627.12	18.31
2	5	5	12.41	5.99	2.67
3	5	5	81.2	68.92	4.15
4	5	5	7.38	-8.78	8.81

h	k	l	F_c^2	F_o^2	σF_o^2
5	5	5	348.12	336.86	15.14
6	5	5	21.67	18.21	3.25
7	5	5	15.47	18.7	3.62
-6	6	5	17.29	4.1	9.64
-5	6	5	59.11	60.2	3.41
-4	6	5	102.49	103.68	5.46
-3	6	5	467.76	471.2	16.38
-2	6	5	54.42	53.45	3.15
-1	6	5	159.92	162.92	8.3
0	6	5	39.3	41.04	2.04
1	6	5	160.16	172.51	9.5
2	6	5	54.13	49.25	3.17
3	6	5	467.97	476.83	16.81
4	6	5	102.72	101.2	4.94
5	6	5	59.22	57.52	3.65
6	6	5	17.34	16.61	3.44
-6	7	5	39.61	39.03	3.79
-5	7	5	25.64	25.79	3.24
-4	7	5	59.76	67.17	3.98
-3	7	5	118.24	118.48	6.61
-2	7	5	46.46	44.31	2.98
-1	7	5	130.93	129.47	7.02
0	7	5	83.02	80.8	2.98
1	7	5	129.84	125.34	6.27
2	7	5	46.92	44.59	3.31
3	7	5	118.08	114.51	6.15
4	7	5	59.64	62.53	3.68
5	7	5	25.77	24.53	3.43
6	7	5	39.93	40.63	4.08
-5	8	5	18.54	-3.41	10.55
-4	8	5	179.21	170.37	9.37
-3	8	5	13.47	3.48	8.83
-2	8	5	10.6	5.77	8.16
-1	8	5	58.11	57.88	3.79
0	8	5	486.08	495.37	23.49
1	8	5	58.36	54.06	3.46
2	8	5	10.73	10.97	3.13
3	8	5	13.74	14.31	3.24
4	8	5	179.82	184.66	9.97
5	8	5	18.61	8.5	11.67
-4	9	5	5.08	14.65	3.56
-3	9	5	3.84	9.04	3.36
-2	9	5	67.97	76.87	4.29
-1	9	5	0.65	2.36	2.93
0	9	5	259.63	275.84	10.07
1	9	5	0.63	4.51	9.18
2	9	5	67.95	62.8	3.93
3	9	5	3.77	-1.64	10.93
4	9	5	5.18	-17.73	11.77
-1	10	5	111.13	113.58	5.92
0	10	5	216.25	230.46	15.97
1	10	5	111.3	115.16	6.37
2	10	5	9.27	6.01	3.96
0	0	6	287.37	320.4	10.49
1	0	6	0.82	-7.68	5.72
2	0	6	5.35	5.53	1.95
3	0	6	410.89	380.59	12.75
4	0	6	55.64	57.97	2.79
5	0	6	12.02	13.32	2.6
6	0	6	135.03	139.37	7.15
7	0	6	18.17	12.33	2.98
8	0	6	7.18	7.83	9.38
-8	1	6	289.01	283.98	14.27
-7	1	6	58.56	55.05	3.41
-6	1	6	2.41	-3.55	8.13
-5	1	6	133.84	152.63	8.3
-4	1	6	51.33	44.73	2.65
-3	1	6	157.37	152.73	7.83
-2	1	6	1118.98	1206.09	28.16
-1	1	6	300.24	308.55	10.42
0	1	6	517.18	534	10.98
1	1	6	299.84	315.92	10.75
2	1	6	1118.67	1193.37	28.03
3	1	6	157.17	150.11	8.33
4	1	6	50.37	51.04	2.77
5	1	6	134.65	133.92	7.46
6	1	6	2.37	0.76	8.11
7	1	6	58.71	58.95	3.43
8	1	6	289.45	271.96	14.57
-8	2	6	64.5	64.9	3.99
-7	2	6	3.55	7.33	2.84
-6	2	6	50.7	49.25	3.1
-5	2	6	9.39	6.95	7.76
-4	2	6	0.38	-0.98	7.2
-3	2	6	218.79	229.66	10.38
-2	2	6	106.79	95.59	4.87
-1	2	6	208.88	205.94	8.87
0	2	6	40.36	35.9	1.61
1	2	6	209.06	207.92	9.37
2	2	6	107.19	106.82	5.63
3	2	6	219.39	233.81	10.44
4	2	6	0.4	4.06	7.57
5	2	6	9.3	-0.67	7.87
6	2	6	50.53	47.45	3.24
7	2	6	3.52	8.45	8.88
8	2	6	64.53	63.42	4.06
-7	3	6	1.32	-4.39	8.78
-6	3	6	314.06	312.93	14.02
-5	3	6	29.99	31.06	2.74
-4	3	6	80.8	73.55	3.96

h	k	l	F_c^2	F_o^2	σF_o^2
-3	3	6	34.71	37.1	2.46
-2	3	6	415.06	417.88	13.56
-1	3	6	43.49	48.19	2.82
0	3	6	1184.63	1168	21.69
1	3	6	43.7	44.07	2.6
2	3	6	414.38	450.2	14.43
3	3	6	35.08	37.25	2.72
4	3	6	79.89	84.29	4.27
5	3	6	30.22	30.59	3
6	3	6	315.1	326.86	14.48
7	3	6	1.27	-5.94	9.23
-7	4	6	15.47	11.71	3.34
-6	4	6	63.88	65.04	3.41
-5	4	6	24.19	4.29	8.25
-4	4	6	175.55	173.2	9.37
-3	4	6	304.18	293.78	12.14
-2	4	6	30.23	33	2.41
-1	4	6	146.58	144.41	8.01
0	4	6	66.99	81.86	3.36
1	4	6	146.2	146.1	8.02
2	4	6	30.02	35.58	2.81
3	4	6	304.26	283.63	12.83
4	4	6	176.83	168.36	9.37
5	4	6	23.78	8.3	9.4
6	4	6	63.83	64.68	3.84
7	4	6	15.56	10.17	10.88
-7	5	6	80.68	76.89	4.17
-6	5	6	42.03	37.86	3.27
-5	5	6	110.94	110.79	5.84
-4	5	6	78.58	69.72	4.1
-3	5	6	70.2	73.84	3.62
-2	5	6	40.16	37.68	2.62
-1	5	6	41.64	48.13	2.67
0	5	6	2.36	2.04	5.22
1	5	6	42.13	44.86	3.05
2	5	6	40.34	39.85	3
3	5	6	71.05	70.88	3.87
4	5	6	78.23	76.99	3.86
5	5	6	111.15	105.14	5.65
6	5	6	42.21	46.86	3.55
7	5	6	80.48	82.03	4.89
-6	6	6	16.6	19.21	3.39
-5	6	6	38.86	35.22	3.22
-4	6	6	35.45	35.1	3.05
-3	6	6	30.46	28.35	2.86
-2	6	6	57.1	61.68	3.15
-1	6	6	149.52	144.75	7.89
0	6	6	320.68	334.88	9.66
1	6	6	150.42	159.68	8.51
2	6	6	56.97	55.64	3.56
3	6	6	30.58	24.32	3.22
4	6	6	35.54	30.26	3.34
5	6	6	36.33	41.25	3.55
6	6	6	16.54	16.11	3.74
-5	7	6	25.63	28.52	3.48
-4	7	6	28.04	29.33	3.12
-3	7	6	69.54	63.22	3.34
-2	7	6	4.07	3.34	7.88
-1	7	6	209.15	222.22	11.57
0	7	6	292.39	293.49	10.92
1	7	6	209.77	218.12	11.85
2	7	6	4.11	4.06	3.17
3	7	6	70.19	74.27	4.32
4	7	6	27.8	7.66	10.43
5	7	6	25.46	30.18	3.8
-4	8	6	31.72	33.1	3.67
-3	8	6	22.26	21.67	3.08
-2	8	6	23.64	23.48	3.05
-1	8	6	82.34	85.18	4.65
0	8	6	12.36	14.55	3.14
1	8	6	81.99	80.71	4.13
2	8	6	23.72	25.7	3.36
3	8	6	22.23	20.88	3.48
4	8	6	31.77	32.04	3.91
-3	9	6	22.81	20.45	3.55
-2	9	6	65.06	69.69	4.36
-1	9	6	15.75	17.08	3.31
0	9	6	0.04	3.12	3.04
1	9	6	15.6	14.68	3.68
2	9	6	64.77	67.04	4.27
3	9	6	22.72	22.55	3.96
1	0	7	2.78	-3.65	6.42
2	0	7	429.27	427.95	13.69
3	0	7	2.18	4.34	6.89
4	0	7	8.62	2.86	7.42
5	0	7	167.78	174.62	9.35
6	0	7	41.9	39.22	3.1
7	0	7	4.73	0.31	8.52
-7	1	7	39.74	37.12	3.24
-6	1	7	50.88	51.35	3.2
-5	1	7	51.94	64.66	4.3
-4	1	7	5.8	3.1	7.06
-3	1	7	109.02	97.91	5.42
-2	1	7	519.44	502.6	15.21
-1	1	7	406.01	421.61	13.38
0	1	7	935.55	917.12	16.15
1	1	7	407.54	412	13.42
2	1	7	519.29	532.34	15.8
3	1	7	109.29	115.7	5.84
4	1	7	6.15	6.83	2.44
5	1	7	51.9	49.65	3.08
6	1	7	51.66	47.88	3.43
7	1	7	39.82	34.53	3.22
-7	2	7	17.84	20.9	3.27
-6	2	7	38.99	37.96	3.08
-5	2	7	108.22	111.61	6.09
-4	2	7	283.69	283.81	12.3
-3	2	7	604.92	612.4	18.02
-2	2	7	439.11	466.98	14.45
-1	2	7	183.71	183.63	9.21
0	2	7	319.5	317.59	8.21
1	2	7	183.19	180.96	9.01
2	2	7	439.9	440.38	14.42
3	2	7	604.69	620.24	18.23
4	2	7	284.82	283.98	12.73
5	2	7	108.01	111.46	6.27
6	2	7	39	43.16	3.24
7	2	7	17.8	7.08	10
-7	3	7	1.47	2.67	9.14
-6	3	7	120.34	114.11	6.66
-5	3	7	47.31	45.65	3.01
-4	3	7	44.96	45.59	2.91
-3	3	7	40.57	43.54	2.67
-2	3	7	170.25	180.81	9.69
-1	3	7	148.71	162.59	8.52
0	3	7	597.45	584.79	12.13
1	3	7	149.72	166.77	8.68
2	3	7	170.64	166.59	9.02
3	3	7	40.61	52.49	3.12
4	3	7	45.02	44.85	3.08
5	3	7	47.15	40.87	3.24
6	3	7	119.73	113.96	5.87
7	3	7	1.4	7.25	3.37
-7	4	7	18.62	20.88	3.49
-6	4	7	66.38	66.85	4.05
-5	4	7	268.46	259.22	13
-4	4	7	34.45	30.85	2.77
-3	4	7	552.96	566.62	17.9
-2	4	7	15.69	20.31	2.43
-1	4	7	150.2	148.28	7.9
0	4	7	111.67	112.59	8.36
1	4	7	149.46	155.91	8.16
2	4	7	15.76	18.42	2.79
3	4	7	553.65	568.34	18.35
4	4	7	34.69	35.45	3.13
5	4	7	268.01	260.43	13.38
6	4	7	66.52	66.24	3.82
7	4	7	18.57	30.07	3.77
-6	5	7	40.24	40.39	3.58
-5	5	7	17.54	16.2	2.93
-4	5	7	22.75	19.81	2.79
-3	5	7	28.41	35.03	2.77
-2	5	7	1.35	-18.71	7.44
-1	5	7	114.69	112.62	5.47
0	5	7	28.66	23.27	1.88
1	5	7	115.07	117.06	6.09
2	5	7	1.36	-5.11	8.71
3	5	7	28.5	25.17	3.15
4	5	7	22.77	19.44	3.15
5	5	7	17.95	18.76	3.25
6	5	7	40.43	46.17	3.86
-6	6	7	17.47	21.26	3.49
-5	6	7	92.66	103.83	5.85
-4	6	7	8.66	4.6	8.76
-3	6	7	503.51	512.56	17.71
-2	6	7	49.99	54.87	3.2
-1	6	7	187.22	203	10.3
0	6	7	261.56	252.38	8.97
1	6	7	186.29	204.16	10.83
2	6	7	49.88	46.71	3.44
3	6	7	503.6	527.07	18.74
4	6	7	8.71	5.42	9.88
5	6	7	92.07	87.41	5.7
6	6	7	17.67	13.6	3.89
-5	7	7	3.4	6.18	9.45
-4	7	7	16.08	16.04	3.29
-3	7	7	51.26	52.64	3.31
-2	7	7	0.26	0.28	7.73
-1	7	7	79.83	74.15	3.82
0	7	7	32.16	36.03	3.12
1	7	7	80.02	80.9	4.92
2	7	7	0.26	-1.1	9.98
3	7	7	51.16	50.99	3.68
4	7	7	16.08	15.73	3.68
5	7	7	3.19	7.87	11.12
-4	8	7	64.9	61.01	4.06
-3	8	7	65.28	68.14	3.94
-2	8	7	55.46	56.31	3.49
-1	8	7	32.29	32.59	3.13
0	8	7	10.03	2.51	6.78
1	8	7	31.83	34.69	3.68
2	8	7	55.27	54.42	3.89
3	8	7	65.5	71.41	4.3
4	8	7	64.99	66.57	4.48
-2	9	7	8	3.12	10.33
-1	9	7	92.89	97.39	5.54
0	9	7	0.17	3.72	4.78
1	9	7	93.17	91.21	4.92
2	9	7	8.07	8.87	3.99
0	0	8	1854.57	1866.81	42.17
1	0	8	8.34	3.17	7.13
2	0	8	188.03	187.25	9.85
3	0	8	88.58	82.02	5.18
4	0	8	508.31	474.97	16.48
5	0	8	12.85	10.38	2.75
6	0	8	1.94	3.82	8.47
7	0	8	0.72	-3.01	9.86
-7	1	8	21.82	23.21	3.55
-6	1	8	98.82	96.38	4.91
-5	1	8	52.18	50.05	3.12
-4	1	8	166.68	172.66	9.16
-3	1	8	631.85	614	18.45
-2	1	8	244.44	238.22	10.9
-1	1	8	89.83	89.2	4.92
0	1	8	198.9	189	6.96
1	1	8	90.51	95.47	4.92
2	1	8	243.89	223.12	10.87
3	1	8	632.51	606.81	18.38
4	1	8	167.34	155.67	7.97
5	1	8	51.97	50.13	3.25
6	1	8	98.63	102.78	5.08
7	1	8	21.77	23.05	3.53
-7	2	8	24.31	27.44	3.49
-6	2	8	199.05	186.8	9.8
-5	2	8	94.15	90.04	4.67
-4	2	8	264.61	285.42	12.47
-3	2	8	401.04	387.83	14.09
-2	2	8	32.86	31.66	2.48
-1	2	8	283.82	299.61	11.81
0	2	8	102.14	102.24	3.86
1	2	8	284.23	279.22	11.99
2	2	8	32.73	28.01	2.65
3	2	8	401.61	404.5	14.85
4	2	8	265.19	263.65	12.97
5	2	8	95.05	93.21	5.11
6	2	8	198.73	190.53	10.11
7	2	8	24.42	30.49	3.68
-7	3	8	16.2	6.73	10.69
-6	3	8	83.67	80.64	4.2
-5	3	8	79.85	80.98	3.53
-4	3	8	271.82	261.77	12.79
-3	3	8	58.4	55.07	3.03
-2	3	8	128.46	118.9	6.65
-1	3	8	40.46	37.46	2.6
0	3	8	126.14	119.98	4.44
1	3	8	41.11	40.2	2.89
2	3	8	128.8	107.99	5.85
3	3	8	58.4	59.57	3.67
4	3	8	272.31	243.74	13.05
5	3	8	79.46	81.12	4.15
6	3	8	83.93	88.51	4.63
7	3	8	16.36	10.59	10.98
-6	4	8	7.07	-6.9	9.74
-5	4	8	59.18	55.5	3.63
-4	4	8	1.04	-18.8	7.97
-3	4	8	74.89	74.87	3.6
-2	4	8	37.34	36.69	2.98
-1	4	8	8.08	0.21	7.44
0	4	8	43.62	46.01	1.99
1	4	8	7.9	7.71	6.44
2	4	8	37.14	36.58	3.12
3	4	8	74.99	82.36	3.65
4	4	8	1.08	-16.61	8.83
5	4	8	59.6	59.39	3.63
6	4	8	7	3.92	10.17
-6	5	8	254.9	260.88	13.74
-5	5	8	6.71	4.7	8.74
-4	5	8	125.28	122.48	6.15
-3	5	8	553.2	516.05	17.95
-2	5	8	195.7	193.22	9.93
-1	5	8	106.37	102.99	5.15
0	5	8	379.52	398.82	10.61
1	5	8	105.77	110.75	6.39
2	5	8	195.11	202.93	10.81
3	5	8	553.19	557.14	18.98
4	5	8	125.1	126.44	7.23
5	5	8	6.61	4.7	3.34
6	5	8	256.05	282.85	14.69
-5	6	8	169.6	159.83	8.3
-4	6	8	58.73	64.59	3.48
-3	6	8	49.17	50.15	3.2
-2	6	8	49.16	43.83	3.1
-1	6	8	54.7	50.68	3.12
0	6	8	231.16	232.77	8.56
1	6	8	54.2	56.66	3.67
2	6	8	49.54	50.17	3.53
3	6	8	49.18	44.5	3.77
4	6	8	58.54	63.52	3.91
5	6	8	170.17	177.56	6.88
-4	7	8	53.85	50.99	3.77
-3	7	8	5.57	-4.41	9.26
-2	7	8	22.07	26.94	3.01
-1	7	8	108.49	107.81	5.27
0	7	8	175.28	200.12	7.58
1	7	8	106.24	109.81	5.68
2	7	8	22.11	18.87	3.58
3	7	8	5.46	-0.62	10.78
4	7	8	53.41	51.3	4.27
-3	8	8	6.89	-7.28	9.78
-2	8	8	2.04	-3.31	9.67

h	k	l	F_c^2	F_o^2	σF_o^2
-1	8	8	61.89	61.7	3.84
0	8	8	53.43	57.74	3.88
1	8	8	62.14	60.06	4.49
2	8	8	2.02	7.25	11.03
3	8	8	6.91	3.8	11.53
1	0	9	163.08	159.35	8.42
2	0	9	35.93	34.93	2.79
3	0	9	7.12	3.92	7.76
4	0	9	23.61	26.13	2.87
5	0	9	99.9	101.75	5.22
6	0	9	5.15	-5.41	9.61
-6	1	9	12.02	4.48	9.36
-5	1	9	21.53	27.65	2.91
-4	1	9	23.25	20.38	2.81
-3	1	9	225.41	201.36	10.4
-2	1	9	11.74	11.79	2.51
-1	1	9	285.47	296.13	12.33
0	1	9	112.01	107.55	4.3
1	1	9	285.11	280.25	12.14
2	1	9	11.91	11.22	2.63
3	1	9	224.67	232.85	11.64
4	1	9	23.34	23.03	2.87
5	1	9	21.57	19.88	3.03
6	1	9	12.12	15.06	3.29
-6	2	9	71.36	72.87	3.96
-5	2	9	172.44	173.1	9.44
-4	2	9	78.39	72.34	3.58
-3	2	9	7.85	4.8	7.69
-2	2	9	16.99	14.8	2.6
-1	2	9	240.67	237.51	11.3
0	2	9	706.24	683.33	14.02
1	2	9	241.21	253.16	11.59
2	2	9	17.21	6.01	8.4
3	2	9	7.89	4.92	2.75
4	2	9	77.81	79.3	3.65
5	2	9	172.2	164.63	9.37
6	2	9	71.88	81.46	4.54
-6	3	9	113.21	133.06	7.42
-5	3	9	68.83	69.38	3.55
-4	3	9	61.71	63.84	3.31
-3	3	9	2.19	4.77	7.47
-2	3	9	79.33	80.19	4.03
-1	3	9	29.72	24.17	2.67
0	3	9	165.24	152.91	5.95
1	3	9	29.56	33.16	2.96
2	3	9	79.59	78.94	3.56
3	3	9	2.17	6.27	8.3
4	3	9	62.01	60.06	3.49
5	3	9	68.6	69.9	3.79
6	3	9	113.37	117.81	6.63
-6	4	9	10.06	7.4	10.04
-5	4	9	169.27	171.26	9.31
-4	4	9	42.1	37.62	3.08
-3	4	9	4.98	4.8	7.85
-2	4	9	9.09	12.76	2.62
-1	4	9	195.56	211.94	10.66
0	4	9	528.53	519.03	12.33
1	4	9	196.04	209.8	11.24
2	4	9	9.2	7.25	3.03
3	4	9	4.86	12.93	3.01
4	4	9	41.83	40.3	3.37
5	4	9	169.44	156.95	8.78
6	4	9	9.94	3.17	10.6
-5	5	9	76.27	71.22	3.98
-4	5	9	0.24	-9.3	8.93
-3	5	9	52.22	51.13	3.24
-2	5	9	43.81	47.79	3.03
-1	5	9	39.29	39.03	3.01
0	5	9	53.02	51.51	2.32
1	5	9	39.74	38.61	3.43
2	5	9	44.27	42.71	3.46
3	5	9	52.09	55.4	3.65
4	5	9	0.21	4.01	9.83
5	5	9	75.91	72.22	4.36
-4	6	9	32.01	38.44	3.49
-3	6	9	17.08	18.42	2.98
-2	6	9	4.27	-2.67	8.59
-1	6	9	64.34	66.9	3.87
0	6	9	86.92	81.23	3.25
1	6	9	64.55	65.52	3.93
h	k	l	F_c^2	F_o^2	σF_o^2
1	2	12	28.86	6.44	9.85
2	2	12	20.93	20.3	3.41
3	2	12	10.95	14.63	3.49
-3	3	12	68.55	75.49	4.05
-2	3	12	13.42	13.29	3.29
-1	3	12	2.75	8.26	8.71
0	3	12	2.34	3.76	2.92
1	3	12	2.85	9.5	10.26
2	3	12	13.39	19.38	3.51
3	3	12	68.7	80.43	4.27
-2	4	12	52.7	60.53	3.77
-1	4	12	39.35	38.92	3.49
0	4	12	178.97	178.93	6.28
1	4	12	39.09	38.97	3.98
2	4	12	52.82	51.82	4.11
0	5	12	11.45	13.17	6.54
1	0	13	24.89	27.89	3.49
2	0	13	66.8	81.6	4.46
2	6	9	4.32	8.81	9.73
3	6	9	17.08	-3.72	10.48
4	6	9	31.78	38.8	3.99
-3	7	9	24.73	21.21	3.48
-2	7	9	28.3	30.07	3.37
-1	7	9	3.6	-1.57	8.66
0	7	9	59.17	58.17	2.62
1	7	9	3.71	1.26	11.07
2	7	9	28.49	30.11	3.99
3	7	9	24.75	22.59	4.01
-1	8	9	8.01	7.25	9.55
0	8	9	20.09	23.34	8.44
1	8	9	7.85	10.98	4.22
0	0	10	866.57	842.36	23.4
1	0	10	0.83	-6.75	7.87
2	0	10	1.9	5.58	7.99
3	0	10	1.84	2.96	2.72
4	0	10	91.66	81.76	3.99
5	0	10	9.48	6.51	3.01
6	0	10	3.34	-0.91	3.46
-6	1	10	1.49	-9.04	9.93
-5	1	10	31.85	35.74	3.2
-4	1	10	62.23	65.71	3.39
-3	1	10	28.62	29.28	2.87
-2	1	10	59.19	57.22	3.12
-1	1	10	383.72	399.28	14.93
0	1	10	20.1	18.91	1.93
1	1	10	383.14	376.47	14.83
2	1	10	59.1	53.94	3.18
3	1	10	28.81	28.22	2.96
4	1	10	62.42	56.12	3.6
5	1	10	32.75	34.19	3.27
6	1	10	1.48	1.29	3.44
-5	2	10	80.33	73.53	3.91
-4	2	10	7.81	4.58	2.84
-3	2	10	30.03	26.12	2.87
-2	2	10	80.5	82.77	4.15
-1	2	10	83.9	91.88	4.92
0	2	10	988.49	973.89	18.66
1	2	10	83.89	88.28	4.55
2	2	10	80.24	85.86	4.84
3	2	10	30.19	25.29	3.05
4	2	10	7.67	7.56	8.64
5	2	10	80.09	87.11	5.27
6	2	10	70.22	65.18	4.17
-5	3	10	14.14	17.46	3.29
-4	3	10	9.58	13.58	2.89
-3	3	10	61.79	55	3.46
-2	3	10	37.95	41.13	2.93
-1	3	10	86.79	87.58	4.27
0	3	10	79.26	81.15	6.04
1	3	10	86.45	98.13	5.77
2	3	10	37.98	36.63	3.18
3	3	10	61.66	57.67	3.43
4	3	10	9.63	1.74	3.17
5	3	10	14.47	12.69	3.82
-5	4	10	4.61	-2.75	9.61
-4	4	10	17.33	14.34	3.24
-3	4	10	4.39	-5.32	8.83
-2	4	10	37.77	38.37	3
-1	4	10	5.57	6.39	2.65
0	4	10	4.9	2.25	5.94
1	4	10	5.61	6.7	8.93
2	4	10	37.77	35.64	3.34
3	4	10	4.47	7.37	3.1
4	4	10	17.28	16.9	3.56
5	4	10	4.62	-18.97	10.83
-4	5	10	87.86	91.92	5.44
-3	5	10	9.67	9.52	3.08
-2	5	10	13.48	5.37	8.47
-1	5	10	52.35	51.82	3.22
0	5	10	17.63	18.99	5.72
1	5	10	52.14	49.72	3.67
2	5	10	13.57	14.93	3.36
3	5	10	9.63	-7.85	10.28
4	5	10	88.56	98.94	5.73
-3	6	10	11.33	15.54	3.24
-2	6	10	22.34	25.68	3.22
-1	6	10	97.23	108.55	6.13
0	6	10	4.86	2.74	3.21
h	k	l	F_c^2	F_o^2	σF_o^2
1	6	10	97.02	97.22	5.18
2	6	10	22.1	25.86	3.82
3	6	10	11.36	8.44	11.12
-2	7	10	52.63	58.36	3.86
-1	7	10	3.57	4.1	3.29
0	7	10	115.57	128.87	5.11
1	7	10	3.55	2.7	11.74
2	7	10	52.85	56.36	4.49
1	0	11	39.42	40.09	3.05
2	0	11	72.28	66.69	3.41
3	0	11	0.04	1.74	8.3
4	0	11	4.1	8.19	2.98
5	0	11	2.18	3.08	9.81
-5	1	11	52.68	48.56	3.79
-4	1	11	23.01	22.53	3.27
-3	1	11	327.45	301.06	14.24
-2	1	11	61.19	52.85	3.27
-1	1	11	50.4	54.37	3.56
0	1	11	13.59	19.66	2.01
1	1	11	50.95	50.13	3.44
2	1	11	61.1	52.7	3.39
3	1	11	328.03	299.94	14.72
4	1	11	23.22	21.35	3.34
5	1	11	52.8	53.35	3.82
-5	2	11	111.98	112.09	4.68
-4	2	11	27.17	25.43	3.41
-3	2	11	22.6	7.78	9.18
-2	2	11	11.32	8.88	2.79
-1	2	11	7.86	8.97	2.74
0	2	11	63.38	66.77	2.59
1	2	11	7.99	-1.38	8.54
2	2	11	11.47	6.21	8.68
3	2	11	22.49	19.68	3.2
4	2	11	27.29	33.16	3.56
5	2	11	111.71	105.29	5.53
-4	3	11	20.85	20.93	3.36
-3	3	11	272.18	277.54	14.26
-2	3	11	3.55	-13.82	8.38
-1	3	11	45.3	44.28	3.1
0	3	11	47.74	47.18	2.31
1	3	11	45.87	47.43	3.37
2	3	11	3.42	1.69	3.1
3	3	11	272.83	256.29	13.22
4	3	11	20.65	20.59	3.62
-4	4	11	5.32	0.71	9.59
-3	4	11	45.37	51.94	3.49
-2	4	11	24.44	22.86	3.03
-1	4	11	20.06	3.6	8.69
0	4	11	14.2	17.88	5.43
1	4	11	20.14	17.59	3.37
2	4	11	24.37	8.02	10.14
3	4	11	45.34	49.24	3.94
4	4	11	5.35	0.71	10.24
-3	5	11	19.5	20.98	3.39
-2	5	11	61.17	54.97	3.68
-1	5	11	21.53	23.89	3.31
0	5	11	23.32	22.77	3.6
1	5	11	21.51	23.19	3.77
2	5	11	60.76	60.46	4.22
3	5	11	19.52	20.81	3.91
-1	6	11	1.37	5.47	8.76
0	6	11	131.9	138.76	5.04
1	6	11	1.4	-15.37	11.6
0	0	12	34.02	30.92	3.08
1	0	12	3.4	-10.72	8.85
2	0	12	99.12	94.26	4.55
3	0	12	26.39	22.71	3.41
4	0	12	110.97	115.37	7.2
-4	1	12	10.54	10.74	3.43
-3	1	12	52.78	47.12	3.63
-2	1	12	40.72	40.78	3.55
-1	1	12	47.51	48.32	3.27
0	1	12	0.02	-3.7	3.21
1	1	12	47.01	44.86	3.39
2	1	12	40.61	40.52	3.37
3	1	12	52.94	58.05	3.79
4	1	12	10.54	8.93	3.56
-3	2	12	11.02	11.1	3.32
-2	2	12	20.94	21.71	3.24
-1	2	12	29.01	24.39	3.03
0	2	12	175.75	174.83	6.62

A3.4 MEOXAL

h	k	l	F_c^2	F_o^2	σF_o^2
1	0	0	393.06	409.81	1.05
2	0	0	18.99	22.31	0.22
3	0	0	284.39	296.48	2.33
4	0	0	29.38	26.85	0.17
5	0	0	28.03	30.3	0.34
6	0	0	90.66	90.01	1.67
7	0	0	34.02	34.45	0.54
1	1	0	1184.76	1376.23	96.1
2	1	0	251.32	254.23	3.21
3	1	0	92.05	98.27	0.82
4	1	0	0.19	0.26	0.01
5	1	0	1.53	1.59	0.17
6	1	0	0.62	0.73	0.02
7	1	0	21.26	20.86	0.11
0	2	0	46.29	50.73	0.34
1	2	0	161.06	171.14	3.08
2	2	0	289.92	298.6	8.3
3	2	0	1.91	2.39	0.04
4	2	0	71.37	70.71	0.25
5	2	0	9.68	10.3	0.1
6	2	0	0.5	0.4	0.02
1	3	0	1.83	2.56	0.07
2	3	0	10.88	10.36	0.12
3	3	0	29.69	30.22	0.2
4	3	0	0.03	0.01	0.02
5	3	0	33.84	30.72	0.61
0	4	0	0.55	0.54	0.02
1	4	0	4.28	4.35	0.06
2	4	0	1.68	2.15	0.05
3	4	0	1.23	1.28	0.03
-7	1	1	2.26	2.26	0.07
-6	1	1	0.85	1.19	0.05
-5	1	1	44.84	42.94	0.47
-4	1	1	73.07	79.35	0.88
-3	1	1	231.46	240.62	2.14
-2	1	1	88.97	90.67	1.74
-1	1	1	2802.4	3296.64	126.96
0	1	1	461.54	551.16	42.66
1	1	1	19.98	21.18	0.11
2	1	1	63.36	75.61	1.11
3	1	1	290.2	281.59	8.71
4	1	1	81.96	84.15	1.05
5	1	1	53.24	53.47	0.23
6	1	1	76.88	77.36	0.26
7	1	1	0.01	0.02	0.05
-6	2	1	27.33	26.5	0.22
-5	2	1	1.61	1.59	0.13
-4	2	1	31.75	32.71	0.47
-3	2	1	69.94	72.51	2.23
-2	2	1	75.21	74.15	1.64
-1	2	1	125.53	140.03	1.87
0	2	1	49.98	51.17	0.2
1	2	1	151.46	148.49	5.66
2	2	1	0.13	0.14	0.01
3	2	1	2.6	2.51	0.05
4	2	1	18.35	17.41	0.32
5	2	1	13.14	14.36	0.2
6	2	1	4.85	5	0.09
-5	3	1	4.26	4.71	0.22
-4	3	1	2.03	2.01	0.07
-3	3	1	0.04	0.04	0.05
-2	3	1	54.81	57.97	0.2
-1	3	1	2.6	3.48	0.07
0	3	1	10.48	11.51	0.24
1	3	1	16.15	16.77	0.69
2	3	1	1	1.13	0.04
3	3	1	0.32	0.3	0.02
4	3	1	12.92	12.89	0.12
5	3	1	1.34	1.15	0.05
-3	4	1	6.08	5.37	0.1
-2	4	1	10.15	9.11	0.11
-1	4	1	0.78	0.93	0.06
0	4	1	0.34	0.4	0.03
1	4	1	1	0.7	0.03
2	4	1	2.12	2	0.07
3	4	1	2.89	2.4	0.08
-7	0	2	2.37	2.22	0.1
-6	0	2	82.16	81.96	0.36
-5	0	2	46.34	47.78	0.24
-4	0	2	580.31	597.88	3.27
-3	0	2	12.75	13.95	0.1
-2	0	2	590.09	577.72	2.47
-1	0	2	779.87	648.87	2.3
0	0	2	133.42	128.93	0.73
1	0	2	19.25	17.96	0.08
2	0	2	3052.35	3380.15	8.47
3	0	2	143.14	144.73	1.33
4	0	2	0.4	0.8	0.04
5	0	2	354.51	335.75	2.77
6	0	2	16.14	16.39	0.18
7	0	2	8.41	9.4	0.16
-7	1	2	22.15	22.11	0.32
-6	1	2	2.09	2.03	0.06
-5	1	2	104.59	104.39	1.58
-4	1	2	34.07	36.51	0.67
-3	1	2	27.17	32.5	0.93
-2	1	2	406.23	449.07	5
-1	1	2	162.99	186.31	4.28
0	1	2	65.31	62.42	1.04
1	1	2	326.7	329.23	28.6
1	1	2	326.7	329.23	28.6
2	1	2	1.45	1.26	0.09
3	1	2	267.4	255.89	4.23
4	1	2	106.08	102.46	0.66
5	1	2	33.14	32.42	0.23
6	1	2	15.94	16.45	0.13
7	1	2	0.03	-0.06	0.1
-7	2	2	0.15	0.04	0.05
-6	2	2	4.29	4.6	0.08
-5	2	2	0.01	0.04	0.02
-4	2	2	8.01	6.99	0.15
-3	2	2	62.4	71.3	1.83
-2	2	2	335.03	363.45	1.7
-1	2	2	3.6	4.14	0.08
0	2	2	97.74	99.52	1.48
1	2	2	8.63	10.92	0.21
2	2	2	0.05	0.14	0.02
3	2	2	144.51	147.21	2.39
4	2	2	118.17	120.14	0.31
5	2	2	8.67	7.89	0.09
6	2	2	0	0.06	0.05
-5	3	2	0.39	0.59	0.08
-4	3	2	4.45	4.21	0.08
-3	3	2	92.11	86.35	0.27
-2	3	2	30.03	29.54	0.15
-1	3	2	16.23	16.52	0.32
0	3	2	56.15	54.12	0.2
1	3	2	13.86	13.28	0.19
2	3	2	42.96	43.82	0.18
3	3	2	5	5.66	0.18
4	3	2	1.89	2.55	0.07
5	3	2	1.26	1.14	0.04
-3	4	2	0.41	0.36	0.03
-2	4	2	8.89	8.73	0.11
-1	4	2	2.28	2.14	0.07
0	4	2	11.6	12.09	0.17
1	4	2	6.84	6.96	0.1
2	4	2	0.22	0.14	0.1
3	4	2	0.03	0.05	0.04
-7	1	3	2.46	2.33	0.07
-6	1	3	0.14	0.06	0.03
-5	1	3	15.42	16.85	0.38
-4	1	3	1.69	0.74	0.05
-3	1	3	121.86	124.59	1
-2	1	3	8.6	9.61	1.93
-1	1	3	284.45	274.17	1.15
0	1	3	54.57	56.98	1.08
1	1	3	735.43	762.94	82.31
2	1	3	385.47	407.96	21.35
3	1	3	13.99	13.24	0.24
4	1	3	154.05	149.97	1.11
5	1	3	5.96	6.25	0.1
6	1	3	7.64	8.06	0.15
-7	2	3	8.97	9.09	0.17
-6	2	3	12.22	12.82	0.47
-5	2	3	6	5.76	0.08
-4	2	3	41.1	38.25	0.87
-3	2	3	129.38	132.73	0.53
-2	2	3	2.3	1.96	0.05
-1	2	3	152.49	157.57	6.59
0	2	3	0.6	0.48	0.02
1	2	3	248.67	248.99	16.15
2	2	3	16.4	14.6	0.09
3	2	3	56.46	54.41	0.71
4	2	3	40.88	40.54	0.18
5	2	3	8.93	9.15	0.37
6	2	3	0.91	1.03	0.04
-5	3	3	2.32	2.52	0.08
-4	3	3	0.01	0.59	0.32
-3	3	3	0.33	0.32	0.02
-2	3	3	3.74	3.59	0.11
-1	3	3	2.93	3.71	0.07
0	3	3	22.4	21.5	0.55
1	3	3	0.42	0.43	0.02
2	3	3	2.76	2.62	0.07
3	3	3	40.5	39.58	0.19
4	3	3	0.85	0.53	0.02
5	3	3	0.89	0.83	0.03
-3	4	3	22.55	20.55	0.16
-2	4	3	2.98	3.22	0.1
-1	4	3	0.02	0.02	0.05
0	4	3	1.01	1.16	0.07
1	4	3	7.75	7.78	0.33
2	4	3	11.85	11.5	0.13
3	4	3	4.61	4.44	0.1
-7	0	4	16.77	15.25	0.18
-6	0	4	1.58	1.64	0.08
-5	0	4	9.92	8.33	0.11
-4	0	4	65.44	76.42	0.28
-3	0	4	61.73	61.89	0.22
-2	0	4	1550.07	1346.47	4.76
-1	0	4	696.11	589.54	2.55
0	0	4	58.34	49.05	0.59
1	0	4	1575.34	1767.83	5.34
2	0	4	9.62	10.22	0.09
3	0	4	22.03	20.61	0.14
4	0	4	13.25	12.58	0.13
5	0	4	4.14	4.88	0.1
6	0	4	1.89	1.56	0.08
-7	1	4	0.03	0.15	0.08
-6	1	4	16.58	15.16	0.4
-5	1	4	40.25	39.89	1.35
-4	1	4	16.68	16.06	0.49
-3	1	4	101.74	104.24	1.28
-2	1	4	253.8	252.07	7.2
-1	1	4	174.62	181.02	0.95
0	1	4	1086.49	1174.84	161.18
1	1	4	73.17	80.93	1.43
2	1	4	6.58	6.33	0.06
3	1	4	6.2	5.85	0.06
4	1	4	3.55	2.88	0.09
5	1	4	16.06	15.63	0.22
6	1	4	18.39	18.78	0.25
-7	2	4	0.3	0.26	0.04
-6	2	4	0.19	0.2	0.02
-5	2	4	28.7	25.58	0.43
-4	2	4	17.01	15.69	0.45
-3	2	4	17.64	19.59	0.36
-2	2	4	4.65	5.34	0.09
-1	2	4	77.03	79.37	0.38
0	2	4	117.35	121.35	1.53
1	2	4	2.29	2.41	0.07
2	2	4	0.01	0.25	0.14
3	2	4	76.16	72.37	0.22
4	2	4	17.1	16.32	0.18
5	2	4	19.37	19.09	0.59
6	2	4	9.08	9.3	0.27
-5	3	4	6.41	5.19	0.09
-4	3	4	90.22	90.22	0.75
-3	3	4	10.13	10.25	0.14
-2	3	4	1.32	2	0.06
-1	3	4	15.9	14.9	0.11
0	3	4	38.08	38.74	0.17
1	3	4	2.35	3.08	0.11
2	3	4	74.58	75.53	0.31
3	3	4	44.4	43.6	0.4
4	3	4	14.91	14.95	0.18
-3	4	4	4.5	5.18	0.1
-2	4	4	0.89	1.08	0.04
-1	4	4	0.1	0.1	0.12
0	4	4	2.24	2.23	0.08
1	4	4	0.47	0.42	0.03
2	4	4	11.66	11.63	0.13
-7	1	5	0.95	0.93	0.04
-6	1	5	49.69	48.24	0.74
-5	1	5	12.64	11.34	0.27
-4	1	5	1.88	3	0.33
-3	1	5	141.46	135.58	3.74
-2	1	5	11.85	13.17	0.07
-1	1	5	3.19	3.38	0.18
0	1	5	69.17	67.91	1
1	1	5	70.61	72.43	0.58
2	1	5	25.1	22.36	0.14
3	1	5	0.99	1.23	0.04
4	1	5	43.67	44.3	0.35
5	1	5	0.03	-0.06	0.05
6	1	5	20.49	21.7	0.18
-6	2	5	2.34	1.91	0.06
-5	2	5	87.91	88.13	2.71
-4	2	5	0.52	0.51	0.02
-3	2	5	4.76	5.5	0.32
-2	2	5	3.93	5.28	0.19
-1	2	5	245.78	243.9	3.78
0	2	5	49.18	56.46	0.86
1	2	5	55.8	56.53	0.34
2	2	5	69.46	69.24	0.57
3	2	5	22.26	22.71	0.19
4	2	5	0.88	0.96	0.03
5	2	5	8.91	8.07	0.1
-5	3	5	0.43	0.42	0.02
-4	3	5	9.39	10.2	0.2
-3	3	5	8.09	7.94	0.24
-2	3	5	1.93	2.06	0.07
-1	3	5	0.61	0.53	0.02
0	3	5	1.17	1.72	0.12
1	3	5	2.64	2.49	0.06
2	3	5	0.01	0.02	0.03
3	3	5	2.81	2.64	0.07
4	3	5	0.18	0.18	0.04
-3	4	5	1.54	1.2	0.04
-2	4	5	6.42	5.99	0.1
-1	4	5	25.68	23.31	0.27
0	4	5	11.71	11.83	0.13
1	4	5	11.54	10.9	0.23
2	4	5	9.95	8.83	0.12
-7	0	6	69.71	69.54	0.39
-6	0	6	53.92	55.33	0.31
-5	0	6	53.76	54.28	0.27
-4	0	6	25.35	25.39	0.17
-3	0	6	11.41	8.93	0.09
-2	0	6	124.91	106.52	1.13

h	k	l	F_c^2	F_o^2	σF_o^2
-1	0	6	131.5	122.55	1.16
0	0	6	721.37	753.45	3.37
1	0	6	169.61	135.84	1.3
2	0	6	8.39	7.09	0.09
3	0	6	374.77	364.7	2.7
4	0	6	5.07	3.98	0.09
5	0	6	3.75	3.08	0.1
6	0	6	16.3	18.88	0.21
-7	1	6	1.95	2.45	0.15
-6	1	6	51.49	52.99	0.41
-5	1	6	3.36	3.39	0.06
-4	1	6	92.43	90.88	1.46
-3	1	6	0.7	0.61	0.35
-2	1	6	1.53	1.25	0.06
-1	1	6	3.78	4.97	0.05
0	1	6	223.02	211.37	8.4
1	1	6	135.16	137.38	5.12
2	1	6	240.14	220.7	7.08
3	1	6	5.06	5.29	0.07
4	1	6	18.68	16.98	0.12
5	1	6	25.53	27.37	0.36
6	1	6	7.53	7.73	0.13
-6	2	6	0.51	0.39	0.02
-5	2	6	18.79	18.62	0.59
-4	2	6	1.83	1.71	0.06
-3	2	6	96.74	99.35	0.89
-2	2	6	40.71	42.4	0.45
-1	2	6	18.88	17.43	0.1
0	2	6	7.68	9.11	0.08
1	2	6	56.89	58.26	0.19
2	2	6	1.01	1.07	0.13
3	2	6	11.34	10.94	0.18
4	2	6	0.63	0.68	0.02
5	2	6	16.69	17.05	0.14
-5	3	6	0.07	0.05	0.03
-4	3	6	3.14	2.28	0.09
-3	3	6	0.02	0.03	0.05
-2	3	6	137.95	138.32	0.08
-1	3	6	37.13	39.04	0.75
0	3	6	0.2	0.13	0.03
1	3	6	24.6	24.49	0.15
2	3	6	0.14	0.08	0.02
3	3	6	4.63	4.5	0.09
4	3	6	21.12	22.23	0.17
-2	4	6	0.02	-0.06	0.07
-1	4	6	12.1	13.21	0.25
0	4	6	1.41	1.53	0.05
1	4	6	2.39	2.31	0.12
-7	1	7	13.11	13.05	0.13
-6	1	7	0.55	0.51	0.02
-5	1	7	0.18	0.08	0.02
-4	1	7	58.17	58.35	0.19
-3	1	7	188.24	191.23	7.02
-2	1	7	11.86	13.72	0.09
-1	1	7	298.82	305.6	12.64
0	1	7	26.27	29.42	0.26
1	1	7	24.61	22.93	0.11
2	1	7	30.25	29.89	0.31
3	1	7	11.1	9.64	0.09
4	1	7	5.95	4.89	0.08
5	1	7	3.76	4.6	0.08
-6	2	7	0.41	0.4	0.02
-5	2	7	3.08	3.28	0.16
-4	2	7	0.35	0.39	0.02
-3	2	7	92.68	92.04	1.96
-2	2	7	18.43	19.26	0.42
-1	2	7	0.58	0.53	0.02
0	2	7	89.64	93.84	0.39
1	2	7	34.73	33.53	0.4
2	2	7	36.63	38.52	1.29
3	2	7	0.36	0.53	0.02
4	2	7	44.76	46.98	0.38
5	2	7	3.54	3.66	0.09
-5	3	7	1.77	1.95	0.09
-4	3	7	3.43	3.33	0.11
-3	3	7	5.98	6.05	0.12
-2	3	7	23.07	24.83	0.38
-1	3	7	0.58	0.45	0.02
0	3	7	0.14	0.13	0.02
1	3	7	3.79	3.55	0.08
2	3	7	6.65	7.09	0.27
3	3	7	0	-0.07	0.06
-2	4	7	10.02	9.42	0.21
-1	4	7	7.49	6.81	0.15
0	4	7	1.26	1.18	0.11
-7	0	8	0.1	-0.01	0.08
-6	0	8	0.75	0.82	0.05
-5	0	8	110.61	112.11	0.42
-4	0	8	272.67	251.76	2.3
-3	0	8	8.53	6.44	0.09
-2	0	8	269.41	264.02	2.11
-1	0	8	370.7	343.43	2.39
0	0	8	191.96	165.18	1.62
1	0	8	42.17	37.02	0.2
2	0	8	48.5	48.49	0.24
3	0	8	8.55	6.3	0.11
4	0	8	0.13	-0.13	0.06
5	0	8	48.61	48.69	0.32
-7	1	8	0.27	0.15	0.02
-6	1	8	0.63	0.59	0.02
-5	1	8	1.81	2.07	0.06
-4	1	8	75.42	74.29	0.68
-3	1	8	8.04	7.34	0.08
-2	1	8	145.14	139.03	2.04
-1	1	8	44.1	45.14	0.92
0	1	8	23.12	21.94	0.11
1	1	8	59.6	56.89	0.45
2	1	8	29.24	30.11	0.48
3	1	8	14.03	15.67	0.15
4	1	8	10.13	9.38	0.1
5	1	8	0.18	0.31	0.06
-6	2	8	1.11	1.55	0.08
-5	2	8	2.83	2.85	0.07
-4	2	8	42.93	44.55	0.67
-3	2	8	94.41	98.6	2.74
-2	2	8	18.18	19.05	0.52
-1	2	8	20.44	18.48	0.62
0	2	8	0.78	0.76	0.03
1	2	8	6.85	6.63	0.12
2	2	8	23.37	22.97	0.17
3	2	8	39.29	38.14	0.68
4	2	8	0.1	0.24	0.03
-5	3	8	1.83	1.57	0.05
-4	3	8	0.37	0.27	0.03
-3	3	8	9.34	10.53	0.11
-2	3	8	6.97	6.37	0.23
-1	3	8	5.74	5.18	0.08
0	3	8	24.73	23.46	0.23
1	3	8	9.54	9.28	0.23
2	3	8	0.63	0.72	0.03
3	3	8	29.65	31.18	0.88
-6	1	9	10.6	11.19	0.12
-5	1	9	106.1	109.98	0.73
-4	1	9	23.36	23.84	0.14
-3	1	9	27.86	28.77	0.33
-2	1	9	16	16.73	0.11
-1	1	9	90.61	84.99	0.88
0	1	9	19.16	17.85	0.11
1	1	9	101.78	103.83	0.73
2	1	9	99.86	95.71	1.22
3	1	9	0.31	0.06	0.02
4	1	9	10.76	10.57	0.27
-6	2	9	6.71	6.81	0.11
-5	2	9	0	0.01	0.06
-4	2	9	11.88	12.99	0.3
-3	2	9	12.64	12.65	0.48
-2	2	9	2.27	1.99	0.06
-1	2	9	2.61	1.95	0.06
0	2	9	22.75	21.17	0.5
1	2	9	1.14	1.01	0.04
2	2	9	29.69	31.46	0.35
3	2	9	0.59	0.53	0.07
4	2	9	4.68	4.36	0.09
-4	3	9	3.14	3.46	0.12
-3	3	9	4.83	5.29	0.09
-2	3	9	2.23	2.41	0.15
-1	3	9	1.28	1.27	0.07
0	3	9	7.01	6.96	0.16
1	3	9	2.54	2.42	0.26
2	3	9	1.6	1.51	0.05
-6	0	10	80.43	81.92	0.41
-5	0	10	39.22	40.84	0.27
-4	0	10	0.11	0.08	0.02
-3	0	10	0.51	0.51	0.03
-2	0	10	91.07	85.24	0.33
-1	0	10	3.95	3.29	0.08
0	0	10	211.22	226.59	0.55
1	0	10	412.47	384.16	3.01
2	0	10	10.16	9.89	0.13
3	0	10	0.37	0.22	0.03
4	0	10	4.68	4.27	0.12
-6	1	10	10.63	10.99	0.22
-5	1	10	9.27	9.49	0.11
-4	1	10	0.01	0.01	0.02
-3	1	10	4.61	4.75	0.08
-2	1	10	15.62	13.85	0.26
-1	1	10	0.3	0.14	0.07
0	1	10	60.75	58.59	0.38
1	1	10	27.01	27.45	0.76
2	1	10	20.85	20.15	0.13
3	1	10	31.64	30.48	0.38
4	1	10	0.55	0.47	0.03
-5	2	10	0.03	0.02	0.03
-4	2	10	13.52	12.88	0.12
-3	2	10	4.36	4.23	0.08
-2	2	10	45.14	47.19	0.38
-1	2	10	61.45	60.66	0.75
0	2	10	12.88	12.06	0.11
1	2	10	6.26	6.42	0.23
2	2	10	20.45	19.75	0.33
3	2	10	6.05	5.62	0.14
-4	3	10	10.49	10.46	0.29
-3	3	10	7.04	6.75	0.13
-2	3	10	4.5	5.24	0.09
-1	3	10	9.99	9.94	0.16
0	3	10	0.05	0.02	0.06
1	3	10	0.03	0.09	0.06
-6	1	11	1.26	1.21	0.04
-5	1	11	0.5	0.32	0.02
-4	1	11	1.64	1.47	0.05
-3	1	11	72.01	72.46	0.86
-2	1	11	41.12	37.94	0.18
-1	1	11	32.02	31.7	0.21
0	1	11	124.15	126.15	0.31
1	1	11	1.05	1.05	0.04
2	1	11	0.52	0.42	0.02
3	1	11	1.47	1.92	0.06
-5	2	11	8.79	8.85	0.62
-4	2	11	2.11	2.11	0.07
-3	2	11	5.64	6.57	0.16
-2	2	11	9.43	8.97	0.1
-1	2	11	21.22	23.23	0.15
0	2	11	2.02	2.2	0.1
1	2	11	4.98	5.18	0.14
2	2	11	9.22	9.13	0.14
-2	3	11	3.23	2.79	0.08
-1	3	11	13.34	13.51	0.14
0	3	11	0	-0.01	0.06
-6	0	12	0.22	0.11	0.03
-5	0	12	11.17	11.83	0.17
-4	0	12	74.35	73.66	0.37
-3	0	12	65.79	63.77	0.33
-2	0	12	3.24	3.83	0.1
-1	0	12	60.75	59.65	0.31
0	0	12	13.06	13.47	0.16
1	0	12	2.34	1.72	0.08
2	0	12	21.69	23.28	0.22
3	0	12	88.9	98.22	0.46
-5	1	12	3.46	3.54	0.1
-4	1	12	18.56	20.45	0.3
-3	1	12	16.94	16.59	0.13
-2	1	12	1.7	1.83	0.06
-1	1	12	38.68	40.35	0.59
0	1	12	0	0.27	0.21
1	1	12	0.76	0.96	0.03
2	1	12	5.57	6.13	0.19
-4	2	12	0.01	0.02	0.06
-3	2	12	0.79	0.55	0.02
-2	2	12	31.49	31.25	0.19
-1	2	12	18.98	18.28	0.45
0	2	12	4.09	4.63	0.08
1	2	12	2.72	2.79	0.08
-5	1	13	1.3	1	0.06
-4	1	13	6.01	5.29	0.09
-3	1	13	0.05	0.03	0.05
-2	1	13	14.51	13.57	0.12
-1	1	13	0.87	1.48	0.53
0	1	13	8.35	7.53	0.1
1	1	13	1.32	1.38	0.05
2	1	13	40.8	45.78	0.23
-3	2	13	9.89	10.28	0.31
-2	2	13	8.8	9.76	0.12
-1	2	13	1.3	1.49	0.06
0	2	13	3.28	3.13	0.09
-4	0	14	0.06	0.25	0.03
-3	0	14	5.1	5.06	0.12
-2	0	14	12.44	13.91	0.18
-1	0	14	19.07	18.79	0.21
0	0	14	13.6	15.54	0.19
1	0	14	26.83	30.43	0.27
-4	1	14	2.96	3.44	0.08
-3	1	14	0.04	0.06	0.02
-2	1	14	2.5	2.73	0.07
-1	1	14	11.52	12.01	0.16
0	1	14	1.18	1.5	0.11

A3.5 CITXL

h	k	l	F_c^2	F_o^2	σF_o^2
1	0	0	135.23	172.4	5.04
2	0	0	3141.67	3279.33	4.13
3	0	0	1139.96	1111.36	23.09
4	0	0	29.4	20.86	6.12
5	0	0	258.44	237.91	11.24
6	0	0	247.96	259.03	9.19
7	0	0	5.15	0.11	13.04
8	0	0	1.13	9.88	7.07
-9	1	0	1	1.12	17.38
-8	1	0	7.51	-17.5	13.36
-7	1	0	58.19	57.8	7.46
-6	1	0	1.12	6.21	11.61
-5	1	0	0.19	7.84	5.74
-4	1	0	129.09	132.81	10.24
-3	1	0	261.05	265.87	40.41
-2	1	0	1.96	58.48	10.73
-1	1	0	1037.65	1037.04	9.5
0	1	0	436.48	446.17	7.18
1	1	0	73.67	99.45	3.47
2	1	0	181.85	214.41	11.53
3	1	0	161.68	179.56	8.65
4	1	0	510.51	496.72	16.89
5	1	0	382.2	361.43	13.45
6	1	0	77.91	72.72	5.15
7	1	0	0.37	4.72	6.91
8	1	0	32.03	33.87	6.06
-9	2	0	0.97	-10.58	24.48
-8	2	0	2.13	1.8	12.5
-7	2	0	156.31	162.19	5.57
-6	2	0	39.3	45.29	9.76
-5	2	0	60.23	55.14	4.25
-4	2	0	12.2	19.76	18.19
-3	2	0	167.97	199.91	5.99
-2	2	0	936.97	891.28	16.69
-1	2	0	2259.27	2328.32	20.48
0	2	0	37.43	79.47	4.98
1	2	0	156.76	196.19	8.58
2	2	0	50.47	52.95	5.86
3	2	0	272.82	229.85	10.37
4	2	0	58.77	47.78	6.39
5	2	0	215.16	234.95	9.26
6	2	0	4.89	7.1	17.21
7	2	0	35.68	-10.29	19.88
8	2	0	6	9.4	9.58
-9	3	0	0.37	-17.56	18.45
-8	3	0	0.15	-0.53	16.85
-7	3	0	19.03	7.98	15.26
-6	3	0	0.34	-0.35	14.37
-5	3	0	47.77	56.83	5.68
-4	3	0	0	-4.79	4.61
-3	3	0	612.74	565.59	15.02
-2	3	0	96.7	112.53	4.99
-1	3	0	500.26	471.67	13.59
0	3	0	144.97	182.52	6.6
1	3	0	162.23	151.08	7.49
2	3	0	0.11	2.31	11.71
3	3	0	26.07	20.23	6.03
4	3	0	279.16	264.39	12.49
5	3	0	31.34	50.94	7.1
6	3	0	3.11	17.21	17.21
7	3	0	0.22	0	20.4
-9	4	0	0.34	16.85	7.63
-8	4	0	5.33	9.58	7.1
-7	4	0	4.07	12.24	15.26
-6	4	0	16.21	-2.48	14.2
-5	4	0	44.95	49.36	5.5
-4	4	0	107.97	106.9	5.69
-3	4	0	422.87	384.74	14.54
-2	4	0	108.78	134.03	6.23
-1	4	0	0.74	3.19	9.58
0	4	0	4.58	7.81	10.29
1	4	0	54.45	57.02	4.97
2	4	0	13.82	13.66	5.68
3	4	0	88.43	89.03	7.11
4	4	0	28.36	29.28	7.1
5	4	0	12.96	15.61	17.39
6	4	0	7.11	21.11	8.16
-9	5	0	24.49	6.21	18.81
-8	5	0	11.51	2.31	16.5
-7	5	0	141.78	145.62	7.47
-6	5	0	48.03	43.85	6.39
-5	5	0	17.51	20.41	5.86
-4	5	0	5.55	1.42	12.24
-3	5	0	288.48	251.35	12.51
-2	5	0	37.91	37.46	4.79
-1	5	0	215.56	197.99	10.35
0	5	0	7.82	7.1	12.06
1	5	0	30.22	20.59	5.5
2	5	0	0.27	-5.85	13.66
3	5	0	0.42	-4.08	15.25
4	5	0	18.62	24.84	7.1
5	5	0	2.29	1.24	18.8
6	5	0	0	0.71	20.75
-9	6	0	22.33	-18.63	18.99
-8	6	0	30.15	26.62	7.28
-7	6	0	0.3	1.6	14.55
-6	6	0	56.76	67.47	6.39
-5	6	0	44.95	46.69	6.04
-4	6	0	119.39	117.71	7.47
-3	6	0	86.25	80.86	5.86
-2	6	0	196.58	189.73	9.44
-1	6	0	35.24	36.57	5.33
0	6	0	0.07	-7.98	13.48
1	6	0	146.62	172.73	9.96
2	6	0	11.89	24.13	6.39
3	6	0	33.61	28.04	7.1
4	6	0	2.44	8.51	17.21
5	6	0	9.61	25.19	8.52
-8	7	0	13.54	2.66	17.39
-7	7	0	47.61	44.2	7.1
-6	7	0	36.28	41.71	6.21
-5	7	0	117.61	97.58	6.75
-4	7	0	1.39	-5.5	13.84
-3	7	0	71.43	66.79	6.22
-2	7	0	274.21	259.44	13.19
-1	7	0	20.76	14.2	5.86
0	7	0	35.03	2.84	15.09
1	7	0	8.27	4.97	15.08
2	7	0	12.05	12.24	15.79
3	7	0	0.4	-9.93	17.03
4	7	0	15.11	0	18.98
-8	8	0	4.66	-12.24	18.63
-7	8	0	11.44	-15.08	16.5
-6	8	0	7.78	7.27	15.43
-5	8	0	0.04	7.27	14.19
-4	8	0	2.91	-28.38	14.72
-3	8	0	68.5	68.37	6.57
-2	8	0	118.8	125.66	7.47
-1	8	0	12.53	17.92	6.03
0	8	0	17.4	23.95	6.39
1	8	0	45.03	47.75	7.28
2	8	0	6.18	15.79	16.5
3	8	0	62.79	83.62	8.7
-7	9	0	3.41	-17.21	17.03
-6	9	0	17.59	11.36	16.86
-5	9	0	1.52	-0.71	15.61
-4	9	0	13.07	16.68	6.74
-3	9	0	26.71	29.81	6.74
-2	9	0	19.27	33	6.74
-1	9	0	1.9	14.37	15.79
0	9	0	2.02	-27.49	16.14
1	9	0	2.81	16.14	17.74
-5	10	0	6.13	-0.71	16.85
-4	10	0	33.69	44.9	7.28
-3	10	0	7.1	19.87	7.27
-2	10	0	4.94	6.39	16.32
-1	10	0	6.25	-7.98	17.38
1	-10	1	0.07	-9.05	7.27
2	-10	1	2.45	1.42	16.32
3	-10	1	6.95	14.55	16.5
4	-10	1	30.9	4.97	17.21
5	-10	1	6.84	9.22	7.45
-1	-9	1	0.89	-0.35	7.27
0	-9	1	8.46	12.77	15.26
1	-9	1	4.01	2.48	6.74
2	-9	1	22.2	12.07	6.74
3	-9	1	1.84	4.43	6.39
4	-9	1	3.05	-40.8	15.79
5	-9	1	6.79	0	16.85
6	-9	1	10.47	16.85	7.27
-3	-8	1	2.7	15.26	18.8
-2	-8	1	22.5	12.95	7.45
-1	-8	1	37.89	35.5	7.1
0	-8	1	29.82	35.32	6.57
1	-8	1	88.41	104.46	6.75
2	-8	1	0.37	11.71	13.3
3	-8	1	42.2	43.49	6.39
4	-8	1	18.09	9.05	14.02
5	-8	1	0.36	-7.27	15.25
6	-8	1	6.24	11.18	6.56
7	-8	1	3.17	4.08	7.27
-4	-7	1	12.04	28.56	7.81
-3	-7	1	26.05	15.97	17.57
-2	-7	1	54.03	63.2	6.92
-1	-7	1	17.89	-3.37	14.73
0	-7	1	25.51	12.6	14.02
1	-7	1	0.75	2.13	13.13
2	-7	1	215.24	200.2	11.76
3	-7	1	18.63	10.47	14.2
4	-7	1	440.59	417.3	19.31
5	-7	1	2.38	-4.43	13.66
6	-7	1	52.61	49.89	6.75
7	-7	1	11.26	18.98	6.92
8	-7	1	0.56	8.87	17.56
-5	-6	1	1.82	-16.67	18.98
-4	-6	1	22.43	20.23	7.63
-3	-6	1	5.36	8.52	15.43
-2	-6	1	1.47	7.98	14.72
-1	-6	1	15.15	-16.86	14.02
0	-6	1	88.34	78.37	6.04
1	-6	1	107.59	105.97	5.69
2	-6	1	6.54	5.5	5.14
3	-6	1	22.07	22.89	5.5
4	-6	1	19.04	12.95	13.66
5	-6	1	12.91	10.29	5.85
6	-6	1	187.47	199.13	9.79
7	-6	1	30.76	15.08	15.44
8	-6	1	11.69	5.85	17.21
-6	-5	1	5.89	5.5	8.87
-5	-5	1	0.34	3.02	18.27
-4	-5	1	13.31	0	15.97
-3	-5	1	55.75	52.03	6.93
-2	-5	1	5.12	10.82	14.37
-1	-5	1	4.46	6.56	12.6
0	-5	1	102.65	104.21	5.51
1	-5	1	74.56	71.62	4.98
2	-5	1	0.72	3.19	11
3	-5	1	58.86	53.11	5.15
4	-5	1	4.53	13.3	5.32
5	-5	1	4.1	14.19	5.68
6	-5	1	5.65	4.97	14.01
7	-5	1	44.61	38.52	6.75
8	-5	1	2.68	-9.93	16.67
9	-5	1	0.29	-15.08	18.45
-7	-4	1	0.93	-0.71	22.17
-6	-4	1	0.22	-6.03	19.51
-5	-4	1	3.85	-34.41	17.74
-4	-4	1	3.42	3.02	15.97
-3	-4	1	30.44	25.91	6.21
-2	-4	1	73.11	60.42	5.51
-1	-4	1	127.07	121.59	6.76
0	-4	1	4.25	5.5	10.11
1	-4	1	39.07	38.01	5.15
2	-4	1	42.75	31.26	4.26
3	-4	1	1.1	8.87	10.11
4	-4	1	0	2.66	11.53
5	-4	1	6.47	-20.22	13.84
6	-4	1	15.42	12.95	6.21
7	-4	1	0.86	2.13	15.06
8	-4	1	17.9	14.55	17.21
9	-4	1	0.61	9.58	8.16
-7	-3	1	0.19	-21.29	20.22
-6	-3	1	7.34	-12.95	17.92
-5	-3	1	35.95	35.86	7.46
-4	-3	1	16.9	4.79	16.15
-3	-3	1	467.29	448.47	17.41
-2	-3	1	0	1.95	4.61
-1	-3	1	2621.42	2475.85	25.72
0	-3	1	2182.72	2222.23	22.72
1	-3	1	457.13	476.21	13.55
2	-3	1	1462.19	1399	19.61
3	-3	1	69.34	80.71	5.51
4	-3	1	6.81	5.85	4.79
5	-3	1	63.09	60.57	6.04
6	-3	1	16.4	17.57	6.39
7	-3	1	3.55	-9.76	15.43
8	-3	1	1.25	-5.5	7.45
9	-3	1	0	-1.42	19.69
-8	-2	1	13.46	28.03	9.23
-7	-2	1	38.28	54.67	8.34
-6	-2	1	1.59	7.27	17.03
-5	-2	1	129.53	134.63	8.18
-4	-2	1	22.4	21.47	6.03
-3	-2	1	101.04	95.89	5.34
-2	-2	1	14.68	-6.03	10.83
-1	-2	1	77.47	126.78	5.16
0	-2	1	44.06	76.3	4.8
1	-2	1	40.78	88.36	4.8
2	-2	1	648.8	528.51	13.86
3	-2	1	147.32	158.03	12.66
4	-2	1	1.27	-8.22	8.7
5	-2	1	430.4	418.41	18
6	-2	1	50.28	60.64	16.25
7	-2	1	55.57	62.85	5.31
8	-2	1	0.96	-2.87	7.63
9	-2	1	2.05	0.76	6.29
-8	-1	1	0	2.23	7.23
-7	-1	1	8.44	10.24	11.69
-6	-1	1	5.28	5.85	11.7
-5	-1	1	428.9	438.73	13.7
-4	-1	1	82.08	88.91	4.02
-3	-1	1	6.09	-9.59	7.82
-2	-1	1	1629.43	1605.29	63.19
-1	-1	1	940.73	956.35	10.91
0	-1	1	2060.64	2216.69	12.24
1	-1	1	170.56	222.47	6.6
2	-1	1	268.97	289.26	9.21
3	-1	1	435.37	420.18	10.29
4	-1	1	202.67	197.22	6.75
5	-1	1	87.02	74.37	4.63
6	-1	1	5.24	-7.37	12.06
7	-1	1	1.91	-15.92	12.45
8	-1	1	0.2	4.98	13.04
-9	0	1	0.07	9.29	7.49
-8	0	1	17.32	11.85	5.61
-7	0	1	9.77	2.58	11.59
-6	0	1	115.35	119.43	5.42
-5	0	1	18.4	11.3	7.81
-4	0	1	17.06	20.19	3.56

h	k	l	F_c^2	F_o^2	σF_o^2
-3	0	1	1346.31	1320.86	13.72
-2	0	1	696.38	632.72	40.25
-1	0	1	1217.96	1202.6	10.98
0	0	1	108.12	164.22	7.2
1	0	1	251.27	249.42	7.63
2	0	1	1056.24	1018.03	65.01
3	0	1	43.51	63.67	4.07
4	0	1	8.8	-0.63	9.21
5	0	1	27.89	26.88	5.24
6	0	1	12.57	3.2	11.49
7	0	1	20.32	7.39	7.24
8	0	1	3.83	-0.29	17.65
-9	1	1	0.78	-15.64	31.13
-8	1	1	14.46	7.97	7.43
-7	1	1	3.43	-3.99	7.54
-6	1	1	92.18	101.68	16.44
-5	1	1	50.89	48.92	4.07
-4	1	1	0.53	-7.99	9.05
-3	1	1	464.61	500.62	59.02
-2	1	1	837.27	864.1	11.45
-1	1	1	53.19	96.77	2.96
0	1	1	585.08	632.94	25.27
1	1	1	322.69	322.77	9.51
2	1	1	2247	2261.71	16.78
3	1	1	101.87	93.74	7.21
4	1	1	80.8	86.63	7.91
5	1	1	135.42	153.04	11.83
6	1	1	4.07	-1.66	11.47
7	1	1	47.35	66.25	5.95
8	1	1	0.12	-1.39	26.25
-9	2	1	0.35	-13.75	13.46
-8	2	1	28.33	18.93	5.31
-7	2	1	19.67	7.38	8.61
-6	2	1	143.13	128.63	5.29
-5	2	1	601.51	579.28	13.42
-4	2	1	417.17	411.93	15.9
-3	2	1	59.33	80.2	4.44
-2	2	1	1695.93	1581.51	18.8
-1	2	1	2856.02	2854.37	22.68
0	2	1	450.67	485.25	14.15
1	2	1	166.59	201.8	8.04
2	2	1	0.28	-9.93	11.18
3	2	1	26.04	25.56	5.5
4	2	1	25.29	23.6	6.39
5	2	1	27.22	14.02	7.28
6	2	1	4.64	10.11	7.27
7	2	1	0.52	4.97	8.34
-9	3	1	8.19	-2.66	17.92
-8	3	1	4.19	3.9	16.32
-7	3	1	4.39	1.42	15.43
-6	3	1	1.77	2.66	14.19
-5	3	1	49.38	55.23	5.51
-4	3	1	297.42	282.11	13.06
-3	3	1	133.94	125.98	5.7
-2	3	1	668.22	666.06	15.1
-1	3	1	76.63	84.52	4.8
0	3	1	18.36	34.79	11.54
1	3	1	20.28	30.71	5.5
2	3	1	14.81	-3.55	12.24
3	3	1	25.83	15.44	6.03
4	3	1	37.49	45.98	6.92
5	3	1	44.03	51.83	7.63
6	3	1	4.08	3.55	18.45
7	3	1	0.11	-10.47	22
-9	4	1	0.32	2.66	16.67
-8	4	1	3.13	11.71	15.61
-7	4	1	5.07	8.34	8.39
-6	4	1	148.39	139.48	6.94
-5	4	1	48.45	38.89	5.5
-4	4	1	210.43	201.35	9.63
-3	4	1	268.51	268.31	13.41
-2	4	1	210.97	226.02	11.25
-1	4	1	18.31	20.06	4.26
0	4	1	19.93	13.84	4.44
1	4	1	5.89	13.66	4.97
2	4	1	31.38	34.08	5.68
3	4	1	104.08	102.38	7.11
4	4	1	39.42	41.71	7.1
5	4	1	8.56	-12.42	18.45
6	4	1	7.22	11.53	8.69
-9	5	1	20.51	42.05	7.63
-8	5	1	5.75	-13.3	16.85
-7	5	1	3.11	12.42	15.26
-6	5	1	6.06	-17.74	14.19
-5	5	1	1.65	11.35	13.13
-4	5	1	0.42	3.9	5.14
-3	5	1	11.3	12.42	4.97
-2	5	1	208.5	181.35	9.63
-1	5	1	31.06	28.94	4.97
0	5	1	866.87	877.17	21.17
1	5	1	36.81	36.39	5.86
2	5	1	124.27	114.51	7.11
3	5	1	148.63	124.85	7.65
4	5	1	1.12	14.55	7.1
5	5	1	11.05	21.82	7.98
-9	6	1	33.24	48.27	7.99
-8	6	1	2.53	-1.77	16.14
-7	6	1	133.76	128.35	7.29
-6	6	1	4.76	4.79	14.37
-5	6	1	148.88	157.25	7.83
-4	6	1	1.83	9.4	12.59
-3	6	1	135.11	156.01	8.18
-2	6	1	11.14	12.24	5.32
-1	6	1	18.42	26.44	5.5
0	6	1	31.41	3.55	14.73
1	6	1	8.5	-18.45	14.02
2	6	1	24.87	-9.76	15.97
3	6	1	6.17	-6.03	16.85
4	6	1	7.61	6.39	17.56
5	6	1	1.63	-11.53	19.34
-8	7	1	11.78	-1.24	17.21
-7	7	1	70.1	83.99	7.28
-6	7	1	1.59	-2.13	13.84
-5	7	1	0.13	1.42	13.84
-4	7	1	199.72	210.43	10.15
-3	7	1	107	99	6.58
-2	7	1	139.67	138.19	8
-1	7	1	6.88	3.73	14.19
0	7	1	10.31	5.32	14.37
1	7	1	32.26	33.9	6.57
2	7	1	19.41	33.36	7.27
3	7	1	56.54	68.7	8.34
4	7	1	0.42	-11.71	19.87
-8	8	1	0.1	-9.93	18.27
-7	8	1	0.19	1.95	16.14
-6	8	1	0.37	2.48	6.56
-5	8	1	35.35	43.13	6.57
-4	8	1	0.78	-1.6	14.72
-3	8	1	82.18	92.37	6.57
-2	8	1	0.75	-12.24	14.19
-1	8	1	3.18	7.63	14.55
0	8	1	66.44	68.72	7.46
1	8	1	6.6	29.27	7.1
2	8	1	32.31	18.63	18.63
-7	9	1	10.92	13.66	16.5
-6	9	1	2.76	-44.88	17.74
-5	9	1	0.08	5.14	15.25
-4	9	1	13.46	13.31	7.1
-3	9	1	13.02	18.98	6.74
-2	9	1	0.52	-4.43	15.43
-1	9	1	1.05	3.19	16.32
0	9	1	4.59	-31.58	17.56
1	9	1	5.21	0.71	18.45
-5	10	1	1.8	-29.09	17.74
-4	10	1	0.86	-54.28	18.27
-3	10	1	20.9	29.45	7.63
-2	10	1	5.37	6.74	7.27
1	-10	2	20.23	26.08	7.45
2	-10	2	2.43	-2.13	16.32
3	-10	2	88	127.87	7.99
4	-10	2	35.79	49.69	7.63
-2	-9	2	6.26	29.63	7.81
-1	-9	2	7.44	0.89	7.45
0	-9	2	0.36	10.64	16.5
1	-9	2	10.11	6.74	15.97
2	-9	2	2.47	5.32	15.43
3	-9	2	68.9	70.14	7.28
4	-9	2	13.11	-2.48	15.79
5	-9	2	21.33	29.1	7.1
6	-9	2	2.27	-2.13	16.5
-3	-8	2	2.54	7.81	7.63
-2	-8	2	0.05	-31.4	16.85
-1	-8	2	41.26	36.56	7.1
0	-8	2	3.83	-1.06	14.9
1	-8	2	0.72	-7.27	13.66
2	-8	2	0.25	-1.95	13.66
3	-8	2	13.02	17.56	5.85
4	-8	2	32.83	41.88	6.21
5	-8	2	12.55	15.79	6.39
6	-8	2	5.32	-26.25	16.32
7	-8	2	3.27	1.42	16.85
-4	-7	2	32.6	47.38	7.99
-3	-7	2	20	29.28	7.27
-2	-7	2	2.38	8.34	14.72
-1	-7	2	3.24	0.89	13.84
0	-7	2	62.9	61.98	6.22
1	-7	2	70.44	74.07	6.22
2	-7	2	185.77	174.62	8.72
3	-7	2	8.46	8.87	13.13
4	-7	2	0.86	12.24	13.13
5	-7	2	0.12	7.27	5.85
6	-7	2	2.85	7.27	6.56
7	-7	2	1.44	1.42	6.92
8	-7	2	5.81	9.4	18.09
-5	-6	2	0.25	-1.06	7.8
-4	-6	2	6.86	6.21	17.03
-3	-6	2	1.96	23.06	6.21
-2	-6	2	82.47	78.88	6.57
-1	-6	2	14.77	23.78	5.68
0	-6	2	76.78	65.56	5.86
1	-6	2	11.55	6.39	12.42
2	-6	2	142.69	129.88	7.65
3	-6	2	46.11	41.37	5.68
4	-6	2	63.48	57.01	5.86
5	-6	2	0.55	-1.77	13.84
6	-6	2	96.9	96.29	6.75
7	-6	2	20.65	19.7	7.1
8	-6	2	0.24	8.87	16.85
-6	-5	2	1.96	12.42	19.69
-5	-5	2	24.99	24.13	7.45
-4	-5	2	121.53	113.41	7.64
-3	-5	2	1.12	-5.5	15.43
-2	-5	2	23.24	12.78	14.2
-1	-5	2	8.67	-2.31	12.6
0	-5	2	4.28	1.77	4.79
1	-5	2	62.79	55.25	4.8
2	-5	2	4.23	11.35	4.61
3	-5	2	7.08	7.45	11.53
4	-5	2	20.74	4.79	12.95
5	-5	2	13.52	12.07	5.86
6	-5	2	0.6	-14.19	14.55
7	-5	2	1.27	5.14	15.96
8	-5	2	13.71	1.24	17.39
-7	-4	2	0.12	-29.27	21.82
-6	-4	2	1.65	-6.92	18.8
-5	-4	2	197.68	189.74	10.68
-4	-4	2	18.77	83.4	18.1
-3	-4	2	204.64	170.34	9.98
-2	-4	2	451.67	417.78	16.68
-1	-4	2	42.64	33.21	4.62
0	-4	2	1451.63	1442.3	21.46
1	-4	2	293.13	279	12.89
2	-4	2	511.25	468.1	14.94
3	-4	2	4.62	7.1	11
4	-4	2	105.83	108.29	5.87
5	-4	2	155.95	146.8	8.9
6	-4	2	41.2	44.02	6.57
7	-4	2	3.33	-11.18	16.32
8	-4	2	0.09	2.13	7.63
-8	-3	2	0.13	2.31	9.58
-7	-3	2	6.2	-2.48	19.34
-6	-3	2	10.61	18.63	7.45
-5	-3	2	90.04	88.84	7.46
-4	-3	2	37.85	29.82	6.39
-3	-3	2	29.14	25.21	5.5
-2	-3	2	23.16	6.21	11.18
-1	-3	2	285.27	251.53	12.36
0	-3	2	76.8	81.3	4.98
1	-3	2	1313.71	1340.95	19.15
2	-3	2	182.63	208.8	9.99
3	-3	2	9.62	1.77	10.82
4	-3	2	285.08	278.26	13.75
5	-3	2	6.47	16.68	6.21
6	-3	2	3.44	-3.19	14.9
7	-3	2	9.43	7.63	7.1
8	-3	2	5.98	14.37	17.74
-8	-2	2	0	19.16	19.33
-7	-2	2	45.85	50.24	8.17
-6	-2	2	37.49	35.32	7.28
-5	-2	2	217.6	172.31	9.8
-4	-2	2	97.9	92.28	6.22
-3	-2	2	113.66	105.55	5.34
-2	-2	2	81.87	112.63	5.69
-1	-2	2	192.12	230.84	10.2
0	-2	2	1137.71	1170.61	17.05
1	-2	2	0.62	42.93	12.24
2	-2	2	1363.44	1351.13	19.74
3	-2	2	63.32	69.63	6.66
4	-2	2	352.11	335.14	11.01
5	-2	2	123.55	123.81	15.74
6	-2	2	84.58	90.24	5.2
7	-2	2	19.41	28.44	7.19
8	-2	2	0.68	-3.33	13.68
-9	-1	2	1.27	8.26	15.1
-8	-1	2	21.24	26.8	7.41
-7	-1	2	13.31	11.42	12.44
-6	-1	2	207.28	218.51	14.34
-5	-1	2	260.18	267.76	9.52
-4	-1	2	21.33	22.83	7.37
-3	-1	2	3638.71	3796.68	62.33
-2	-1	2	469.62	513.86	10.89
-1	-1	2	170.11	242.27	12.37
0	-1	2	1828.52	1658.7	12.44
1	-1	2	150.3	200.62	5.74
2	-1	2	35.97	63.04	7.28
3	-1	2	704.38	708.86	17.57
4	-1	2	7.54	2.35	9.44
5	-1	2	1.99	4.13	10.71
6	-1	2	144.43	130.83	9.07
7	-1	2	8.59	12.66	6.82
8	-1	2	8.07	-11.91	13.97
-9	0	2	8.69	1.97	15.61
-8	0	2	15.6	12.18	13.13
-7	0	2	1.27	-6.3	11.79
-6	0	2	146.61	142.67	7.47
-5	0	2	17.78	20.28	4.07
-4	0	2	46.56	52.19	5.6
-3	0	2	31.24	63.04	3.7
-2	0	2	618.69	573.96	39.5
-1	0	2	94.36	119.19	4.38
0	0	2	2781.94	2675.33	22.67
1	0	2	1327.54	1294.96	37.89
2	0	2	1643.44	1546.82	17.19
3	0	2	367.11	353.15	13.44
4	0	2	100.07	101.15	4.45
5	0	2	13.66	16.52	7.9
6	0	2	0.1	-5.31	17.92
7	0	2	74.8	80.28	5.89
8	0	2	5.38	1.6	7.8
-9	1	2	8.98	-7.39	14.24

h	k	l	F_c^2	F_o^2	σF_o^2
-8	1	2	1.88	10.71	7.01
-7	1	2	52.97	54.7	8.88
-6	1	2	91.53	76.77	5.01
-5	1	2	6.87	9	9.35
-4	1	2	159.53	154.72	19.97
-3	1	2	102.29	112.29	4.72
-2	1	2	32.13	66.11	3.52
-1	1	2	5159.61	5726.42	55.44
0	1	2	1327.02	1237.08	28.89
1	1	2	364.92	423.19	12.34
2	1	2	780.5	797.98	12.54
3	1	2	0.97	-4.16	8.78
4	1	2	128.67	132.14	4.83
5	1	2	43.9	58.46	12.34
6	1	2	0.07	-7.11	12.19
7	1	2	2.07	-5.62	13.43
-9	2	2	3.48	-5.71	13.44
-8	2	2	10.58	15	7.19
-7	2	2	0.59	7.2	10.96
-6	2	2	0.18	-8.39	10.68
-5	2	2	72.06	61.95	6.13
-4	2	2	88.69	98.29	10.23
-3	2	2	355.82	333.98	19.14
-2	2	2	69.78	111.74	4.8
-1	2	2	1759.68	1705.17	19.72
0	2	2	2081.97	2076.56	22.3
1	2	2	877.58	942.9	17.35
2	2	2	463.35	470.04	15.81
3	2	2	2.88	5.5	14.01
4	2	2	68.38	70.16	6.93
5	2	2	0.02	-11.88	16.5
6	2	2	5.98	0.53	18.45
7	2	2	23.58	44.36	9.05
-9	3	2	0.06	-6.39	17.92
-8	3	2	3.23	-6.03	16.5
-7	3	2	347.46	345.61	16.42
-6	3	2	28.78	35.32	6.21
-5	3	2	288.06	276.87	14.29
-4	3	2	6.97	6.39	10.82
-3	3	2	29.08	26.28	4.26
-2	3	2	309.95	272.06	12.37
-1	3	2	277.41	265.29	12.18
0	3	2	16.51	6.57	10.65
1	3	2	4.97	-0.71	10.64
2	3	2	5.23	-12.24	13.48
3	3	2	27.42	22.54	6.57
4	3	2	31.13	28.22	6.92
5	3	2	2.89	-22	17.56
6	3	2	2.78	8.16	8.34
-9	4	2	0.89	-5.85	17.38
-8	4	2	0.14	0.53	16.5
-7	4	2	0.17	-3.73	15.08
-6	4	2	27.7	24.49	6.21
-5	4	2	22.69	21.65	5.32
-4	4	2	34.22	31.78	4.79
-3	4	2	33.07	29.12	4.44
-2	4	2	784.91	744.92	17.23
-1	4	2	67.49	75.35	5.51
0	4	2	145.39	149.93	8.19
1	4	2	55.55	46	5.51
2	4	2	18.32	23.78	6.21
3	4	2	183.06	191.16	10.32
4	4	2	1.61	10.47	16.5
5	4	2	4.23	-26.25	19.16
6	4	2	6.61	5.32	8.87
-9	5	2	11.56	6.56	18.63
-8	5	2	10.73	9.23	16.32
-7	5	2	44.84	34.79	6.57
-6	5	2	16.45	14.37	14.73
-5	5	2	21.68	20.76	5.86
-4	5	2	198.46	211.49	10.87
-3	5	2	6.78	9.93	4.79
-2	5	2	11.11	10.29	4.79
-1	5	2	91.24	78.22	5.51
0	5	2	28.77	29.46	5.5
1	5	2	6.19	13.13	14.01
2	5	2	11.77	-0.53	15.26
3	5	2	21.58	27.15	6.74
4	5	2	0.16	-6.56	17.56
5	5	2	0.61	6.92	19.16
-9	6	2	30.35	1.42	19.17
-8	6	2	76.75	89.86	7.64
-7	6	2	2.96	-9.22	15.61
-6	6	2	35.42	29.46	6.39
-5	6	2	17.31	-3.37	13.66
-4	6	2	53.71	58.42	5.86
-3	6	2	23.98	4.26	13.13
-2	6	2	206.74	212.52	10.15
-1	6	2	19.24	22.71	5.68
0	6	2	5.91	0.89	13.48
1	6	2	44.99	39.23	6.21
2	6	2	10.75	8.69	15.79
3	6	2	0.26	-8.16	16.85
4	6	2	3.24	7.27	19.16
-9	7	2	3.22	8.87	17.74
-8	7	2	7.3	10.29	7.1
-7	7	2	1.54	-11.88	15.61
-6	7	2	57.12	53.97	8.75
-5	7	2	66.49	57.01	6.22
-4	7	2	42.82	45.44	6.39
-3	7	2	97.53	81.74	6.57
-2	7	2	87.86	86.17	6.4
-1	7	2	3.76	-0.89	6.03
0	7	2	124.53	129.23	7.82
1	7	2	0.05	1.06	15.25
2	7	2	22.26	-16.32	17.57
3	7	2	1.11	-2.66	17.38
-8	8	2	1.01	13.48	7.63
-7	8	2	0.41	-17.74	14.9
-6	8	2	10.45	0.53	15.26
-5	8	2	7.59	-2.84	15.61
-4	8	2	0	-11	14.19
-3	8	2	22.9	11.89	14.73
-2	8	2	0.49	10.47	14.37
-1	8	2	33.91	57.5	6.57
0	8	2	3.26	-2.48	15.61
1	8	2	0.25	-12.42	17.38
2	8	2	0.03	0.71	7.8
-7	9	2	7.59	2.84	17.74
-6	9	2	1.85	6.74	16.67
-5	9	2	1.81	-1.24	15.96
-4	9	2	13.81	25.9	6.74
-3	9	2	0.39	-1.24	15.43
-2	9	2	22.47	13.66	16.86
-1	9	2	3.92	-13.48	16.5
0	9	2	1.22	-2.13	17.03
-4	10	2	0.04	6.03	7.1
-3	10	2	0.4	5.85	17.38
1	-10	3	8.36	0.71	17.39
2	-10	3	11.09	28.03	7.27
3	-10	3	4.19	-9.05	16.67
-2	-9	3	0.8	14.9	17.38
-1	-9	3	5.48	-4.61	16.32
0	-9	3	29.57	40.64	6.92
1	-9	3	18.1	30.52	6.92
2	-9	3	0.43	-8.51	14.55
3	-9	3	5.97	-1.77	14.9
4	-9	3	0.54	2.48	15.61
5	-9	3	1.39	-6.03	15.96
-3	-8	3	2.05	0.71	17.03
-2	-8	3	17.1	-6.03	16.68
-1	-8	3	13.9	12.95	15.79
0	-8	3	13.43	12.95	6.21
1	-8	3	85.77	80.11	6.39
2	-8	3	0.07	-0.53	5.85
3	-8	3	0.01	-7.98	14.37
4	-8	3	20.37	11.18	14.2
5	-8	3	3.45	2.48	15.43
6	-8	3	8.15	11	7.1
-5	-7	3	0.51	-9.93	18.27
-4	-7	3	1.56	7.98	7.45
-3	-7	3	24.14	27.68	7.28
-2	-7	3	25.84	22	6.57
-1	-7	3	0.09	-15.25	14.19
0	-7	3	3.17	2.31	13.3
1	-7	3	8.69	19.52	5.68
2	-7	3	31.7	28.09	6.03
3	-7	3	65.3	73.34	6.22
4	-7	3	9.06	3.02	14.19
5	-7	3	0.52	-0.53	14.55
6	-7	3	35.44	31.41	6.92
7	-7	3	0.04	-10.82	17.56
-6	-6	3	3.03	-41.33	20.93
-5	-6	3	6.73	20.93	7.45
-4	-6	3	0.2	8.16	15.79
-3	-6	3	19.94	18.1	6.39
-2	-6	3	0.01	-28.56	14.55
-1	-6	3	0.03	0	13.13
0	-6	3	195.73	181.48	8.37
1	-6	3	45.79	39.59	5.86
2	-6	3	1	3.73	12.77
3	-6	3	29.65	32.66	5.88
4	-6	3	106.12	114.64	7.64
5	-6	3	21.11	18.5	6.03
6	-6	3	9.2	-3.37	15.43
7	-6	3	10.81	-3.9	17.03
-6	-5	3	2.24	-24.66	19.34
-5	-5	3	11.67	27.14	7.1
-4	-5	3	36.93	37.27	6.92
-3	-5	3	25.31	53.6	7.81
-2	-5	3	8.73	-1.42	13.48
-1	-5	3	56.18	58.79	5.51
0	-5	3	10.34	18.81	4.97
1	-5	3	3.99	-2.31	4.97
2	-5	3	73.37	68.76	5.51
3	-5	3	217.04	195.5	9.8
4	-5	3	136.1	126.81	6.58
5	-5	3	85.86	77.64	8.75
6	-5	3	23.68	28.75	6.74
7	-5	3	8.58	13.13	17.39
8	-5	3	0.04	-4.26	18.45
-7	-4	3	0.85	0	19.51
-6	-4	3	13.35	7.45	7.81
-5	-4	3	0.78	1.06	6.92
-4	-4	3	35.37	36.57	6.75
-3	-4	3	351.93	339.99	16.62
-2	-4	3	33.7	34.97	5.33
-1	-4	3	28.74	26.27	4.79
0	-4	3	30.58	24.68	4.62
1	-4	3	138.45	117.7	5.7
2	-4	3	4.92	11.53	11.53
3	-4	3	1.24	0.35	4.97
4	-4	3	1.77	-12.06	13.48
5	-4	3	50.31	48.12	6.57
6	-4	3	53.66	53.8	6.92
7	-4	3	41.89	45.79	7.63
8	-4	3	2.19	20.04	7.81
-8	-3	3	0.36	18.63	9.05
-7	-3	3	0.59	8.87	19.16
-6	-3	3	0	-11	17.56
-5	-3	3	16.34	21.12	6.92
-4	-3	3	1.65	1.06	14.9
-3	-3	3	50.41	42.63	5.68
-2	-3	3	35.01	30.36	4.97
-1	-3	3	80.43	85.72	4.62
0	-3	3	908.68	826.45	17
1	-3	3	38.03	43.87	5.15
2	-3	3	560.6	540.27	15.68
3	-3	3	41.62	31.96	4.97
4	-3	3	87.07	98.81	6.22
5	-3	3	0.34	3.02	14.55
6	-3	3	61.38	60.55	6.93
7	-3	3	18.08	18.28	7.27
8	-3	3	5.82	0.71	18.8
-8	-2	3	13.93	1.24	21.11
-7	-2	3	15.55	-4.97	18.81
-6	-2	3	57.35	70.67	7.46
-5	-2	3	45.51	54.86	7.1
-4	-2	3	70.77	68.41	6.04
-3	-2	3	5.37	12.42	4.79
-2	-2	3	90.37	93.06	5.52
-1	-2	3	6.6	58.91	11.36
0	-2	3	1742.16	1651.81	20.67
1	-2	3	361.68	372.81	13.48
2	-2	3	45.26	61.46	5.33
3	-2	3	186.25	167.77	5.99
4	-2	3	28.15	22.9	4.32
5	-2	3	15.47	-2.06	11.47
6	-2	3	3.25	5.74	6.59
7	-2	3	0.35	-10.37	12.83
8	-2	3	5.77	2.45	13.97
-9	-1	3	6.89	12.3	8.4
-8	-1	3	4.71	10.15	12.97
-7	-1	3	3.11	3.18	6.79
-6	-1	3	0.02	-5.58	11.45
-5	-1	3	34.6	37.41	4.44
-4	-1	3	53.37	55.25	5.77
-3	-1	3	662.18	611.8	11.41
-2	-1	3	151.54	208.7	13.12
-1	-1	3	58.88	95.26	3.52
0	-1	3	13.54	57.62	8.41
1	-1	3	264.92	261.64	8.87
2	-1	3	434.18	400.27	10.17
3	-1	3	46.66	50.93	3.76
4	-1	3	53.12	52.53	7.19
5	-1	3	4.01	10.94	6.3
6	-1	3	32.18	30.31	5.13
7	-1	3	0.01	-7.37	13.21
-9	0	3	2.44	-20.26	17.3
-8	0	3	20.46	24.03	5.57
-7	0	3	80.93	83.89	5.27
-6	0	3	4.98	7.28	11.06
-5	0	3	173.36	181.35	6.05
-4	0	3	1.12	-0.96	9.58
-3	0	3	197.63	193.68	6.7
-2	0	3	173.75	237.5	7.21
-1	0	3	91.25	138.14	6.15
0	0	3	235.52	247.58	7.51
1	0	3	64.39	80.8	3.46
2	0	3	26.7	21.53	3.32
3	0	3	0.79	-7.32	13.39
4	0	3	12.48	10.8	7.27
5	0	3	6.7	15.24	4.76
6	0	3	1.59	1.39	8.6
7	0	3	6.72	2.09	14.01
-9	1	3	10.2	11.64	7.29
-8	1	3	24.53	20.18	5.25
-7	1	3	33.04	26.75	5
-6	1	3	0.22	-18.49	10.77
-5	1	3	288.07	281.57	9.92
-4	1	3	221.35	187.38	6.58
-3	1	3	122.47	106.57	3.84
-2	1	3	3221.54	3377.43	19.45
-1	1	3	320.73	366.68	9.67
0	1	3	1942.25	1879.23	15.33
1	1	3	123.65	112.99	4.44
2	1	3	4.01	-4.43	8.96
3	1	3	2.97	0.71	9.87
4	1	3	27.44	34.4	13.84
5	1	3	31.58	25.61	8.7
6	1	3	2.09	-3.97	12.75
7	1	3	4.11	15.82	8.01
-9	2	3	1.97	7.37	7.12
-8	2	3	13.37	25.06	7.01
-7	2	3	114.82	114	5.26
-6	2	3	0.52	-1.28	10.41
-5	2	3	52.65	62.31	4
-4	2	3	11.76	17.1	3.26
-3	2	3	81.12	90.62	3.83
-2	2	3	1.56	-5.85	9.58

h	k	l	F_c^2	F_o^2	σF_o^2
-1	2	3	54.67	61.86	4.8
0	2	3	13.29	34.25	5.15
1	2	3	154.75	142.19	7.13
2	2	3	308.75	283.47	13.94
3	2	3	2.24	-15.97	15.43
4	2	3	23.76	8.87	15.97
5	2	3	0	-24.3	17.74
6	2	3	11.12	-11.89	19.34
-9	3	3	44.02	48.99	7.45
-8	3	3	30.64	21.65	6.92
-7	3	3	160.68	157.8	7.65
-6	3	3	24.95	21.3	6.03
-5	3	3	0	-8.51	12.95
-4	3	3	38.65	47.06	4.79
-3	3	3	473.01	442.54	14.57
-2	3	3	1198.62	1251.69	20.05
-1	3	3	251.6	243.46	11.44
0	3	3	24.32	8.17	11.18
1	3	3	301.92	315.79	15.37
2	3	3	39.61	14.38	14.56
3	3	3	0.02	4.97	14.72
4	3	3	1.57	-3.02	15.96
5	3	3	12.72	-0.53	18.1
6	3	3	0.76	-21.82	20.22
-9	4	3	0.95	19.51	7.1
-8	4	3	0.42	-14.55	16.5
-7	4	3	20.79	27.5	6.21
-6	4	3	3.95	-14.19	14.55
-5	4	3	482.68	461.46	17.75
-4	4	3	7.04	-3.9	11.18
-3	4	3	1447.84	1484.51	23.73
-2	4	3	226.28	255	12.49
-1	4	3	61.29	64.49	4.97
0	4	3	273.23	264.77	12.5
1	4	3	42.81	40.84	5.86
2	4	3	2.31	-9.93	14.72
3	4	3	66.49	80.09	7.1
4	4	3	0	4.97	7.45
5	4	3	0.81	-13.84	18.27
-9	5	3	3.99	5.32	17.38
-8	5	3	7.38	16.32	6.92
-7	5	3	2.01	-5.85	14.19
-6	5	3	13.23	11	6.03
-5	5	3	16.52	24.31	5.86
-4	5	3	0.38	7.45	12.24
-3	5	3	143.37	152.69	7.83
-2	5	3	43.2	34.27	5.33
-1	5	3	44.71	42.26	5.5
0	5	3	0.22	-0.35	13.66
1	5	3	50.74	45.81	6.39
2	5	3	31.54	20.94	6.74
3	5	3	53.47	46.69	7.28
4	5	3	9.83	-16.63	16.45
-9	6	3	0.67	-2.84	17.58
-8	6	3	3.05	-4.79	16.32
-7	6	3	8.19	5.85	14.72
-6	6	3	0.86	-7.1	13.84
-5	6	3	39.2	42.25	6.04
-4	6	3	24.81	28.22	5.68
-3	6	3	10.88	10.65	12.95
-2	6	3	37.52	42.43	5.86
-1	6	3	2.78	12.59	12.77
0	6	3	26.73	10.83	14.02
1	6	3	10.61	-11	14.9
2	6	3	36.45	53.96	7.1
3	6	3	0	-4.43	17.38
4	6	3	2.18	3.19	8.16
-9	7	3	4.08	17.03	18.09
-8	7	3	6.67	12.6	16.85
-7	7	3	0.03	-4.08	15.43
-6	7	3	45.72	45.44	6.75
-5	7	3	0.44	7.1	13.3
-4	7	3	12.87	7.63	14.19
-3	7	3	0.59	-6.21	13.84
-2	7	3	2.42	0.53	13.3
-1	7	3	4.75	6.56	13.3
0	7	3	71.86	73.34	6.93
1	7	3	2.11	-3.02	16.14
2	7	3	18.29	11.71	17.57
-8	8	3	0.02	0.89	7.45
-7	8	3	24.53	38.15	7.1
-6	8	3	11.53	-3.02	15.97
-5	8	3	2.07	-19.16	15.79
-4	8	3	5.73	11.35	14.9
-3	8	3	6.88	-3.37	14.72
-2	8	3	0.01	7.63	6.39
-1	8	3	0.47	-0.53	6.56
0	8	3	3.95	-2.31	6.74
1	8	3	3.95	-5.5	17.74
-7	9	3	9.98	-25.72	17.74
-6	9	3	5.76	12.95	7.27
-5	9	3	2.13	-1.95	16.14
-4	9	3	0.69	6.56	15.43
-3	9	3	8.58	1.24	17.21
-2	9	3	10.92	5.32	16.68
-1	9	3	6.11	-7.63	17.21
2	-10	4	0.02	12.06	16.14
-2	-9	4	0.03	-16.32	18.98
-1	-9	4	3.69	1.42	16.85
0	-9	4	0.62	-3.02	6.74
1	-9	4	0.16	-15.61	15.43
2	-9	4	5.03	-9.93	15.97
3	-9	4	0.34	12.77	14.55
4	-9	4	6.29	-3.9	16.32
5	-9	4	33.13	49.87	7.63
-3	-8	4	0.06	0.71	17.38
-2	-8	4	3.82	1.42	6.92
-1	-8	4	15.85	4.61	14.9
0	-8	4	23.69	26.26	6.39
1	-8	4	11.1	9.76	13.13
2	-8	4	21.81	33.18	6.21
3	-8	4	24.83	10.11	15.62
4	-8	4	0.73	-10.64	15.79
5	-8	4	26	10.82	16.33
6	-8	4	2.44	9.76	16.85
-5	-7	4	0.32	-4.61	8.16
-4	-7	4	15.91	9.4	18.27
-3	-7	4	5.5	15.79	6.74
-2	-7	4	3.25	5.14	6.21
-1	-7	4	106.4	100.05	6.75
0	-7	4	44.79	46.87	6.21
1	-7	4	4.06	-9.22	13.13
2	-7	4	1.54	0	13.66
3	-7	4	108.42	91.7	6.58
4	-7	4	74.92	80.27	6.75
5	-7	4	3.46	14.9	6.39
6	-7	4	7.09	14.01	7.1
7	-7	4	5.21	-18.98	18.27
-6	-6	4	0	0.71	18.98
-5	-6	4	5.14	7.45	17.74
-4	-6	4	55.86	61.25	7.28
-3	-6	4	1.43	5.85	6.21
-2	-6	4	0.76	-15.96	14.55
-1	-6	4	0.87	-11.18	13.3
0	-6	4	7.88	-3.55	13.31
1	-6	4	1.22	9.93	12.59
2	-6	4	188.3	176.61	7.66
3	-6	4	7.91	10.11	13.31
4	-6	4	41.42	46.86	6.21
5	-6	4	0	-6.56	14.37
6	-6	4	2.37	-3.73	16.14
7	-6	4	0.17	-17.56	18.8
-7	-5	4	1.67	-16.5	21.11
-6	-5	4	8.73	-8.16	19.16
-5	-5	4	0.02	-20.22	16.67
-4	-5	4	0.05	-17.74	15.96
-3	-5	4	121.03	125.88	7.11
-2	-5	4	81.32	74.63	6.57
-1	-5	4	173.28	165.23	8.9
0	-5	4	3.24	-5.5	12.6
1	-5	4	105.75	126.77	7.11
2	-5	4	191.25	185.64	8.55
3	-5	4	0.17	-28.38	14.37
4	-5	4	79.95	90.78	8.75
5	-5	4	9.29	11	6.39
6	-5	4	63.32	74.4	7.81
7	-5	4	1.82	-26.25	17.74
-7	-4	4	2.9	1.95	19.69
-6	-4	4	6.35	-5.68	17.58
-5	-4	4	182.86	178.84	8.01
-4	-4	4	9.14	7.98	15.79
-3	-4	4	88.77	101.3	6.4
-2	-4	4	74.73	69.66	5.88
-1	-4	4	1.3	7.81	4.97
0	-4	4	0.81	2.31	11
1	-4	4	198.87	188.43	8.38
2	-4	4	159.08	166.12	8.72
3	-4	4	42.5	34.98	5.5
4	-4	4	91.57	97.73	6.57
5	-4	4	27.05	31.23	6.39
6	-4	4	7.59	6.74	15.26
7	-4	4	11.33	15.08	7.45
-8	-3	4	6.39	-30.87	21.47
-7	-3	4	6.74	20.58	8.16
-6	-3	4	4.93	-3.02	7.45
-5	-3	4	0.18	9.58	16.32
-4	-3	4	3.81	5.14	14.55
-3	-3	4	218.47	237.71	12.13
-2	-3	4	7.35	4.81	11.89
-1	-3	4	1261.05	1226.84	20.96
0	-3	4	243.01	240.12	11.81
1	-3	4	279.14	262.08	12.34
2	-3	4	44	41.55	4.97
3	-3	4	198.91	182.28	9.44
4	-3	4	48.49	53.62	8.39
5	-3	4	49.25	54.5	6.75
6	-3	4	4.42	8.87	15.97
7	-3	4	0.01	25.72	7.27
-8	-2	4	0.04	-0.71	20.04
-7	-2	4	9.52	-5.32	18.1
-6	-2	4	22.55	15.44	17.04
-5	-2	4	64.29	63.77	7.1
-4	-2	4	56.74	68.38	6.22
-3	-2	4	1056.19	981.42	20.44
-2	-2	4	60.55	70.55	5.51
-1	-2	4	328.59	319.4	13.27
0	-2	4	68.08	88.89	5.33
1	-2	4	353.32	407.17	14.34
2	-2	4	5.34	4.26	11.35
3	-2	4	641.37	603.04	13.8
4	-2	4	2.38	-1.54	11.97
5	-2	4	2.06	5.82	11.21
6	-2	4	0.14	-14.29	14.37
7	-2	4	5.68	-12.82	13.68
-9	-1	4	1.31	12.7	23.95
-8	-1	4	10.88	2.54	7.42
-7	-1	4	27.33	21.34	20.14
-6	-1	4	39.47	40.21	5.02
-5	-1	4	9.43	4.22	5.44
-4	-1	4	96.04	88.58	4.89
-3	-1	4	78.33	82.05	9.33
-2	-1	4	194.98	194.31	7.23
-1	-1	4	44.86	71.14	3.58
0	-1	4	74.07	90.94	3.77
1	-1	4	337.99	326.32	21.6
2	-1	4	4.99	11.38	5.5
3	-1	4	63.86	69.9	6.4
4	-1	4	39.12	40.21	4.7
5	-1	4	8.34	3.85	11
6	-1	4	0	-6.81	12.5
7	-1	4	1.7	6.09	13.59
-9	0	4	10.52	5.88	8.18
-8	0	4	12.65	16.67	12.4
-7	0	4	0.24	5.07	6.26
-6	0	4	19.13	25.1	12.33
-5	0	4	4.11	0.97	5.35
-4	0	4	450.02	473.74	11.49
-3	0	4	111.92	111.25	4.34
-2	0	4	244.7	207.55	7
-1	0	4	20.82	22.36	13.94
0	0	4	15	26.04	12.25
1	0	4	36.86	58.92	3.83
2	0	4	474.65	434.72	11.74
3	0	4	36.17	31.94	4.14
4	0	4	103.1	108.3	5.02
5	0	4	0.17	-15.12	27.14
6	0	4	3.14	-6.83	17.47
7	0	4	0.62	-0.24	14.15
-9	1	4	3.65	8.74	13.41
-8	1	4	10.57	17.64	7.98
-7	1	4	6.88	-0.68	12.95
-6	1	4	30.65	31.11	4.82
-5	1	4	39.42	43.75	4.01
-4	1	4	58.73	44.59	3.45
-3	1	4	1077.36	963.36	12.91
-2	1	4	0.32	-2.44	6.96
-1	1	4	64.64	79.3	4.36
0	1	4	6.75	32.45	9.05
1	1	4	418.25	407.26	12.74
2	1	4	0.25	0.02	5.32
3	1	4	4.17	10.85	5.8
4	1	4	0.24	8.58	10.46
5	1	4	2.13	2.87	11.53
6	1	4	23.57	24.07	20.23
-10	2	4	22.87	27.73	12.07
-9	2	4	0.37	4.84	12.78
-8	2	4	2.58	3.98	11.54
-7	2	4	43.43	33.51	4.88
-6	2	4	18.99	18.95	4.44
-5	2	4	0.2	-18.42	9.26
-4	2	4	105.72	100.92	4.15
-3	2	4	37.35	32.56	3.14
-2	2	4	46.14	36.77	4.26
-1	2	4	122.65	115.38	6.23
0	2	4	304.18	301.09	13.78
1	2	4	3.27	-7.81	12.24
2	2	4	74.08	78	8.22
3	2	4	0.5	-1.6	15.08
4	2	4	0	-11.88	16.5
5	2	4	2.18	12.95	17.74
6	2	4	0	-22.17	19.69
-10	3	4	0.2	-18.09	18.98
-9	3	4	7.8	24.68	7.45
-8	3	4	3.33	-8.51	15.97
-7	3	4	48.17	51.49	8.57
-6	3	4	49.47	60.37	6.21
-5	3	4	433.16	420.78	17.38
-4	3	4	76.71	73.22	5.15
-3	3	4	58.88	67.87	4.8
-2	3	4	98.91	96.76	4.8
-1	3	4	1.35	-3.19	10.47
0	3	4	599.33	552.18	17.82
1	3	4	0.02	1.77	5.5
2	3	4	5.4	6.39	14.37
3	3	4	0.15	-8.34	15.08
4	3	4	24.3	15.26	17.57
5	3	4	1.08	15.96	18.27
-9	4	4	0.85	7.98	7.27
-8	4	4	47.02	61.24	6.75
-7	4	4	11.82	11	6.21
-6	4	4	23.32	28.57	6.03
-5	4	4	12.12	10.65	13.48
-4	4	4	7.38	0	12.24
-3	4	4	63.73	61.29	5.15
-2	4	4	26.09	42.78	4.97
-1	4	4	6.81	6.03	4.97
0	4	4	36.14	48.46	5.68
1	4	4	0.78	0.89	14.37
2	4	4	7.46	-4.08	15.26
3	4	4	27.74	29.99	6.92

h	k	l	F_c^2	F_o^2	σF_o^2
4	4	4	0.23	-15.96	17.74
5	4	4	9.68	-13.48	20.76
-9	5	4	0	-6.39	17.56
-8	5	4	23.39	25.91	6.92
-7	5	4	79.42	100.71	6.75
-6	5	4	110.28	97.58	6.58
-5	5	4	143.41	135.19	6.58
-4	5	4	7.71	21.11	5.68
-3	5	4	26.9	30.35	5.5
-2	5	4	6.58	15.97	5.5
-1	5	4	0.26	-2.84	5.85
0	5	4	70.19	64.3	6.39
1	5	4	1.13	6.74	14.37
2	5	4	8.58	15.97	6.56
3	5	4	4.14	-14.01	16.5
4	5	4	0.06	-11.18	18.63
-9	6	4	2.54	10.11	17.21
-8	6	4	9.59	12.6	6.92
-7	6	4	0.08	-3.73	15.08
-6	6	4	40.57	37.99	6.21
-5	6	4	8.44	-4.61	12.95
-4	6	4	17.51	23.78	5.68
-3	6	4	1.03	4.61	5.5
-2	6	4	94.77	90.8	6.75
-1	6	4	1.19	-17.21	13.66
0	6	4	61.52	64.46	6.57
1	6	4	7.9	17.39	6.39
2	6	4	4.45	-9.22	16.5
3	6	4	1.6	-5.5	18.09
-8	7	4	0.17	5.85	7.1
-7	7	4	0.63	-22.71	15.61
-6	7	4	1.49	-17.03	14.55
-5	7	4	12.64	12.6	14.55
-4	7	4	10.83	0	13.48
-3	7	4	1.12	4.79	5.68
-2	7	4	0	-9.76	14.37
-1	7	4	49.99	39.06	6.57
0	7	4	21.79	29.99	6.74
1	7	4	0.37	-18.45	17.38
2	7	4	12.2	26.26	7.81
-8	8	4	2.23	-9.4	17.56
-7	8	4	11.87	6.92	6.92
-6	8	4	0.93	-22.53	15.61
-5	8	4	15.47	-19.69	15.97
-4	8	4	0.03	2.84	14.55
			F_c^2	F_o^2	σF_o^2
-3	8	4	0.06	-1.24	14.55
-2	8	4	1.53	7.27	14.37
-1	8	4	11.46	-13.31	15.97
0	8	4	2.58	-10.11	17.21
-6	9	4	2.19	-1.95	7.27
-5	9	4	5.61	-5.5	16.14
-4	9	4	0.13	-0.18	6.92
-3	9	4	6.44	2.66	6.92
-2	9	4	0.01	14.01	15.08
-1	-9	5	1.77	10.29	16.5
0	-9	5	1.99	4.61	15.43
1	-9	5	29.07	32.12	6.92
2	-9	5	20.52	34.42	6.92
3	-9	5	6.59	10.11	6.92
4	-9	5	5.16	-0.71	16.5
-3	-8	5	2.73	-1.95	17.21
-2	-8	5	3.94	-4.43	16.5
-1	-8	5	16.08	9.05	6.92
0	-8	5	9.78	12.6	14.19
1	-8	5	15.19	-13.13	15.44
2	-8	5	17.48	18.1	6.56
3	-8	5	43.45	44.2	6.92
4	-8	5	0.01	-3.19	16.32
5	-8	5	1.33	0	15.79
-5	-7	5	1.03	13.66	8.16
-4	-7	5	0.01	-1.95	16.67
-3	-7	5	1.36	8.69	15.08
-2	-7	5	2.36	18.45	6.39
-1	-7	5	1.08	-9.76	14.37
0	-7	5	65.57	68.37	6.39
1	-7	5	0.03	-1.42	14.19
2	-7	5	8.84	11.71	5.85
3	-7	5	0.78	-14.72	14.37
4	-7	5	39.12	55.55	7.1
5	-7	5	2.82	3.19	15.79
6	-7	5	13.29	31.05	7.45
-6	-6	5	0.01	-41.51	20.75
-5	-6	5	0.21	-15.08	18.09
-4	-6	5	8.8	0	16.5
-3	-6	5	21.71	17.21	6.57
-2	-6	5	11.32	26.08	6.03
-1	-6	5	29.76	11.71	14.55
0	-6	5	102.19	110.19	6.4
1	-6	5	133.99	134.08	6.58
2	-6	5	30.51	36.38	5.86
3	-6	5	0.71	-22.17	14.72
4	-6	5	7.96	6.21	6.39
5	-6	5	17.3	-1.24	15.79
6	-6	5	1.14	13.3	16.67
-7	-5	5	0.86	-7.98	20.93
-6	-5	5	0.85	-9.05	19.16
-5	-5	5	0.97	16.5	17.21
-4	-5	5	9.27	6.56	16.14
-3	-5	5	89.5	80.67	6.93

h	k	l	F_c^2	F_o^2	σF_o^2
-2	-5	5	178.49	154.69	7.48
-1	-5	5	19.07	-2.31	14.37
0	-5	5	10.74	8.34	13.48
1	-5	5	8.28	8.16	13.66
2	-5	5	1.38	-11.53	13.84
3	-5	5	239.17	225.74	10.69
4	-5	5	42.19	42.43	6.39
5	-5	5	0.95	6.74	14.9
6	-5	5	9.15	-27.85	17.74
7	-5	5	7.57	0	18.8
-7	-4	5	3.84	-7.45	20.05
-6	-4	5	0.04	-1.77	17.74
-5	-4	5	47.33	39.77	7.28
-4	-4	5	2.22	-11	15.61
-3	-4	5	0.35	1.95	14.55
-2	-4	5	38.46	52.19	5.68
-1	-4	5	14.84	12.07	5.32
0	-4	5	133.99	128.83	5.87
1	-4	5	10.15	9.58	5.15
2	-4	5	6.95	6.21	12.95
3	-4	5	36.69	35.15	5.86
4	-4	5	32.28	31.59	6.21
5	-4	5	0.33	10.11	6.21
6	-4	5	2.49	1.77	15.96
7	-4	5	0	-39.38	19.87
-8	-3	5	0.4	-3.55	20.04
-7	-3	5	1.38	-3.02	18.45
-6	-3	5	9.83	-28.21	17.39
-5	-3	5	2.42	-7.45	15.79
-4	-3	5	37.29	33.02	6.57
-3	-3	5	358.26	341.76	15.74
-2	-3	5	32.8	18.64	5.33
-1	-3	5	9.76	7.98	4.79
0	-3	5	105.24	100.85	5.34
1	-3	5	24.7	31.06	4.97
2	-3	5	21.83	12.78	12.96
3	-3	5	200.67	207.85	9.97
4	-3	5	19.79	9.58	14.73
5	-3	5	26.09	14.91	15.79
6	-3	5	2.45	-35.3	17.38
7	-3	5	4.64	7.1	18.8
-8	-2	5	6.41	-25.19	20.93
-7	-2	5	3.05	15.97	17.92
-6	-2	5	3.84	-9.4	16.85
-5	-2	5	9.77	14.37	15.61
-4	-2	5	73.99	66.81	6.22
-3	-2	5	34.76	33.2	5.15
-2	-2	5	52.17	58.62	4.8
-1	-2	5	324.85	313.65	13.43
0	-2	5	90.85	87.49	4.98
1	-2	5	73.33	58.65	4.98
2	-2	5	118.6	123.8	5.87
3	-2	5	117.8	119.82	9.34
4	-2	5	13.54	-7.39	10.78
5	-2	5	20.22	12.07	8.07
6	-2	5	0.36	-1.55	7.21
7	-2	5	36.83	36.26	25.2
-9	-1	5	1.75	-34.68	14.52
-8	-1	5	0.01	-11.08	21.82
-7	-1	5	22.07	7.2	16.5
-6	-1	5	37.31	51.81	4.89
-5	-1	5	1.89	-14.55	10.28
-4	-1	5	4.98	8.52	3.76
-3	-1	5	38.42	39.42	3.45
-2	-1	5	101.43	105.35	3.77
-1	-1	5	13.24	13.46	3.01
0	-1	5	633.58	612.02	11.68
1	-1	5	1.32	8.59	4.28
2	-1	5	17.55	15.25	3.83
3	-1	5	6.14	2.71	5.68
4	-1	5	17.41	4.23	10.78
5	-1	5	0.71	-0.66	12.06
6	-1	5	4.99	1.45	13.11
-9	0	5	2.79	-13.67	13.85
-8	0	5	34.49	32.45	5.58
-7	0	5	50.18	48.8	5.02
-6	0	5	1.73	-1.52	5.93
-5	0	5	338.16	320.34	24.13
-4	0	5	345.83	346.35	11.07
-3	0	5	488.86	465.39	10.87
-2	0	5	27.7	33.57	4.26
-1	0	5	78.25	80.09	3.54
0	0	5	130.64	135.17	12.46
1	0	5	1.71	-20.82	8.39
2	0	5	247.49	246.79	10.79
3	0	5	29.34	27.37	4.51
4	0	5	50.81	44.6	8.52
5	0	5	3.59	-3.24	12.19
6	0	5	12.08	9.74	13.2
-9	1	5	0.22	-22.53	13.48
-8	1	5	29.77	27.35	5.31
-7	1	5	1.08	-1	11.29
-6	1	5	49.67	50.66	4.77
-5	1	5	2.45	6.37	5.21
-4	1	5	49.48	52.06	3.7
-3	1	5	2.77	4.39	10.38
-2	1	5	82.01	83.32	3.33
-1	1	5	79.99	103.89	3.77
0	1	5	0.48	1.6	4.24
1	1	5	174.54	172.43	9.26

h	k	l	F_c^2	F_o^2	σF_o^2
2	1	5	31.11	24.98	4.26
3	1	5	3.76	-2.3	12.51
4	1	5	0.67	8.68	6.29
5	1	5	0.63	-21.06	12.16
6	1	5	4.08	6.94	7.51
-9	2	5	17.26	-12.36	12.89
-8	2	5	45.98	35.75	12.43
-7	2	5	0.35	-22.68	10.96
-6	2	5	42.18	54.71	10.21
-5	2	5	294.44	296.4	10.79
-4	2	5	133.58	118.84	8.28
-3	2	5	177.83	161.91	10.43
-2	2	5	14.96	15.97	4.61
-1	2	5	417.92	424.24	15.42
0	2	5	45.6	36.94	5.15
1	2	5	46.13	45.46	5.86
2	2	5	66.67	76.2	6.57
3	2	5	0.36	5.85	15.08
4	2	5	9.04	-3.9	16.85
5	2	5	0.42	-5.32	18.98
-10	3	5	1.65	-5.85	19.16
-9	3	5	5.94	16.32	16.85
-8	3	5	29.43	31.59	6.92
-7	3	5	21.37	26.79	6.21
-6	3	5	75.23	71.59	6.57
-5	3	5	59.67	65.89	6.04
-4	3	5	0.56	4.61	4.97
-3	3	5	223.21	204.91	10.34
-2	3	5	246.97	249.1	12.31
-1	3	5	40.27	39.59	5.15
0	3	5	555.7	509.45	18.67
1	3	5	58.82	66.95	6.22
2	3	5	1.36	1.42	14.37
3	3	5	13.54	11	6.92
4	3	5	4.98	2.48	17.38
5	3	5	2.98	4.97	20.04
-9	4	5	1.79	14.19	16.5
-8	4	5	1.96	-4.43	16.14
-7	4	5	53.85	69.07	6.57
-6	4	5	42.09	52.19	6.21
-5	4	5	23.03	16.5	5.68
-4	4	5	16.79	23.42	5.5
-3	4	5	87.4	80.68	5.69
-2	4	5	50.27	54.87	5.5
-1	4	5	58.51	43.69	5.86
0	4	5	95.64	109.12	6.4
1	4	5	78.89	79.76	6.57
2	4	5	23.68	23.96	8.74
3	4	5	16.14	12.42	16.32
4	4	5	4.03	-14.01	8.16
-9	5	5	4.2	-5.32	16.85
-8	5	5	0.02	3.55	14.37
-7	5	5	28.07	32.3	6.39
-6	5	5	7.62	-21.82	14.55
-5	5	5	0.1	-15.43	13.66
-4	5	5	3.74	7.63	5.68
-3	5	5	0.3	-2.48	13.48
-2	5	5	7.63	13.68	5.85
-1	5	5	118.8	120.35	7.82
0	5	5	0.62	-10.64	14.55
1	5	5	3.6	6.92	15.08
2	5	5	7.13	-0.53	16.32
3	5	5	0.51	-14.01	18.63
-9	6	5	4.34	16.32	7.45
-8	6	5	0.18	-16.14	17.03
-7	6	5	5.68	-16.32	15.79
-6	6	5	79.83	88.99	6.57
-5	6	5	33.33	34.96	6.03
-4	6	5	30.08	11.36	13.84
-3	6	5	88.25	88.91	6.22
-2	6	5	6.01	12.42	5.85
-1	6	5	49.91	47.93	6.39
0	6	5	1.26	0	14.55
1	6	5	1.71	8.51	15.26
2	6	5	0	1.95	17.21
-8	7	5	0.6	9.4	15.96
-7	7	5	14.98	4.97	16.32
-6	7	5	5.49	-30.87	16.14
-5	7	5	1.32	6.21	14.19
-4	7	5	0.81	8.16	14.01
-3	7	5	1.59	0	6.21
-2	7	5	23.9	29.1	6.57
-1	7	5	0.41	0	15.25
0	7	5	5.3	-8.87	16.68
1	7	5	2.19	-23.59	17.74
-7	8	5	3.4	10.29	16.5
-6	8	5	8.78	3.9	16.32
-5	8	5	11.6	18.81	6.74
-4	8	5	8.17	-6.92	16.14
-3	8	5	1.3	-19.69	15.26
-2	8	5	4.57	7.27	16.32
-1	8	5	12.05	16.14	7.27
-5	9	5	3.1	-12.06	15.79
-4	9	5	0.89	-33.53	18.09
-1	-9	6	0.01	7.8	17.38
0	-9	6	0.65	11.71	16.5
1	-9	6	7.18	12.24	7.27
2	-9	6	0.99	-25.19	16.67
3	-9	6	1.69	2.13	16.67
-3	-8	6	4.08	-6.21	17.56

h	k	l	F_c^2	F_o^2	σF_o^2
-2	-8	6	11.44	-4.61	17.03
-1	-8	6	10.04	13.66	7.1
0	-8	6	3.68	0.89	6.74
1	-8	6	1.76	-0.53	16.14
2	-8	6	6.64	-1.24	15.61
3	-8	6	2.26	-11.88	17.21
4	-8	6	6.03	15.43	7.45
-4	-7	6	0.03	10.82	7.45
-3	-7	6	0.02	11.71	16.32
-2	-7	6	0.06	9.22	16.14
-1	-7	6	51.59	52.37	6.75
0	-7	6	3.32	2.13	14.01
1	-7	6	3.28	0.53	14.37
2	-7	6	0.36	-15.25	15.61
3	-7	6	1.08	3.02	15.79
4	-7	6	0.1	-9.58	15.61
5	-7	6	0.61	-41.33	17.38
-6	-6	6	0.01	-3.73	20.22
-5	-6	6	0.65	-5.85	18.27
-4	-6	6	0.59	13.66	16.67
-3	-6	6	3.64	-1.06	15.08
-2	-6	6	120.95	132.42	7.29
-1	-6	6	13.11	16.86	6.21
0	-6	6	0	2.31	14.01
1	-6	6	30.81	28.22	6.03
2	-6	6	62.95	53.63	6.39
3	-6	6	19.55	15.44	6.21
4	-6	6	11.52	19.16	6.74
5	-6	6	0.52	-5.85	16.32
6	-6	6	0.64	2.13	17.74
-6	-5	6	20.75	-17.92	19.87
-5	-5	6	33.75	46.32	7.63
-4	-5	6	36.27	34.26	6.92
-3	-5	6	4.37	-2.31	14.55
-2	-5	6	255.95	239.37	11.23
-1	-5	6	146.65	135.01	8.18
0	-5	6	15.53	8.34	14.02
1	-5	6	9.15	6.56	5.85
2	-5	6	11.7	-13.66	14.55
3	-5	6	63.28	78.84	6.39
4	-5	6	0.02	1.6	14.9
5	-5	6	5.06	14.72	15.43
6	-5	6	0.8	12.59	17.21
-7	-4	6	6.76	3.9	6.69
-6	-4	6	0.14	-1.77	17.56
-5	-4	6	24.12	27.15	6.92
-4	-4	6	110.57	99.71	7.11
-3	-4	6	326.3	313.29	13.75
-2	-4	6	82.15	83.69	6.4
-1	-4	6	146.43	155.87	7.65
0	-4	6	33.68	10.83	13.31
1	-4	6	17.68	10.82	13.66
2	-4	6	243.96	267.32	14.26
3	-4	6	154.88	151.55	6.94
4	-4	6	94.73	95.76	6.93
5	-4	6	11.86	16.14	16.5
6	-4	6	7.4	-34.42	18.8
-8	-3	6	5.75	-23.24	22
-7	-3	6	2.57	-9.22	18.27
-6	-3	6	1.11	2.66	17.21
-5	-3	6	25.62	21.3	8.92
-4	-3	6	1.4	10.64	14.01
-3	-3	6	31.07	27.51	6.21
-2	-3	6	18.22	18.99	5.5
-1	-3	6	0.55	3.02	5.14
0	-3	6	14.82	8.52	12.78
1	-3	6	45.04	47.05	5.68
2	-3	6	304.77	288.93	14.46
3	-3	6	189.34	172.84	8.01
4	-3	6	8.99	14.02	14.37
5	-3	6	73.44	82.4	7.64
6	-3	6	52.37	72.25	8.17
-8	-2	6	6.43	-15.61	20.58
-7	-2	6	14.19	20.4	7.63
-6	-2	6	3.05	9.22	16.5
-5	-2	6	144.75	141.41	7.29
-4	-2	6	1.43	6.74	14.01
-3	-2	6	49.99	44.4	5.68
-2	-2	6	22.22	0.89	12.07
-1	-2	6	82.66	83.72	5.33
0	-2	6	17.17	18.28	4.97
1	-2	6	0.14	-10.47	12.59
2	-2	6	38.19	31.78	6.04
3	-2	6	33.11	38.41	7.72
4	-2	6	0.11	-8.06	11.41
5	-2	6	0.6	-5.87	6.65
6	-2	6	0	-4.49	7.53
-9	-1	6	0.15	-9.8	14.29
-8	-1	6	7.26	10.13	12.66
-7	-1	6	0.49	-1.94	17.12
-6	-1	6	20.57	25.95	7.1
-5	-1	6	2.48	2.8	5.85
-4	-1	6	27.33	36.68	6.3
-3	-1	6	7.91	-2.22	8.59
-2	-1	6	361.58	353.65	10.88
-1	-1	6	353.95	334.91	10.75
0	-1	6	172.48	184.56	8.02
1	-1	6	128.6	108.46	4.27
2	-1	6	0.23	6.11	5.53
3	-1	6	27.51	33.85	8.61
4	-1	6	6.52	7.97	6.09
5	-1	6	3.31	2.84	12.17
6	-1	6	0.56	-7.07	13.92
-9	0	6	4.21	10.09	13.71
-8	0	6	0.17	4.43	12.39
-7	0	6	0.06	-12.77	11.29
-6	0	6	3.39	-1.65	10.79
-5	0	6	0.04	2.29	9.97
-4	0	6	10.96	-1.66	8.97
-3	0	6	0.72	-1.2	8.08
-2	0	6	135.69	140.53	6.1
-1	0	6	11.46	20.17	3.32
0	0	6	48.19	47.24	4.26
1	0	6	9.74	6.62	6.83
2	0	6	58.31	68.82	16.34
3	0	6	65.8	63.05	10.21
4	0	6	9.1	10.61	11.03
5	0	6	17.9	28.29	5.59
-9	1	6	2.24	-22.85	13.96
-8	1	6	9.48	14.34	6.9
-7	1	6	14.11	13.63	4.83
-6	1	6	10.66	-6.92	11.04
-5	1	6	1.35	-3.2	9.58
-4	1	6	106.47	120.49	7.2
-3	1	6	2.8	2.51	6.34
-2	1	6	23.12	24.06	3.45
-1	1	6	5.73	-3.36	10.02
0	1	6	1.52	6.59	8.64
1	1	6	10.15	-5.56	9.83
2	1	6	2.15	-11.41	10.21
3	1	6	0.33	-20.93	10.93
4	1	6	3.89	-14.2	17.12
5	1	6	0.99	0.23	14.28
-9	2	6	2.87	9.23	12.47
-8	2	6	1.82	-3.67	7.81
-7	2	6	16.4	8.11	24.31
-6	2	6	0.01	24.11	9.14
-5	2	6	103.99	92.13	4.46
-4	2	6	3.55	3.64	9.03
-3	2	6	49.65	49.37	3.76
-2	2	6	20.55	25.73	5.15
-1	2	6	13.72	9.23	12.6
0	2	6	61.29	48.13	6.04
1	2	6	63.73	61.45	6.57
2	2	6	9.73	1.42	6.39
3	2	6	8.04	-32.64	17.03
4	2	6	0.04	-5.14	17.56
5	2	6	3.14	-12.59	19.16
-9	3	6	2.63	5.14	16.85
-8	3	6	12.72	2.31	16.32
-7	3	6	10.97	18.27	6.21
-6	3	6	50.5	43.85	6.21
-5	3	6	73.67	57.73	6.22
-4	3	6	28.89	21.48	5.5
-3	3	6	216.17	199.95	9.62
-2	3	6	32.41	22.37	5.68
-1	3	6	70.76	66.79	6.04
0	3	6	2.5	-15.26	14.37
1	3	6	4.61	-24.84	15.06
2	3	6	35.27	49.34	6.57
3	3	6	5.94	-6.03	17.74
4	3	6	2.33	-10.82	8.16
-9	4	6	4.71	5.85	17.03
-8	4	6	2.87	-23.24	16.32
-7	4	6	1.09	5.68	14.19
-6	4	6	84.67	86.16	6.4
-5	4	6	0.01	-12.42	13.48
-4	4	6	12.98	9.76	13.13
-3	4	6	0.28	13.13	5.32
-2	4	6	0.46	-19.87	13.66
-1	4	6	3.62	-7.27	13.48
0	4	6	185.82	177.25	9.61
1	4	6	3.17	-6.21	15.08
2	4	6	11.08	4.61	16.14
3	4	6	2.95	12.59	17.56
-9	5	6	0.5	-29.27	18.09
-8	5	6	0.55	2.48	16.14
-7	5	6	19.67	2.84	15.79
-6	5	6	8.25	-6.56	14.72
-5	5	6	209.12	227.53	11.04
-4	5	6	4.49	-3.73	13.84
-3	5	6	45.67	41.19	6.04
-2	5	6	26.76	33.54	6.03
-1	5	6	1.77	2.31	6.03
0	5	6	17.55	1.6	15.44
1	5	6	2.34	13.13	6.92
2	5	6	0	-5.5	7.45
-9	6	6	1.94	-12.24	18.63
-8	6	6	6.46	7.98	7.1
-7	6	6	41.89	43.13	6.92
-6	6	6	12.07	7.27	15.26
-5	6	6	10.2	1.6	14.19
-4	6	6	27.77	5.68	14.55
-3	6	6	42.32	34.79	6.39
-2	6	6	6.97	-5.32	13.84
-1	6	6	0.27	-27.14	15.43
0	6	6	0.1	-12.24	15.79
1	6	6	7.46	6.74	17.92
-8	7	6	0.74	-7.8	17.38
-7	7	6	0.36	-5.65	15.61
-6	7	6	3.98	-23.06	16.85
-5	7	6	4.58	7.81	15.26
-4	7	6	0.13	-11.35	16.14
-3	7	6	1.15	-6.03	15.08
-2	7	6	12.46	8.69	15.44
-1	7	6	8.29	11.16	16.14
0	7	6	12.79	-13.31	18.45
-7	8	6	5.14	0.71	17.03
-6	8	6	7.9	13.31	16.68
-5	8	6	1.44	-6.03	16.67
-4	8	6	0.06	-5.5	15.61
-3	8	6	1.59	-1.42	16.5
-2	8	6	2.76	-25.54	17.56
-2	-8	7	9.86	4.26	17.56
-1	-8	7	0.74	16.5	7.1
0	-8	7	0.19	-9.4	16.32
1	-8	7	0.01	3.37	15.96
2	-8	7	10.33	7.63	17.21
3	-8	7	14.25	24.48	7.45
-4	-7	7	1.28	23.41	7.63
-3	-7	7	10.57	8.52	17.39
-2	-7	7	0.01	-15.43	15.79
-1	-7	7	22.73	41.52	6.92
0	-7	7	24.64	29.46	6.74
1	-7	7	17.35	12.77	6.92
2	-7	7	2.89	6.51	15.43
3	-7	7	51.02	52.19	7.46
4	-7	7	1.42	11.18	16.14
-5	-6	7	0.24	8.87	7.8
-4	-6	7	17.67	-12.42	17.92
-3	-6	7	4.8	2.13	6.74
-2	-6	7	8.31	4.26	15.43
-1	-6	7	26.69	9.94	14.73
0	-6	7	0.56	-7.8	14.19
1	-6	7	0.34	11	14.01
2	-6	7	28.78	22.89	6.21
3	-6	7	44.89	55.56	6.92
4	-6	7	52.62	70.65	7.46
5	-6	7	7.88	9.93	17.92
-6	-5	7	0.56	-5.32	8.16
-5	-5	7	25.83	37.09	7.63
-4	-5	7	5.5	8.87	6.74
-3	-5	7	37.14	41.18	6.57
-2	-5	7	0.47	-11.53	14.55
-1	-5	7	2.41	-15.97	14.19
0	-5	7	6.11	-4.26	14.37
1	-5	7	0.93	-7.27	13.84
2	-5	7	0.01	7.27	14.37
3	-5	7	4.97	3.9	14.55
4	-5	7	8.73	13.48	15.97
5	-5	7	1.34	10.29	7.45
-7	-4	7	0.25	-34.59	20.4
-6	-4	7	8.1	14.01	7.63
-5	-4	7	2.45	-26.25	17.03
-4	-4	7	39.38	43.84	6.57
-3	-4	7	276.36	270.45	13.73
-2	-4	7	81.28	86.12	6.57
-1	-4	7	12.18	-2.48	14.19
0	-4	7	261.72	237.1	12.84
1	-4	7	187.51	175.33	9.43
2	-4	7	104.63	89.92	6.75
3	-4	7	0.06	4.26	13.84
4	-4	7	11.81	10.84	16.32
5	-4	7	6.49	-3.37	16.85
-8	-3	7	1.69	4.26	21.64
-7	-3	7	6.12	3.02	8.16
-6	-3	7	26.22	29.99	7.28
-5	-3	7	2.13	13.48	15.43
-4	-3	7	22.44	13.84	14.91
-3	-3	7	143.97	145.51	8.18
-2	-3	7	69.98	70.52	6.22
-1	-3	7	61.87	60.03	6.04
0	-3	7	82.6	76.58	6.22
1	-3	7	24.6	12.6	5.86
2	-3	7	26.16	29.81	6.21
3	-3	7	0.5	-16.14	14.55
4	-3	7	95.52	99.48	7.82
5	-3	7	1.62	-12.59	17.56
-8	-2	7	0.09	-38.85	20.58
-7	-2	7	14.56	17.92	7.63
-6	-2	7	0.14	-4.26	6.74
-5	-2	7	2.17	-4.61	15.43
-4	-2	7	225.56	244.45	11.4
-3	-2	7	94.4	97.04	6.22
-2	-2	7	7.07	-10.82	13.31
-1	-2	7	60.47	45.11	5.68
0	-2	7	8.75	1.6	13.66
1	-2	7	0.07	-5.32	13.66
2	-2	7	140.88	133.38	6.94
3	-2	7	0.84	-6.21	14.72
4	-2	7	13.16	26.05	7.19
5	-2	7	13.87	8.72	13.1
-9	-1	7	0.13	10.55	13.74
-8	-1	7	0.98	4.21	12.89
-7	-1	7	1.1	7.85	7.98
-6	-1	7	2.71	-6.26	10.89
-5	-1	7	27.75	28.07	4.45
-4	-1	7	4.08	1.93	8.16
-3	-1	7	4.19	-8.69	9.76
-2	-1	7	71.24	79.15	4.02

h	k	l	F_c^2	F_o^2	σF_o^2
-1	-1	7	15.93	1.2	9.08
0	-1	7	19.82	24.42	4.08
1	-1	7	408.7	383.76	12.98
2	-1	7	26.19	32.55	16.95
3	-1	7	15.33	23.85	14.64
4	-1	7	12.38	11.56	24.57
5	-1	7	1.83	-5.51	13.35
-9	0	7	0.48	-21.13	13.64
-8	0	7	3.68	13.62	6.9
-7	0	7	3.39	8.61	6.2
-6	0	7	0.12	11.36	10.28
-5	0	7	29.81	44.66	16.06
-4	0	7	22.26	21.06	7.28
-3	0	7	0.34	1.65	8.65
-2	0	7	82.77	77.22	3.9
-1	0	7	12.2	16.47	7.45
0	0	7	0.17	1.22	9.28
1	0	7	119.17	114.8	6.04
2	0	7	0.78	-16.67	10.16
3	0	7	1.49	3.83	5.94
4	0	7	1.18	-18.09	11.92
5	0	7	0.07	-0.85	7.57
-9	1	7	1.76	-24.17	13.9
-8	1	7	0.44	-8.88	14.1
-7	1	7	11.74	16.76	9.14
-6	1	7	42.75	42.38	4.7
-5	1	7	36.52	37.17	4.39
-4	1	7	87.57	93.53	4.46
-3	1	7	3.03	0.17	9.28
-2	1	7	1.92	-0.36	5.04
-1	1	7	0.05	5.62	9.15
0	1	7	91.27	86.44	4.39
1	1	7	17.4	0.5	10.27
2	1	7	16.68	8.16	10.53
3	1	7	0.01	-2.06	6.25
4	1	7	0.05	7.62	6.68
-9	2	7	0.8	-11.01	18.18
-8	2	7	51.85	52.46	11.89
-7	2	7	5.41	4.63	6.28
-6	2	7	179.89	176.8	9.34
-5	2	7	83.33	98.11	4.64
-4	2	7	56.17	56.47	4.33
-3	2	7	167.24	144.14	6.05
-2	2	7	45.17	54.15	5.86
-1	2	7	51.99	41.73	6.21
0	2	7	78.78	79.76	6.4
1	2	7	2.62	-3.02	14.37
2	2	7	24.35	26.09	6.92
3	2	7	0.31	-46.12	17.21
4	2	7	0.08	-38.85	20.4
-9	3	7	6.18	16.32	7.45
-8	3	7	0.14	-17.03	16.32
-7	3	7	36.71	40.82	6.74
-6	3	7	57.36	60.73	6.39
-5	3	7	217.09	205.35	10.86
-4	3	7	59.3	47.59	6.22
-3	3	7	8.36	22	5.68
-2	3	7	122.64	138.68	7.47
-1	3	7	0.71	-16.5	13.66
0	3	7	129.43	131.03	6.93
1	3	7	0.03	7.27	6.21
2	3	7	20.65	23.95	7.27
3	3	7	0.82	-27.67	18.09
-9	4	7	0.28	-18.98	17.74
-8	4	7	0.78	2.48	15.61
-7	4	7	0.03	9.93	15.08
-6	4	7	39.99	31.42	6.39
-5	4	7	4.73	1.77	5.68
-4	4	7	3.33	14.55	5.5
-3	4	7	24.04	-1.42	13.84
-2	4	7	29.21	-3.73	15.09
-1	4	7	213.73	218.8	10.68
0	4	7	20.8	26.62	6.21
1	4	7	19.98	-7.1	16.15
2	4	7	20.34	29.45	7.63
-9	5	7	1.96	-28.2	18.63
-8	5	7	27.48	28.75	7.28
-7	5	7	2.85	1.77	15.97
-6	5	7	0.54	6.03	14.19
-5	5	7	5.3	-6.21	14.19
-4	5	7	0.38	-1.95	14.01
-3	5	7	4.21	1.6	5.85
-2	5	7	0.44	-3.19	14.37
-1	5	7	1.11	-11.71	14.9
0	5	7	9.8	-0.53	15.43
1	5	7	2.07	14.55	16.67
-8	6	7	0.69	8.16	16.67
-7	6	7	23.63	24.13	7.1
-6	6	7	2.32	7.45	6.56
-5	6	7	9.39	9.23	14.37
-4	6	7	0.47	-7.45	14.55
-3	6	7	9.37	-0.89	6.39
-2	6	7	0.55	-19.51	15.61
-1	6	7	8.43	11	6.74
0	6	7	6.6	3.73	7.1
-7	7	7	13.3	8.34	17.92
-6	7	7	0.01	7.27	15.25
-5	7	7	1.09	-37.61	16.32
-4	7	7	0.48	6.03	6.56
-3	7	7	0	3.19	15.43
-2	7	7	0.06	-15.61	16.14
-1	7	7	0.05	-4.26	16.14
-1	-8	8	17.4	12.24	17.39
0	-8	8	0.67	-14.37	17.03
1	-8	8	3.05	4.26	7.45
-4	-7	8	1.64	-23.59	19.34
-3	-7	8	21.21	17.92	18.1
-2	-7	8	17.88	9.76	17.21
-1	-7	8	6.5	-5.14	16.85
0	-7	8	27.54	34.25	7.1
1	-7	8	14.43	10.29	6.92
2	-7	8	11.12	8.16	7.27
3	-7	8	3.52	3.55	17.21
-5	-6	8	10.31	19.51	7.98
-4	-6	8	5.13	7.1	7.1
-3	-6	8	4.98	1.42	6.92
-2	-6	8	11.96	10.29	6.56
-1	-6	8	0.68	8.51	14.72
0	-6	8	19.49	14.73	15.26
1	-6	8	0.24	3.37	6.39
2	-6	8	0.12	-6.21	14.72
3	-6	8	39.3	55.91	7.28
4	-6	8	11.27	33.18	7.27
-6	-5	8	19.27	-10.65	19.52
-5	-5	8	0.05	-24.48	17.92
-4	-5	8	37.92	32.48	7.28
-3	-5	8	0.99	10.82	6.39
-2	-5	8	45.41	43.14	6.57
-1	-5	8	68.2	72.63	6.57
0	-5	8	52.32	42.43	6.57
1	-5	8	72.79	58.96	6.75
2	-5	8	0.37	-5.32	14.37
3	-5	8	0.11	-0.18	6.92
4	-5	8	3.2	10.29	16.32
-7	-4	8	16.49	-3.55	20.05
-6	-4	8	6.06	-24.66	19.34
-5	-4	8	22	34.42	7.28
-4	-4	8	3	6.39	15.61
-3	-4	8	79.63	76.56	6.93
-2	-4	8	167.48	172.39	9.78
-1	-4	8	129.2	118.76	6.76
0	-4	8	211.86	217.56	9.61
1	-4	8	12.78	15.97	6.03
2	-4	8	14.73	16.68	6.21
3	-4	8	34.42	49.52	7.1
4	-4	8	28.98	42.06	7.28
-7	-3	8	0.03	6.56	18.09
-6	-3	8	9.82	12.24	7.27
-5	-3	8	20.88	12.24	15.97
-4	-3	8	47.86	51.31	6.39
-3	-3	8	9.81	13.31	6.03
-2	-3	8	0.21	5.85	12.95
-1	-3	8	6.7	-17.03	13.48
0	-3	8	1.27	-13.84	13.48
1	-3	8	13.74	-4.97	15.08
2	-3	8	50.85	52.37	6.57
3	-3	8	55.25	58.23	7.28
4	-3	8	1.9	7.98	16.14
-8	-2	8	3.98	13.13	19.87
-7	-2	8	0.69	-14.72	17.74
-6	-2	8	0.67	-23.59	16.5
-5	-2	8	12.97	23.77	6.56
-4	-2	8	88.9	84.22	6.75
-3	-2	8	35.52	31.24	6.04
-2	-2	8	0.63	11.88	5.68
-1	-2	8	5.17	8.34	5.85
0	-2	8	8.2	11.18	13.48
1	-2	8	20.35	10.29	6.03
2	-2	8	0.02	-4.26	14.37
3	-2	8	12.07	-10.64	16.14
4	-2	8	26.13	25.99	5.46
-8	-1	8	0.79	-25.08	14.72
-7	-1	8	2.87	-9.15	11.98
-6	-1	8	1.64	8.06	6.04
-5	-1	8	3.51	8.87	10.22
-4	-1	8	69.23	78.64	4.58
-3	-1	8	7.5	10.22	5.39
-2	-1	8	63.22	58.02	4.4
-1	-1	8	0.15	-15.07	10.73
0	-1	8	10.99	10.11	5.85
1	-1	8	4.69	2.89	10.73
2	-1	8	5.7	14.87	7.81
3	-1	8	1.75	2.45	6.45
4	-1	8	2.8	3.64	12.6
-9	0	8	8.42	12.66	8.01
-8	0	8	3.1	-2.66	7.13
-7	0	8	0.76	3.64	11.54
-6	0	8	5.66	3.61	12.86
-5	0	8	108.91	128.62	4.78
-4	0	8	1.43	7.01	9.66
-3	0	8	5.76	4.93	9.71
-2	0	8	55.21	56.3	4.26
-1	0	8	2.99	-14.99	9.72
0	0	8	18.19	15.34	8.78
1	0	8	14.89	13.29	11.71
2	0	8	0.43	6.19	10.82
3	0	8	1.72	-17.32	11.97
4	0	8	4.45	10.4	5.57
-9	1	8	3.49	12.79	7.73
-8	1	8	17.18	12.36	21.47
-7	1	8	17.13	12.88	11.29
-6	1	8	3.5	10.23	5.74
-5	1	8	6.02	-0.39	19.6
-4	1	8	2.88	3.2	5.37
-3	1	8	65.64	73.8	4.46
-2	1	8	6.81	2.75	6.83
-1	1	8	3.18	-0.43	5.35
0	1	8	89.5	99.18	4.77
1	1	8	29.95	28.33	4.45
2	1	8	2.12	-2.71	6.45
3	1	8	9.49	2.38	6.85
-9	2	8	15.8	18.73	5.96
-8	2	8	13.16	9.94	13.57
-7	2	8	25.2	21.18	10.2
-6	2	8	9.59	6.44	5.87
-5	2	8	37.56	29.57	4.39
-4	2	8	107.62	101.88	5.15
-3	2	8	1.69	4.63	5.36
-2	2	8	26.46	29.28	5.86
-1	2	8	21.25	23.6	6.03
0	2	8	6.32	10.64	6.21
1	2	8	8.54	5.5	6.92
2	2	8	0.15	-1.95	16.67
3	2	8	2.56	-2.84	18.27
-9	3	8	5.4	-2.84	18.8
-8	3	8	2.78	7.45	16.14
-7	3	8	0.91	-0.53	15.96
-6	3	8	40.8	38.52	6.21
-5	3	8	26.91	36.91	6.03
-4	3	8	3.73	-2.66	5.85
-3	3	8	180.42	178.84	9.25
-2	3	8	5.22	-1.95	14.01
-1	3	8	24.61	-7.28	15.62
0	3	8	2.43	-10.64	15.08
1	3	8	16.07	4.97	16.5
2	3	8	6.84	-2.66	18.63
-9	4	8	0.9	-1.42	18.27
-8	4	8	12.33	23.6	6.92
-7	4	8	13.46	-14.19	16.15
-6	4	8	0.14	3.37	14.01
-5	4	8	0.09	-4.43	5.85
-4	4	8	19.05	18.99	6.03
-3	4	8	7.36	11.71	5.85
-2	4	8	4.92	12.24	13.48
-1	4	8	5.2	1.6	14.72
0	4	8	12.39	20.58	6.74
1	4	8	44.25	52.36	7.81
-8	5	8	3.84	9.4	17.03
-7	5	8	4.03	13.84	15.79
-6	5	8	14.82	24.13	6.56
-5	5	8	11.26	8.52	14.19
-4	5	8	1.26	7.27	14.37
-3	5	8	2.88	6.03	6.39
-2	5	8	5.6	14.19	15.43
-1	5	8	7.87	9.22	6.92
0	5	8	3.19	14.9	17.21
-7	6	8	4.23	11.53	15.79
-6	6	8	9.13	-6.39	16.14
-5	6	8	0	6.92	14.55
-4	6	8	0	6.92	14.55
-3	6	8	14.65	1.24	15.08
-2	6	8	10.42	8.52	6.92
-1	6	8	7.96	8.52	7.27
-6	7	8	10.4	-5.68	17.03
-5	7	8	3.55	-37.96	17.56
-4	7	8	1.25	11.88	15.43
-3	7	8	12.04	29.1	7.45
-2	-7	9	2.63	4.26	16.85
-1	-7	9	44.54	53.25	7.63
0	-7	9	17.35	-2.13	17.03
1	-7	9	31.81	56.08	7.63
-4	-6	9	1.55	13.13	17.21
-3	-6	9	9.44	9.23	16.85
-2	-6	9	9.95	0	16.5
-1	-6	9	1.8	9.4	15.79
0	-6	9	9	11.89	8.74
1	-6	9	0.45	1.24	15.79
2	-6	9	39.53	61.41	7.45
-5	-5	9	31.52	51.82	7.99
-4	-5	9	10.32	9.58	15.97
-3	-5	9	0.25	-18.98	15.96
-2	-5	9	33.67	33.37	6.92
-1	-5	9	3.43	9.93	15.26
0	-5	9	4.95	14.37	6.56
1	-5	9	2.58	8.69	15.96
2	-5	9	1.68	-9.93	16.32
3	-5	9	18.87	-15.61	18.1
-6	-4	9	7.96	-12.42	18.98
-5	-4	9	12.44	-13.84	18.45
-4	-4	9	3	-15.26	16.5
-3	-4	9	0.53	-2.31	15.61
-2	-4	9	2.38	-20.58	15.96
-1	-4	9	0.18	4.43	14.72
0	-4	9	6.26	9.22	6.21
1	-4	9	16.48	-11.71	15.44
2	-4	9	4.11	-6.56	6.92
3	-4	9	5.33	8.16	16.32
-7	-3	9	7.33	6.39	8.34
-6	-3	9	0.05	-12.06	17.92
-5	-3	9	0.21	6.39	15.61

h	k	l	F_c^2	F_o^2	σF_o^2
-4	-3	9	67.85	72.63	6.93
-3	-3	9	7.09	9.4	14.72
-2	-3	9	1.18	11.53	5.85
-1	-3	9	42.03	38.16	6.39
0	-3	9	14.21	15.61	6.39
1	-3	9	5.72	8.52	14.19
2	-3	9	0.09	9.76	15.61
3	-3	9	11.26	4.08	16.32
-8	-2	9	6.76	-20.4	21.64
-7	-2	9	3.41	-7.27	17.56
-6	-2	9	6.01	11.53	7.27
-5	-2	9	8.17	-19.69	15.61
-4	-2	9	82.15	85.26	6.93
-3	-2	9	35.13	28.22	6.21
-2	-2	9	77.9	79.22	6.39
-1	-2	9	56.44	68.89	6.39
0	-2	9	8.5	14.02	14.55
1	-2	9	9.54	-28.92	15.97
2	-2	9	6.42	12.24	16.5
3	-2	9	3.61	6.03	16.5
-8	-1	9	2.42	-24.04	13.29
-7	-1	9	34.53	32.64	19.7
-6	-1	9	2.29	-11.29	11.52
-5	-1	9	198.57	206.7	7.34
-4	-1	9	4.08	-11.15	9.97
-3	-1	9	5.81	-0.31	9.97
-2	-1	9	29.58	22.11	15.17
-1	-1	9	2.52	2.52	5.39
0	-1	9	2.87	-2.7	19.16
1	-1	9	37.16	41.44	4.77
2	-1	9	0.2	5.33	6.83
3	-1	9	0.55	-13.64	12.65
-8	0	9	4.76	-2.25	7.12
-7	0	9	2.43	8.51	11.67
-6	0	9	30.3	29.37	4.7
-5	0	9	10.45	6.09	5.71
-4	0	9	21.88	32.63	7.19
-3	0	9	75.59	81.18	7.46
-2	0	9	22.22	21.83	8.25
-1	0	9	57.24	57.62	8.61
0	0	9	76.31	69.89	5.24
1	0	9	35.16	40.67	6.83
2	0	9	0	5.72	6.31
3	0	9	52.26	63.61	5.84
-8	1	9	1.16	-4.02	14.99
-7	1	9	9.1	19.95	6.83
-6	1	9	0.12	5.97	8.16
-5	1	9	3.93	-2.38	10.66
-4	1	9	0.25	-12.13	9.9
-3	1	9	5.26	1.49	9.72
-2	1	9	21	25.86	4.33
-1	1	9	9.9	11.73	4.7
0	1	9	145.86	152.04	5.89
1	1	9	4.04	6.11	11.16
2	1	9	21.99	14.79	6.89
-8	2	9	25.79	30.34	5.46
-7	2	9	5.48	12.09	11.66
-6	2	9	1.58	-7.04	10.97
-5	2	9	5.42	-6.67	10.64
-4	2	9	1.53	6.09	4.33
-3	2	9	12.46	13.13	4.27
-2	2	9	4.77	14.72	6.03
-1	2	9	0.22	-26.25	15.25
0	2	9	0	-3.55	16.14
1	2	9	2.19	-7.81	16.14
2	2	9	0.9	-1.42	16.09
-8	3	9	3.22	15.61	16.67
-7	3	9	8.17	13.13	15.61
-6	3	9	2.55	-18.63	14.9
-5	3	9	15.46	15.79	6.39
-4	3	9	86.77	93.26	6.93
-3	3	9	17.34	8.87	14.9
-2	3	9	39.7	54.67	6.74
-1	3	9	0.08	-8.34	16.14
h	k	l	F_c^2	F_o^2	σF_o^2
0	3	9	5	12.24	16.32
1	3	9	8.88	21.29	7.63
-8	4	9	0.03	-9.76	16.5
-7	4	9	0.01	14.19	15.96
-6	4	9	7.84	20.05	6.39
-5	4	9	1.81	5.85	6.39
-4	4	9	0.32	-23.06	15.43
-3	4	9	12.01	8.16	15.08
-2	4	9	2.4	6.03	16.14
-1	4	9	6.27	4.43	15.79
0	4	9	3.66	7.63	16.85
-7	5	9	15.49	-13.48	17.21
-6	5	9	0.01	-8.51	16.32
-5	5	9	2.9	12.59	14.72
-4	5	9	11.96	14.37	6.74
-3	5	9	0	-3.9	15.79
-2	5	9	0.01	-30.15	16.67
-1	5	9	9.84	-2.13	17.92
-6	6	9	0.94	2.84	15.96
-5	6	9	17.75	-8.87	17.57
-4	6	9	0.04	-23.41	16.32
-3	6	9	2.43	5.68	16.5
-3	-6	10	0.98	7.98	7.63
-2	-6	10	0.11	2.13	17.03
-1	-6	10	3.12	17.56	6.92
0	-6	10	10.09	14.37	7.27
1	-6	10	2.37	5.14	17.38
-4	-5	10	0.01	9.76	17.74
-3	-5	10	2.04	3.19	7.27
-2	-5	10	0.46	5.85	15.25
-1	-5	10	10.52	17.92	7.1
0	-5	10	0.17	14.01	15.79
1	-5	10	1.33	-1.24	7.1
-6	-4	10	0.01	14.72	18.63
-5	-4	10	0.02	-15.79	17.21
-4	-4	10	1.06	6.39	15.96
-3	-4	10	1.49	7.45	15.26
-2	-4	10	4.47	0.53	15.79
-1	-4	10	12.33	13.48	15.08
0	-4	10	21.09	13.31	15.61
1	-4	10	0.16	6.56	6.74
2	-4	10	4.66	2.84	17.38
-6	-3	10	0.48	-4.08	17.92
-5	-3	10	10.82	11.53	16.68
-4	-3	10	3.82	7.27	15.79
-3	-3	10	26.89	6.39	16.5
-2	-3	10	0.26	0	14.9
-1	-3	10	0.46	5.32	14.9
0	-3	10	17.5	6.74	15.97
1	-3	10	0.13	-6.39	15.61
2	-3	10	20.07	30.16	7.27
-7	-2	10	18.8	17.57	19.34
-6	-2	10	16.56	-3.19	17.21
-5	-2	10	0.4	11.53	15.79
-4	-2	10	1.27	5.14	15.26
-3	-2	10	2.85	-4.97	15.08
-2	-2	10	1.49	8.87	6.21
-1	-2	10	19.69	12.6	15.44
0	-2	10	4.86	-3.55	14.72
1	-2	10	3.01	-0.89	6.74
2	-2	10	5.51	-28.56	17.38
-7	-1	10	4.23	13.45	7.12
-6	-1	10	0.11	-4.87	6.4
-5	-1	10	1.18	14.2	11.16
-4	-1	10	0.87	4.26	4.52
-3	-1	10	26.67	33.23	4.64
-2	-1	10	39.7	45.66	4.88
-1	-1	10	15.67	9.3	4.7
0	-1	10	2.86	8.47	11.16
1	-1	10	0.6	-10.7	11.6
2	-1	10	8.19	-3.72	17.83
-8	0	10	0.02	-7.2	13.1
-7	0	10	0.11	5.37	11.81
-6	0	10	7.87	14.89	4.83
h	k	l	F_c^2	F_o^2	σF_o^2
-5	0	10	54.26	60.35	4.9
-4	0	10	22.68	8.28	11.04
-3	0	10	71.6	72.93	11.99
-2	0	10	70.89	77.25	4.83
-1	0	10	0.49	-12.08	10.72
0	0	10	10.91	-7.66	14.1
1	0	10	4.46	-2.21	11.72
2	0	10	17.01	16.64	7.29
-8	1	10	2.7	10	7.17
-7	1	10	8.57	-0.27	16.32
-6	1	10	17.68	12.28	11.48
-5	1	10	0.53	3.41	6.12
-4	1	10	0.53	-0.39	5.87
-3	1	10	35.89	36.15	13.22
-2	1	10	1.24	-7.94	6.05
-1	1	10	3.42	9.04	5.99
0	1	10	3.64	12.07	6.24
1	1	10	1.07	-5.9	11.91
-8	2	10	3.28	-19.31	12.97
-7	2	10	2.43	-1.07	6.69
-6	2	10	3.63	10.39	7.36
-5	2	10	4.27	-7.89	10.85
-4	2	10	4.8	10.65	10.65
-3	2	10	9.73	8.15	6.15
-2	2	10	22	26.62	6.74
-1	2	10	18.96	26.79	6.92
0	2	10	0.97	10.29	16.32
-7	3	10	0.79	-30.16	17.03
-6	3	10	0.28	-3.9	16.32
-5	3	10	7.64	12.24	6.92
-4	3	10	1.96	-21.82	16.32
-3	3	10	1.67	-1.6	6.74
-2	3	10	20.05	5.15	17.21
-1	3	10	2.42	-34.95	16.67
0	3	10	2.18	12.42	18.09
-7	4	10	0.73	7.8	16.32
-6	4	10	0.77	8.16	16.85
-5	4	10	1.7	14.01	6.74
-4	4	10	0.88	-16.32	15.61
-3	4	10	0.1	13.3	16.32
-2	4	10	3.92	13.48	7.1
-6	5	10	0.14	-22.17	17.56
-5	5	10	5.75	-5.68	16.68
-4	5	10	2.87	14.19	17.21
-3	-5	11	0.7	-25.19	17.74
-2	-5	11	0.19	8.69	16.85
-1	-5	11	0.41	7.98	16.5
-4	-4	11	2.67	-22	18.09
-3	-4	11	0	-12.42	7.27
-2	-4	11	1.69	3.37	16.32
-1	-4	11	17.51	9.05	16.5
0	-4	11	0.43	4.97	17.03
-5	-3	11	7.91	-3.55	17.56
-4	-3	11	0.74	-25.54	17.03
-3	-3	11	12.05	17.39	7.1
-2	-3	11	48.85	45.8	7.28
-1	-3	11	0.14	-9.93	16.32
0	-3	11	2.17	-9.76	17.74
-6	-2	11	0.58	16.14	7.63
-5	-2	11	7.69	12.06	16.5
-4	-2	11	0.07	15.61	15.79
-3	-2	11	0.51	-16.5	16.14
-2	-2	11	17.65	-4.44	16.15
-1	-2	11	0.01	-15.79	16.67
0	-2	11	0.01	-16.5	16.5
1	-2	11	4.91	0.71	16.85
-6	-1	11	1.59	-12.74	12.23
-5	-1	11	30.66	36.78	5.27
-4	-1	11	20.22	17.63	7.63
-3	-1	11	66.75	70.49	5.27
-2	-1	11	16.07	-4.94	11.67
-1	-1	11	0.02	-7.23	6.42
0	-1	11	3.26	3.57	11.79
-7	0	11	6.71	7.06	19.6
-6	0	11	14.07	15.57	5.33

h	k	l	F_c^2	F_o^2	σF_o^2
-5	0	11	7.63	0.41	19.96
-4	0	11	0.56	7.78	6.21
-3	0	11	40.2	35.99	7.99
-2	0	11	1.53	-2.2	13.48
-1	0	11	10.88	-3.64	11.77
0	0	11	1.1	0.77	5.14
-7	1	11	2.57	-3.49	13.03
-6	1	11	0.08	-0.98	6.53
-5	1	11	6.75	-27.73	12.22
-4	1	11	6.58	3.7	23.15
-3	1	11	2.63	2.26	11.07
-2	1	11	2.08	1.15	11.41
-1	1	11	1.94	0.88	11.66
-7	2	11	1.24	-4.6	18.45
-6	2	11	0.14	-5.54	11.91
-5	2	11	0.68	-16.88	12.42
-4	2	11	0.73	-3.03	11.6
-3	2	11	1.23	-2.37	11.6
-2	2	11	1.62	16.32	7.1
-1	2	11	0.02	-12.59	18.27
-6	3	11	0.16	-4.43	17.38
-5	3	11	0.21	5.68	16.14
-4	3	11	7.06	7.81	16.85
-3	3	11	3.45	13.66	16.67
-4	-2	12	2.58	-0.71	17.56
-3	-2	12	0.51	-12.95	17.03
-2	-2	12	9.89	18.81	7.45
-5	-1	12	1.13	-13.97	12.47
-4	-1	12	0.33	-3.35	12.04
-3	-1	12	6.17	11.44	6.86
-2	-1	12	1.81	8.65	8.34
-5	0	12	1.47	-14.87	12.26
-4	0	12	0.35	-5.19	6.75
-3	0	12	26.87	30.54	5.32
-4	1	12	11.12	-5.08	12.41

A3.6 TRIC2XL

h	k	l	F_c^2	F_o^2	σF_o^2
2	0	0	3114.53	3855.45	35.51
4	0	0	6918.88	9427.54	78.5
6	0	0	378.5	478.2	6.39
8	0	0	58.99	75.31	3.86
10	0	0	94.05	93.8	4.65
12	0	0	358.42	386.39	8.41
14	0	0	155.99	162.79	5.48
2	1	0	250.18	342.88	4.16
4	1	0	1687.61	2337.99	47.53
6	1	0	350.44	439.31	9.11
8	1	0	2362.53	2835.61	17.52
10	1	0	108.9	129.32	8.1
12	1	0	2571.86	2730.74	21.86
14	1	0	32.16	29.58	1.48
2	2	0	259.95	329.64	3.54
4	2	0	82.04	92.52	3.49
6	2	0	148.59	189.36	4.73
8	2	0	475.28	604.58	8.04
10	2	0	307.96	342.41	7.96
12	2	0	559.05	594.45	6.42
14	2	0	56.94	59.79	2.87
2	3	0	8689.56	9401.55	58.64
4	3	0	1368.99	1698.21	8.61
6	3	0	4617.34	5963.98	19.24
8	3	0	29.66	26.1	1.84
10	3	0	26.23	23.47	2.25
12	3	0	66.51	70.45	2.53
14	3	0	105.96	118.24	3.23
0	4	0	8964.25	7562.43	42.2
2	4	0	671.84	815.04	4.88
4	4	0	1857.49	2120.21	9.6
6	4	0	9330.41	10964.4	103.86
8	4	0	9.14	10.42	1.76
10	4	0	15.47	15.71	2.17
12	4	0	834.9	890.99	14.28
14	4	0	78.29	86.53	2.57
2	5	0	2226.39	2307.59	7.92
4	5	0	1674.14	1745.97	9
6	5	0	6.26	27.67	1.87
8	5	0	606.24	814.58	9.25
10	5	0	815.37	912.88	11.06
12	5	0	543.39	558.47	8.65
14	5	0	49.9	42.82	1.76
0	6	0	15902.5	13659.3	70.32
2	6	0	980.45	1012.28	5.76
4	6	0	14973.5	16405.92	110.07
6	6	0	0.1	-11.55	3.67
8	6	0	695.67	809.64	9.21
10	6	0	12.81	12.97	2.17
12	6	0	559.43	591.46	8.6
14	6	0	39.35	32.43	3.25
2	7	0	950.63	916.41	5.75
4	7	0	4843.18	5758.6	16.63
6	7	0	1185.37	1447.91	10.15
8	7	0	692.2	801.76	9.25
10	7	0	460.02	437.5	8.45
12	7	0	525.25	548.52	15.23
14	7	0	7.09	3.02	2.4
0	8	0	3956.83	3215.47	37.68
2	8	0	752.3	645.11	5.09
4	8	0	3.99	17.43	1.5
6	8	0	5532.61	8243.79	20.6
8	8	0	504.41	546	8.04
10	8	0	80.39	77.44	4.28
12	8	0	458.64	482.95	7.94
14	8	0	8.99	6.25	3.63
2	9	0	478.56	515.17	4.85
4	9	0	20.29	36.22	1.76
6	9	0	97.1	120.15	4.65
8	9	0	13.93	15.07	1.87
10	9	0	8.39	6.94	2.1
12	9	0	121.77	117.7	3.3
14	9	0	3.05	8.03	1.98
0	10	0	127.8	111.42	2.85
2	10	0	531.93	526.8	5.16
4	10	0	1106.66	1203.74	8.38
6	10	0	1255.5	1409.52	10.68
8	10	0	308.38	265.6	6.49
10	10	0	286.63	314.47	7.73
12	10	0	220.9	231.79	4.76
14	10	0	49.23	58.08	1.83
2	11	0	2131.31	1940.27	9.43
4	11	0	1230.68	1156.87	8.49
6	11	0	1407.63	1461.31	10.95
8	11	0	84.54	100.66	4.88
10	11	0	69.35	55.8	2.96
12	11	0	79.34	74.44	1.87
0	12	0	253.75	246.09	3.87
2	12	0	3956.6	3743	13.4
4	12	0	439.62	427.18	5.79
6	12	0	75.57	68.15	3.49
8	12	0	1.5	-4.16	4.42
10	12	0	23.36	22.35	2.14
12	12	0	107.41	122.33	3.5
2	13	0	475.54	503.41	6.01
4	13	0	67.75	81.57	4.01
6	13	0	197.22	237.68	5.7
8	13	0	23.65	12.37	2.02
10	13	0	73.51	67.46	3.68
12	13	0	1.98	2.92	1.72
0	14	0	4063.02	3765.48	13.87
2	14	0	96.4	71.65	3.3
4	14	0	498.7	529.16	6.84
6	14	0	30.74	34.2	1.95
8	14	0	1592.49	1512.18	13.31
10	14	0	82.38	114.42	5.78
12	14	0	42.27	35.29	1.54
2	15	0	480.15	422.35	5.71
4	15	0	2404.77	2412.08	13.27
6	15	0	300.76	294.41	6.38
8	15	0	77.2	82.66	4.09
10	15	0	7.37	4.24	5.21
12	15	0	31.5	31.24	1.56
0	16	0	1803.35	1709.27	10.33
2	16	0	159.63	153.95	4.5
4	16	0	25.63	36.03	1.99
6	16	0	0.24	-5.44	4.31
8	16	0	766.44	753.61	10.19
10	16	0	25.7	24.56	2.4
12	16	0	10.89	9.81	2.29
2	17	0	70.55	78.01	3.23
4	17	0	194.25	194.59	5.33
6	17	0	412.57	417.53	7.47
8	17	0	10.06	3.41	4.91
10	17	0	261.74	301.76	8.37
12	17	0	9.84	7.89	2.44
0	18	0	2.55	-1.35	3.3
2	18	0	1597.1	1414.13	10.76
4	18	0	1.35	2.55	3.86
6	18	0	129.43	111.67	5.44
8	18	0	77.75	81.49	3.94
10	18	0	0.9	-0.67	5.59
12	18	0	7.3	11.05	1.55
2	19	0	862.82	867.12	9.22
4	19	0	0.52	-12.11	4.27
6	19	0	371.31	398.88	7.62
8	19	0	266.96	262.97	7.54
10	19	0	12.07	12.15	2.44
0	20	0	286.78	303.81	5.97
2	20	0	21.55	50.99	5.92
4	20	0	1068.36	1066.7	10.46
6	20	0	265.98	266.44	6.98
8	20	0	18.91	25.05	2.62
10	20	0	57.66	61.05	3.34
2	21	0	299.41	317.99	6.91
4	21	0	141.67	118.87	5.7
6	21	0	1.69	23.73	5.02
8	21	0	3.76	3.15	2.17
10	21	0	31.96	36.71	2.66
0	22	0	266.39	252.3	5.97
2	22	0	797.69	897.35	10.26
4	22	0	451.29	469.31	8.19
6	22	0	19.52	18.78	1.99
8	22	0	109.29	130.44	5.93
10	22	0	20.05	17.28	2.77
2	23	0	60.53	450.11	8.44
4	23	0	173.54	186.63	6.53
6	23	0	9.28	4.2	4.46
8	23	0	6.87	6	2.36
0	24	0	37.17	48.07	2.32
2	24	0	72.22	55.84	3
4	24	0	6.3	8.25	2.59
6	24	0	1.98	-0.6	4.5
8	24	0	35.42	40.27	2.59
2	25	0	300.37	361.85	8.37
4	25	0	193.05	203.25	6.53
6	25	0	2.6	-0.11	4.8
8	25	0	14.58	24.6	2.55
0	26	0	156.68	155.37	6
2	26	0	0.08	95.83	8.17
4	26	0	0.02	-11.55	5.02
6	26	0	67.64	69.75	3.49
2	27	0	319.86	333.25	7.84
4	27	0	3.1	0.22	4.8
6	27	0	19.81	5.47	5.62
0	28	0	137.25	148.08	6.45
2	28	0	28.92	89.76	7.24
4	28	0	27.57	24.37	2.29
2	29	0	55.1	50.28	7.12
4	29	0	35.6	47.32	2.89
0	30	0	203.95	248.94	7.62
2	30	0	17.55	28.68	7.01
1	1	1	614.46	591.11	17.92
2	1	1	14661.3	15076.11	237.02
3	1	1	1394.25	1355	25.42
4	1	1	1322.79	1572.75	34.2
5	1	1	961.71	1018.32	32.27
6	1	1	661.19	791.34	20.12
7	1	1	21.94	19.13	1.32
8	1	1	62.87	73.65	2.76
9	1	1	904.67	983.97	40.5
10	1	1	19.18	18.4	1.23
11	1	1	1020.29	1086.74	16.88
12	1	1	51.84	52.55	1.39
13	1	1	27.49	36.23	1.37
14	1	1	23.99	24.68	2.33
0	2	1	1861.24	1485.81	295.36
1	2	1	6483.66	5999.63	360.5
2	2	1	5209.44	5199.6	130.4
3	2	1	1481.82	1443.31	34.29
4	2	1	2827.67	3158.58	24.33
5	2	1	471.38	494.47	4.27
6	2	1	4.46	1.68	1.37
7	2	1	31.49	32.03	1.27
8	2	1	45.15	55.78	2.07
9	2	1	9.78	17.07	1.52
10	2	1	152.25	172.95	4.92
11	2	1	147.39	158.47	5.26
12	2	1	111.57	103.4	3.33
13	2	1	80.25	67.19	1.75
14	2	1	2.11	-6.09	4.49
1	3	1	2869.47	2708.22	194.82
2	3	1	1637.04	1454.57	115.73
3	3	1	2400.94	2299.71	186.87
4	3	1	3623.62	3949.92	285.65
5	3	1	387.6	473.52	28.25
6	3	1	359.32	377.26	19.65
7	3	1	145.67	164.82	6.7
8	3	1	3778.2	4079.15	41.27
9	3	1	1217.9	1397.77	23.7
10	3	1	1113.26	1138.46	8.8
11	3	1	1416.61	1494.22	10.53
12	3	1	56.97	49.56	1.39
13	3	1	39.73	38.47	1.43
14	3	1	6.06	4.56	1.83
0	4	1	2704.82	2576.67	295.38
1	4	1	12178.9	10434.19	1063.2
2	4	1	379.74	411.4	62.43
3	4	1	16764.18	16665.03	1124.63
4	4	1	2170.24	2274.37	224.99
5	4	1	1009.99	1085.85	70.55
6	4	1	32.86	28.24	1.11
7	4	1	33.25	40.49	3.71
8	4	1	16.45	35.53	1.55
9	4	1	16.08	12.77	1.67
10	4	1	413.76	429.89	6.16
11	4	1	319.66	306.66	4.35
12	4	1	31.71	27.9	1.3
13	4	1	18.3	21.15	1.82
14	4	1	0.37	-6.38	3.32
1	5	1	3675.78	3299.52	216.46
2	5	1	273.54	360.82	53.85
3	5	1	825.55	891.65	119.38
4	5	1	1119.15	1239.92	155.29
5	5	1	1838.1	1974.82	186.72
6	5	1	1152.38	1304.41	97.9
7	5	1	410.33	392.14	21.36
8	5	1	372.63	356.92	11.49
9	5	1	6.78	3.32	3.42
10	5	1	1.86	0.54	3.67
11	5	1	149.38	145.24	3.43
12	5	1	20.55	21.15	1.26
13	5	1	147.23	140.59	3.36
14	5	1	108.39	98.86	2.97
0	6	1	172.02	150.72	10.07
1	6	1	0.92	-5.68	1.44
2	6	1	1419.95	1318.67	193.28
3	6	1	29.46	31.21	1.09
4	6	1	143.61	170.52	19.82
5	6	1	598.93	667.22	65.57
6	6	1	97.89	75.39	7.61
7	6	1	40.83	48.34	1.82
8	6	1	199.64	199.52	6.32
9	6	1	55.39	64.54	2.26
10	6	1	261.93	291.48	5.43
11	6	1	58.9	63.65	4.12
12	6	1	86.93	86.55	2.27
13	6	1	91.16	87.73	2.12
14	6	1	62.14	62.1	2.13
1	7	1	9553.93	7493.77	644.06
2	7	1	9529.8	8528.39	613.52
3	7	1	5033.72	4868.42	608.99
4	7	1	36.27	43.73	9.19
5	7	1	55.33	63.86	9.38
6	7	1	1139.06	1114.63	88.96
7	7	1	1004.72	1075.32	90.09
8	7	1	235.46	219.11	4.4
9	7	1	139.06	145.42	4.26
10	7	1	207.73	202.94	11.54
11	7	1	15.27	10.88	2.57
12	7	1	0.44	0.77	2.04
13	7	1	20.22	18.79	1.38
14	7	1	241.8	220.08	4.58
0	8	1	194.42	148.36	3.15
1	8	1	66.3	73.25	2.8
2	8	1	483.83	454.33	46.12
3	8	1	323.39	363.4	44.85
4	8	1	154.19	149.2	14.97

h	k	l	F_c^2	F_o^2	σF_o^2
5	8	1	1438.14	1500.48	159.14
6	8	1	57.86	49.4	4.18
7	8	1	21.99	29.13	2.68
8	8	1	1.64	0.57	3.16
9	8	1	3.2	2.47	1.69
10	8	1	27.26	23.12	1.59
11	8	1	28.45	27.45	1.18
12	8	1	39.62	41.26	1.34
13	8	1	94.89	92.97	3.25
14	8	1	127.09	127.14	4.51
1	9	1	1404.09	1299.76	53.9
2	9	1	186.18	183.2	17.31
3	9	1	180.91	173.64	20.96
4	9	1	218.1	198.39	21.17
5	9	1	934.59	981.08	85.09
6	9	1	2.56	1.45	1.47
7	9	1	1671.92	1639.15	129.08
8	9	1	271.69	276.58	16.59
9	9	1	151.1	134.21	8.97
10	9	1	55.94	52.93	4.14
11	9	1	38.1	31.96	1.19
12	9	1	9.53	8.02	1.41
13	9	1	16.96	19.29	1.38
14	9	1	3.12	1.06	2.52
0	10	1	1613.99	1447.72	32.93
1	10	1	25.76	27.37	0.76
2	10	1	1197.85	1112.66	98.93
3	10	1	512.68	502.03	57.49
4	10	1	248.55	226.21	16.59
5	10	1	1285.76	1253.64	108.59
6	10	1	12.57	8.13	2.27
7	10	1	559.76	542.4	39.18
8	10	1	1.92	-1.37	3.21
9	10	1	7.81	6.2	1.87
10	10	1	3.89	0.94	3.55
11	10	1	38.66	40.98	1.24
12	10	1	82.84	90.55	2.32
13	10	1	7.89	8.49	1.52
1	11	1	518.24	485.98	12.66
2	11	1	1382.02	1321.34	107.25
3	11	1	1.36	0.56	2.03
4	11	1	427.13	381.69	36.81
5	11	1	728.02	728.35	59.89
6	11	1	19.16	19.64	1.84
7	11	1	538.47	507.21	29.86
8	11	1	86.82	98.94	4.76
9	11	1	49.38	47.82	2.62
10	11	1	28.39	31.36	1.63
11	11	1	9.82	10.28	2.13
12	11	1	20	18.25	1.29
13	11	1	58.52	52.58	1.52
0	12	1	284.39	297.81	6.95
1	12	1	65.09	57.68	1.44
2	12	1	315.44	274.8	17.22
3	12	1	368.5	336.73	26.8
4	12	1	640.39	597.34	41.96
5	12	1	155	173.81	11.14
6	12	1	60.28	55.58	4.14
7	12	1	0.64	10.82	8.42
8	12	1	1.04	1.64	3.21
9	12	1	241.99	209.71	4.64
10	12	1	300.54	268.67	8.67
11	12	1	75.1	72.32	2.69
12	12	1	1.66	-1	2.85
13	12	1	17.62	15.05	1.38
1	13	1	779.61	603.7	8.27
2	13	1	3566.01	3241.32	177.35
3	13	1	949.64	826.05	43.63
4	13	1	365.33	315.76	13.15
5	13	1	275.44	251.84	7.32
6	13	1	17.15	17.34	2.59
7	13	1	200.39	183.48	4.71
8	13	1	260.62	251.66	8.78
9	13	1	7.1	0.05	3.38
10	13	1	0	1.4	3.51
11	13	1	38.8	32.39	1.37
12	13	1	5.11	2.87	1.4
13	13	1	4.53	0.3	2.14
0	14	1	71.43	60.31	2.1
1	14	1	54.31	85.76	27.53
2	14	1	1.2	20.52	2.79
3	14	1	268.65	237.46	8.54
4	14	1	0.08	3.04	2.46
5	14	1	19.36	15.56	1.18
6	14	1	11.02	11.3	1.26
7	14	1	0.49	-4.86	3.75
8	14	1	143.28	137.06	4.23
9	14	1	34.02	34.02	1.56
10	14	1	63.38	57.83	2.46
11	14	1	9.84	7.82	1.55
12	14	1	6.18	2.84	2.07
13	14	1	0.47	1.48	1.88
1	15	1	144.85	135.93	4.47
2	15	1	216.31	219.26	12.84
3	15	1	184.05	160.04	10.83
4	15	1	255.25	221.7	13.08
5	15	1	2.02	2.51	1.53
6	15	1	17.71	27.6	2.27
7	15	1	116.27	102.78	5.21
8	15	1	147.57	170.93	5.78
9	15	1	173.92	159.46	5.5
10	15	1	10.23	10.03	2.08
11	15	1	50.09	56.17	2.63
12	15	1	0.6	-4.22	2.98
0	16	1	412.61	356.35	3.85
1	16	1	182.29	192.28	17.24
2	16	1	128.6	115.91	4.01
3	16	1	248.66	255.58	3.87
4	16	1	661.42	598.9	14.64
5	16	1	6.98	6.5	1.28
6	16	1	50.33	51.23	1.8
7	16	1	19.68	28.24	1.44
8	16	1	329.82	317.99	5.45
9	16	1	137.65	126.37	4.2
10	16	1	13.77	11.8	3.07
11	16	1	7.92	2.78	1.71
12	16	1	0.04	0.54	2.57
1	17	1	0.84	56.37	25.24
2	17	1	107.87	99.79	10.02
3	17	1	537.74	507.48	11.44
4	17	1	846.35	763.1	21.01
5	17	1	462.85	404.2	8.11
6	17	1	306.12	294.62	9.87
7	17	1	75.29	66.57	2.38
8	17	1	58.58	57.8	2.33
9	17	1	12.41	11.87	3.09
10	17	1	39.66	36.27	1.79
11	17	1	13.9	15.95	1.27
12	17	1	31.77	30.47	1.41
0	18	1	89.6	77.57	4.56
1	18	1	1.07	-2.27	1.95
2	18	1	114.05	98.66	3.2
3	18	1	395.1	373.82	5.18
4	18	1	538.14	494.56	6.27
5	18	1	716.8	668.75	13.65
6	18	1	0.37	0.27	3.09
7	18	1	89.79	89.49	3.03
8	18	1	16.35	19.24	2.25
9	18	1	183.9	159.11	4.87
10	18	1	10.41	7.9	4.93
11	18	1	27.62	27.49	1.79
1	19	1	59.15	56.55	1.54
2	19	1	201.31	194.36	7.02
3	19	1	91.99	92.32	3.28
4	19	1	99.91	88.43	6.24
5	19	1	4.46	15.88	7.78
6	19	1	122.21	116.26	3.87
7	19	1	83.3	78.55	4.31
8	19	1	125.51	124.05	6.45
9	19	1	17.02	15.96	2.36
10	19	1	52.29	55.71	1.92
11	19	1	2.86	-1.55	2.98
0	20	1	241.15	195.42	3.7
1	20	1	35.69	26.86	5.14
2	20	1	190.57	163.8	7.15
3	20	1	16.9	20.03	3.79
4	20	1	66.01	58.59	2.04
5	20	1	66.77	54.46	2.63
6	20	1	9.94	6.21	1.39
7	20	1	0.19	1.75	3.38
8	20	1	0.01	-0.01	3.68
9	20	1	8.77	8.65	2.79
10	20	1	12.07	17.18	2.16
11	20	1	5.59	2.72	1.74
1	21	1	13.21	15.74	1.66
2	21	1	266.19	304.98	10.88
3	21	1	2.07	-0.22	2.82
4	21	1	59.89	59.52	2.16
5	21	1	142.65	140.97	6.51
6	21	1	99.41	126.16	4.18
7	21	1	238.04	248.98	5.25
8	21	1	176.92	191.53	5.17
9	21	1	158.96	189.87	5.25
10	21	1	38.77	37.47	3.32
0	22	1	223.99	203.65	3.95
1	22	1	0.28	-4.86	10.98
2	22	1	3.29	100.34	19.7
3	22	1	14.52	12.17	1.26
4	22	1	80.72	64.88	2.09
5	22	1	28.01	25.07	1.89
6	22	1	20.89	27.84	1.55
7	22	1	44.48	46.85	1.78
8	22	1	6.48	5.97	7.33
9	22	1	9	11.25	1.79
10	22	1	51.55	55.63	2.2
1	23	1	257.06	260.23	3.24
2	23	1	219.25	218.04	4.39
3	23	1	94.47	102.83	3.5
4	23	1	35.83	36.92	1.42
5	23	1	192.65	202.68	6.08
6	23	1	32.92	33.45	2.59
7	23	1	0.08	3.27	3.6
8	23	1	143.5	158.88	5.08
9	23	1	8.79	14.29	2.32
0	24	1	1.18	2.21	1.59
1	24	1	4.36	-47.02	34.46
2	24	1	0.22	96.33	19.01
3	24	1	21.22	35.54	1.66
4	24	1	9.29	8.61	3.82
5	24	1	57.04	55.85	1.92
6	24	1	21.13	23.52	1.56
7	24	1	67.31	83.04	4.86
8	24	1	4.38	6.37	2.33
1	25	1	386.67	411.61	4.25
2	25	1	1.54	-2.12	3.08
3	25	1	0.36	0.98	3.11
4	25	1	3.72	-3.97	3.21
5	25	1	4.19	-0.85	3.41
6	25	1	9.13	12.27	1.54
7	25	1	0.13	1.41	2.11
8	25	1	147.84	171.4	5.3
0	26	1	5.41	1.37	3.17
1	26	1	51.08	63.16	22.82
2	26	1	7.56	2.66	3.31
3	26	1	0.26	-3.55	5.72
4	26	1	3.06	1.51	3.19
5	26	1	48.69	52.97	1.95
6	26	1	1.89	-0.03	2.01
7	26	1	1.65	2.56	2.16
1	27	1	15.28	2.69	3.95
2	27	1	41.88	37.5	6.64
3	27	1	7.5	9.15	1.44
4	27	1	3.63	4.15	1.93
5	27	1	2.2	0.26	3.63
6	27	1	7.86	4.97	3.49
0	28	1	49.93	59.21	1.93
1	28	1	9.37	12.03	9.55
2	28	1	56.16	72.76	2.23
3	28	1	19.49	18.98	3
4	28	1	25.21	29.46	2.29
5	28	1	41.13	53.19	2.59
1	29	1	131.41	130.22	3.45
2	29	1	33.58	49.51	4.81
3	29	1	1.6	8.67	6.11
0	0	2	380.5	352.03	4.25
1	0	2	1934.82	1761.75	181.56
2	0	2	23632.0	24658.42	34.09
3	0	2	4931.73	4659.28	15.4
4	0	2	1529.97	1374.91	9.46
5	0	2	1870.35	1886.22	11.6
6	0	2	56.33	67.32	3.26
7	0	2	439.88	417.73	7.4
8	0	2	162.95	137.43	5.97
9	0	2	62.83	68.25	3.41
10	0	2	245.47	242.71	7.62
11	0	2	29.77	27.41	1.8
12	0	2	150.34	118	4.08
13	0	2	34.77	34.69	2.05
14	0	2	430.19	357.42	7.62
1	1	2	77.98	92.74	2.79
2	1	2	763.69	702.69	34.68
3	1	2	323.87	324.32	3.91
4	1	2	7.44	14.82	1.97
5	1	2	1212.4	1109.06	6.5
6	1	2	0.47	2.43	1.56
7	1	2	512.98	546.45	5.78
8	1	2	236.03	223.31	4.7
9	1	2	707.94	583.55	7.54
10	1	2	112.57	96.91	3.28
11	1	2	2.76	-3.22	2.82
12	1	2	31.46	24.92	1.36
13	1	2	30.95	32.76	1.77
14	1	2	255.48	243.35	4.76
0	2	2	2641.75	2820.75	9.77
1	2	2	0.24	10.58	2.31
2	2	2	405.98	354.01	4.7
3	2	2	549.24	576.85	6.06
4	2	2	2447.39	2422.83	11.95
5	2	2	15.74	8.62	1.57
6	2	2	208.23	194.38	5.44
7	2	2	0	4.01	1.84
8	2	2	0.01	2.77	4.95
9	2	2	306.76	262.2	7.32
10	2	2	11.05	7.35	2.32
11	2	2	23.3	22.34	1.44
12	2	2	39.36	39.59	1.61
13	2	2	44.83	43.68	1.71
14	2	2	58.93	56.75	1.92
1	3	2	406.25	456.83	22.61
2	3	2	1705.18	1583.67	8.31
3	3	2	296.13	301.94	4.77
4	3	2	5048.17	5336.09	17.51
5	3	2	28.67	33.86	1.99
6	3	2	97.57	95.2	4.65
7	3	2	85.28	74.79	3.94
8	3	2	385.73	358.07	7.47
9	3	2	27.2	32.55	2.74
10	3	2	92.18	90.27	4.88
11	3	2	19.88	18.93	1.44
12	3	2	77.34	71.99	2.11
13	3	2	67.89	66.51	1.87
14	3	2	0.25	1.68	1.96
0	4	2	934.09	825.06	5.82
1	4	2	21.35	24.56	3.56
2	4	2	3497.89	3405.22	11.91
3	4	2	68.81	54.24	2.66
			F_c^2	F_o^2	σF_o^2
4	4	2	9.31	21.41	1.8
5	4	2	105.12	84.71	3.98
6	4	2	73.33	80.75	3.94

h	k	l	F_c^2	F_o^2	σF_o^2
7	4	2	74.25	81.27	4.09
8	4	2	2171.81	2078.56	14.72
9	4	2	69.97	62.82	2.89
10	4	2	738.95	691	10.53
11	4	2	88.07	97.8	2.86
12	4	2	11.92	13.02	2.09
13	4	2	2.06	0.76	3.12
14	4	2	9.44	20.21	1.74
1	5	2	405.75	488.46	11.3
2	5	2	14.1	22.01	1.46
3	5	2	1373.47	1375.78	8.62
4	5	2	4.98	13.35	1.76
5	5	2	0.83	2.74	3.6
6	5	2	0	-1.8	3.9
7	5	2	919.94	956.87	10.01
8	5	2	814.5	770.42	9.67
9	5	2	88.12	77.71	3.83
10	5	2	3.69	4.05	5.25
11	5	2	0.7	-3.66	3.94
12	5	2	0.44	-0.13	3.7
13	5	2	0.38	-1.34	3.66
14	5	2	55.67	55.09	3.08
0	6	2	2800.28	3015.42	10.86
1	6	2	571.39	492.37	3.65
2	6	2	607.13	561.35	5.5
3	6	2	679.18	695	6.48
4	6	2	0.24	-1.35	3.26
5	6	2	226	247.85	5.37
6	6	2	0.04	3.26	3.94
7	6	2	2.01	3.37	4.46
8	6	2	4.99	6.6	2.1
9	6	2	1.52	1.99	4.91
10	6	2	38.82	40.61	2.44
11	6	2	1.52	-2.63	2.11
12	6	2	15.48	16.85	1.53
13	6	2	0.75	-0.33	4.79
14	6	2	173.27	175.59	4.9
1	7	2	938.6	959.81	4.8
2	7	2	8.29	12.56	1.42
3	7	2	271.42	306.92	4.92
4	7	2	10.51	6.45	1.46
5	7	2	440.87	388.88	6.2
6	7	2	631.87	640.65	7.93
7	7	2	28.66	25.65	2.02
8	7	2	833.29	835.93	10.04
9	7	2	436.01	442.94	8.41
10	7	2	6.15	10.05	2.29
11	7	2	4.22	3.04	2
12	7	2	9.16	2.88	3.56
13	7	2	0.88	1.28	2.33
0	8	2	1250.77	1198.66	7.48
1	8	2	0.72	12.87	8.75
2	8	2	93.02	92.36	3.49
3	8	2	1018.06	1133.91	8.18
4	8	2	3756.68	3968.04	15.72
5	8	2	0.26	0.45	1.54
6	8	2	0.1	2.96	4.09
7	8	2	316.93	298.09	6.87
8	8	2	448.16	491.79	8.41
9	8	2	183.81	170.07	6.57
10	8	2	1026	1008.11	12.27
11	8	2	108.03	102.2	4.45
12	8	2	9.38	10.4	2.03
13	8	2	128.53	123.97	3.55
1	9	2	989.09	1051.42	22.84
2	9	2	1311.74	1336.44	8.42
3	9	2	612.57	688.67	6.73
4	9	2	56.84	75.87	3.79
5	9	2	60.1	67.02	3.15
6	9	2	160.21	164	5.55
7	9	2	14.1	15.64	1.95
8	9	2	20.74	21.37	2.1
9	9	2	7.77	5.02	2.1
10	9	2	6.23	10.05	2.32
11	9	2	40.62	35.23	1.53
12	9	2	12.57	11.12	2.9
13	9	2	129.81	124.4	3.54
0	10	2	212.96	197.94	4.05
1	10	2	49.57	40.54	3.02
2	10	2	0.04	0.64	1.24
3	10	2	180.32	204.41	4.62
4	10	2	114.16	107.78	4.43
5	10	2	186.67	189.65	5.18
6	10	2	2240.13	2289.06	14.12
7	10	2	31.78	37.38	2.1
8	10	2	73.78	76.28	3.68
9	10	2	271.12	239.28	7.24
10	10	2	343.33	347.5	8.6
11	10	2	1.1	2.61	3.29
12	10	2	47.87	54.07	1.75
13	10	2	64.28	58.75	1.83
1	11	2	358.79	339.15	3.65
2	11	2	462.53	438.22	5.71
3	11	2	243.2	242.12	4.88
4	11	2	2383.98	2389.76	13.01
5	11	2	61.43	66.42	3.38
6	11	2	143.34	158.24	5.63
7	11	2	93.44	92.9	4.65
8	11	2	26.31	22.65	2.06
9	11	2	0.89	3.26	4.91
10	11	2	231.85	237.02	7.65
11	11	2	24.81	13.46	1.47
12	11	2	31.03	28.97	2.19
13	11	2	5.6	8.25	2.99
0	12	2	1853.81	1772.57	10.14
1	12	2	231.18	252.7	4
2	12	2	407.57	412.81	5.71
3	12	2	219.29	209.95	4.77
4	12	2	683.74	643.13	7.56
5	12	2	10.62	12.22	1.72
6	12	2	12.1	13.8	1.91
7	12	2	89.83	84.57	4.31
8	12	2	13.75	8.92	2.02
9	12	2	11.97	11.51	2.17
10	12	2	138.67	148.54	6.68
11	12	2	25.23	28.72	2.09
12	12	2	35	36.31	1.63
13	12	2	3.52	-1.58	3.79
1	13	2	35.46	37.75	1.91
2	13	2	2.4	1.16	3.34
3	13	2	101.93	99.25	4.28
4	13	2	117.76	98.13	4.69
5	13	2	74.64	73.81	3.68
6	13	2	73.72	73.24	3.53
7	13	2	2.32	2.4	4.61
8	13	2	104.67	82.4	4.01
9	13	2	63.17	55.84	2.55
10	13	2	7.42	15.45	2.32
11	13	2	0.28	4.41	1.63
12	13	2	36.23	34.59	2.06
0	14	2	207.21	191.77	4.69
1	14	2	0.86	49.73	24.88
2	14	2	550.2	525.08	6.69
3	14	2	109.91	111.56	4.39
4	14	2	438.46	399.55	6.69
5	14	2	25.7	31.31	1.87
6	14	2	1973.94	1967.32	14.17
7	14	2	17.66	19.46	2.06
8	14	2	241.1	253.51	6.98
9	14	2	82.61	88.77	4.43
10	14	2	8.75	1.42	5.66
11	14	2	45.84	37.37	1.55
12	14	2	44.62	52.12	1.74
1	15	2	455.44	486.87	6.93
2	15	2	54.69	51.9	2.7
3	15	2	538.73	501.89	6.95
4	15	2	7.73	6	1.72
5	15	2	32.52	34.16	1.87
6	15	2	1775.19	1756.65	13.62
7	15	2	0	0.3	4.84
8	15	2	21.62	22.57	2.14
9	15	2	34.48	39.26	2.36
10	15	2	0.31	-0.04	2.32
11	15	2	0.32	-1.66	3.37
12	15	2	33.03	36.2	1.7
0	16	2	32.52	27.52	1.57
1	16	2	1.09	31.57	20.81
2	16	2	17.06	14.17	1.61
3	16	2	142.48	146.38	5.03
4	16	2	322.01	320.22	6.34
5	16	2	36.66	45.67	2.4
6	16	2	1307.5	1248.79	11.94
7	16	2	16.82	17.58	2.1
8	16	2	2.19	-0.67	4.72
9	16	2	9.72	-0.97	5.29
10	16	2	41.57	31.01	2.51
11	16	2	18.71	15.34	4.66
1	17	2	3.23	-6.79	6
2	17	2	43.28	39.22	2.29
3	17	2	84.29	85.71	3.23
4	17	2	35.99	34.53	1.87
5	17	2	28.34	27.41	1.87
6	17	2	2.12	20.32	5.77
7	17	2	151.54	154.7	6.15
8	17	2	12.33	12.79	2.1
9	17	2	31.11	32.1	2.32
10	17	2	26.82	28.12	2.55
11	17	2	29.16	30.44	1.6
0	18	2	1750.54	1530.57	11.44
1	18	2	20.54	36.08	6.67
2	18	2	1.57	-0.86	3.82
3	18	2	147.76	128.03	5.03
4	18	2	66.06	73.09	3.83
5	18	2	1.47	-0.9	4.35
6	18	2	62.24	58.73	3.15
7	18	2	11.4	6.86	2.1
8	18	2	99.21	88.17	4.13
9	18	2	10.28	10.69	2.36
10	18	2	4.29	-3.37	5.59
11	18	2	16.18	22.61	2.37
1	19	2	78.15	65.97	6.23
2	19	2	31.08	28.35	1.84
3	19	2	17.01	16.72	1.78
4	19	2	6.53	0.07	4.31
5	19	2	190.74	200.08	6.15
6	19	2	70.09	75.83	3.38
7	19	2	37.33	43.76	2.32
8	19	2	0.06	-0.04	2.21
9	19	2	146.3	153.11	6.86
10	19	2	15.58	15	2.51
0	20	2	361.06	320.38	6.61
1	20	2	93.28	95.69	2.63
2	20	2	19.99	37.87	2.32
3	20	2	50.42	48.82	2.47
4	20	2	124.13	126.51	5.51
5	20	2	6.59	5.1	1.87
6	20	2	327.19	308.7	7.62
7	20	2	51.67	51.75	2.44
8	20	2	83.88	78.53	3.38
9	20	2	0.37	-1.09	2.36
10	20	2	33.18	31.68	2.62
1	21	2	2.8	-2.16	5.92
2	21	2	600.39	572.57	8.42
3	21	2	0.08	1.61	4.05
4	21	2	40.84	40.31	2.06
5	21	2	0.24	-1.84	4.35
6	21	2	12.18	10.54	2.14
7	21	2	0.85	-9.45	5.1
8	21	2	9.31	4.57	2.36
9	21	2	0.35	2.1	5.32
0	22	2	1079.82	1008.68	10.8
1	22	2	22.66	28.25	3.28
2	22	2	57.34	208.91	6.9
3	22	2	77.08	79.2	3.79
4	22	2	22.44	21.97	1.95
5	22	2	57.67	67.2	3.04
6	22	2	57.35	49.24	2.32
7	22	2	4.98	0.86	5.29
8	22	2	0.36	-0.94	5.51
9	22	2	11.6	14.51	2.51
1	23	2	0.92	-1.15	11.6
2	23	2	11.72	35.43	5.4
3	23	2	21.73	34.57	2.47
4	23	2	1.04	-4.65	4.54
5	23	2	1.77	1.76	1.99
6	23	2	44.8	44.17	2.44
7	23	2	42.91	48.93	3
8	23	2	30.42	38.13	2.51
0	24	2	10.77	0.71	4.42
1	24	2	5.72	5.14	1.75
2	24	2	8.09	1.54	4.84
3	24	2	5.11	7.95	1.99
4	24	2	22.3	22.31	2.02
5	24	2	1.33	0.04	1.95
6	24	2	68.03	75.15	3.19
7	24	2	5.11	6.04	2.36
1	25	2	0.71	-5.17	3.11
2	25	2	31.07	19.16	2.17
3	25	2	1.16	-0.79	4.76
4	25	2	36.51	45.11	2.25
5	25	2	2.07	1.95	4.91
6	25	2	83.24	106.28	5.81
7	25	2	3.79	6.6	2.36
0	26	2	119.89	147.96	6.08
1	26	2	0.04	9.04	7.1
2	26	2	21.3	-6.82	5.77
3	26	2	40.17	43.38	2.32
4	26	2	20.89	18.63	2.25
5	26	2	0.4	-10.84	5.06
6	26	2	12.12	16.95	2.4
1	27	2	61.06	70.13	2.24
2	27	2	67.74	70.8	3
3	27	2	42.58	61.23	3
4	27	2	14.09	5.36	5.44
5	27	2	41.25	53.21	2.96
0	28	2	7.78	8.75	2.14
1	28	2	2.94	-1.18	4.04
2	28	2	3.04	-7.64	7.61
3	28	2	3.91	6.04	6.97
1	1	3	99.02	95.66	3.9
2	1	3	1075.32	1027.52	24.17
3	1	3	43.44	40.6	1.52
4	1	3	1.51	2.72	1.76
5	1	3	6.08	10.01	2.04
6	1	3	6.99	11.43	7.93
7	1	3	719.18	672.22	6.87
8	1	3	49.94	52.33	1.85
9	1	3	544.3	475.2	7.53
10	1	3	41.39	41.59	1.87
11	1	3	26.57	32.28	1.92
12	1	3	39.45	34.86	1.5
13	1	3	44.67	45.35	1.6
0	2	3	1132.46	1291.67	8.45
1	2	3	595.75	667.46	42.56
2	2	3	406.57	371.32	5.67
3	2	3	274.26	325.97	5.89
4	2	3	4.7	5.21	1.8
5	2	3	75.28	65.33	3.04
6	2	3	23.98	25.5	2.14
7	2	3	208.87	175.24	6.64
8	2	3	158.81	166.26	6.72
9	2	3	0.1	4.39	5.36
10	2	3	2.9	4.72	2.44
11	2	3	36.71	29.45	2.07
12	2	3	1.33	-2.89	3.74
13	2	3	17.49	25.2	1.77
1	3	3	16.65	20.53	1.06
2	3	3	47.04	46.3	2.4
3	3	3	447.05	462.45	6.54
4	3	3	87.9	109.64	5.06

h	k	l	F_c^2	F_o^2	σF_o^2
5	3	3	823.58	810.56	9.11
6	3	3	56.22	66.86	3.64
7	3	3	10.93	13.72	2.25
8	3	3	188.31	136	6.6
9	3	3	66.81	56.63	2.66
10	3	3	245.6	228.7	7.92
11	3	3	40.74	47.99	1.7
12	3	3	60.41	58.27	1.84
13	3	3	211.57	220.08	5.39
0	4	3	256.23	204.4	4.54
1	4	3	98.22	193.62	37.32
2	4	3	20.27	16.54	1.46
3	4	3	714.7	714.8	7.64
4	4	3	33.19	24.9	1.87
5	4	3	460.86	447.65	7.29
6	4	3	15.86	21.15	2.17
7	4	3	768.07	705.77	9.7
8	4	3	135.36	151.92	6.71
9	4	3	0.48	0.22	5.17
10	4	3	2.47	6.3	2.4
11	4	3	225.95	188.65	4.75
12	4	3	42.79	33.7	1.76
13	4	3	282.79	255.04	5.75
1	5	3	2248.8	2399.02	99.85
2	5	3	176.06	176.07	4.62
3	5	3	139.09	126.96	4.76
4	5	3	513.16	478.51	7.14
5	5	3	167.58	165.16	5.59
6	5	3	541.61	548.74	8.3
7	5	3	154.37	148.93	6.45
8	5	3	0	2.85	5.25
9	5	3	16.18	17.4	2.29
10	5	3	14.26	16.31	2.4
11	5	3	112.14	102.27	5.34
12	5	3	83.08	75.79	2.11
13	5	3	72.84	68.07	2.09
0	6	3	71.16	65.3	3.11
1	6	3	215.36	433.24	107.42
2	6	3	34.43	39.26	1.99
3	6	3	29.59	27.15	1.69
4	6	3	53.33	37.95	2.03
5	6	3	1002.89	1003.69	9.75
6	6	3	244.11	217.45	6.42
7	6	3	317.87	333.15	7.51
8	6	3	1.88	4.65	5.32
9	6	3	102.03	90.84	4.73
10	6	3	19.87	21	2.44
11	6	3	210.8	202.01	4.74
12	6	3	24.48	32.12	2.17
13	6	3	90.55	78.55	3.23
1	7	3	5034.13	4927.63	81.41
2	7	3	148.81	127.45	4.39
3	7	3	44.42	51.71	2.51
4	7	3	83.62	61.85	3.26
5	7	3	180.38	188.21	5.74
6	7	3	156.39	120.58	5.74
7	7	3	103.83	107.38	5.44
8	7	3	81.78	73.36	3.6
9	7	3	91.29	93.2	4.46
10	7	3	1.69	2.02	5.66
11	7	3	2.76	3.17	3.69
12	7	3	26.27	31.35	1.76
0	8	3	161.92	181.46	4.69
1	8	3	8.85	28.43	2.14
2	8	3	1.88	3.07	3.64
3	8	3	28.13	25.09	1.65
4	8	3	6.57	10.61	1.76
5	8	3	17.19	21.11	1.99
6	8	3	101	81.54	4.16
7	8	3	843.93	819.49	10.42
8	8	3	10.44	11.32	2.21
9	8	3	43.93	36.75	2.44
10	8	3	65.03	56.92	2.74
11	8	3	232.83	217.06	8.18
12	8	3	40.35	40.54	1.77
1	9	3	82.89	77.16	2.68
2	9	3	176.82	173.36	4.84
3	9	3	149.12	138.78	4.84
4	9	3	3.04	3.9	4.16
5	9	3	702.48	634.48	8.54
6	9	3	104.38	103.71	5.03
7	9	3	823.68	825.36	10.49
8	9	3	39.04	34.76	2.36
9	9	3	0.95	1.99	5.36
10	9	3	180.32	160.56	7.47
11	9	3	7.76	8.69	1.61
12	9	3	2.46	0.68	1.87
0	10	3	489.66	403.55	6.16
1	10	3	0.16	64.46	30.03
2	10	3	33.88	46.8	2.25
3	10	3	139.38	125.79	4.88
4	10	3	18.76	15.56	1.87
5	10	3	1560.79	1553.22	12.3
6	10	3	40.41	41.25	2.17
7	10	3	5.45	9.04	2.29
8	10	3	4.83	-0.86	5.47
9	10	3	118.81	99.66	4.91
10	10	3	17.27	16.98	2.59
11	10	3	85.6	82.32	2.42
12	10	3	27.82	26.16	1.72

h	k	l	F_c^2	F_o^2	σF_o^2
1	11	3	515.99	508.04	7.33
2	11	3	132.09	163.49	4.95
3	11	3	535.14	503.47	7.14
4	11	3	122.35	124.09	5.29
5	11	3	197.68	196.05	6.19
6	11	3	96.16	86.71	4.09
7	11	3	668.41	655.09	9.81
8	11	3	131.76	121.34	6.04
9	11	3	71.1	72.19	3.86
10	11	3	36.25	49.65	2.74
11	11	3	37.13	40.78	1.72
12	11	3	39.93	33.27	1.76
0	12	3	0.49	3.15	3.6
1	12	3	27.83	27.1	4.76
2	12	3	9.76	11.74	1.72
3	12	3	37.43	43.12	2.17
4	12	3	45.05	39.45	1.99
5	12	3	414.22	411.38	7.47
6	12	3	90.37	97.51	4.58
7	12	3	1323.23	1328.65	12.99
8	12	3	61.24	59.29	2.92
9	12	3	378.31	371.17	8.9
10	12	3	2.08	-7.27	5.7
11	12	3	113.49	109.26	3.21
12	12	3	4.84	4.35	2.44
1	13	3	4.23	-5	4.99
2	13	3	261.41	237.43	5.74
3	13	3	356.22	324.7	6.53
4	13	3	230.95	211.53	5.97
5	13	3	931.95	869.97	9.89
6	13	3	27.65	25.68	2.1
7	13	3	6.61	24.03	2.7
8	13	3	13.31	1.24	5.36
9	13	3	51.75	53.36	2.66
10	13	3	22.49	29.17	2.59
11	13	3	36.65	39.18	1.72
0	14	3	19.81	24.9	1.69
1	14	3	132.81	125.9	18.31
2	14	3	24.48	44.06	2.36
3	14	3	265.77	205.6	6.04
4	14	3	72.48	61.58	3.34
5	14	3	115.02	102.81	5.18
6	14	3	114.01	114.06	5.59
7	14	3	112.63	104.83	5.25
8	14	3	3.78	-0.11	5.32
9	14	3	95.67	72.38	3.15
10	14	3	1.35	5.29	5.7
11	14	3	28.34	29.16	2.33
1	15	3	276.01	283.44	61.76
2	15	3	353.17	313.83	6.46
3	15	3	130.97	121.27	5.44
4	15	3	25.76	21.11	1.91
5	15	3	131.19	119.96	5.51
6	15	3	24.27	27.33	2.14
7	15	3	377.9	405.53	8.52
8	15	3	11.42	9.45	2.32
9	15	3	0.11	-9	5.55
10	15	3	12.36	13.42	2.66
11	15	3	48.62	43.1	1.75
0	16	3	70.85	67.13	3.3
1	16	3	644.65	577.83	14.92
2	16	3	34.89	32.1	1.87
3	16	3	100.17	81.35	3.64
4	16	3	1.21	-1.09	1.91
5	16	3	654.37	585.46	9.06
6	16	3	12.31	15.71	2.1
7	16	3	13.66	10.39	2.25
8	16	3	44.11	36.97	2.44
9	16	3	95.56	87.61	4.8
10	16	3	24.82	28.72	2.62
1	17	3	1.26	-23.08	8.79
2	17	3	16.79	13.16	1.8
3	17	3	210.99	182.42	6
4	17	3	247.18	251.38	6.57
5	17	3	218.57	192.36	6.72
6	17	3	94.32	91.77	4.8
7	17	3	9.36	9.45	2.21
8	17	3	4.54	3.6	2.29
9	17	3	103.91	101.3	4.8
10	17	3	0.16	3.07	2.51
0	18	3	1.23	-1.27	3.97
1	18	3	85.74	77.42	6.3
2	18	3	10.61	9.49	1.8
3	18	3	271.17	260.59	6.83
4	18	3	11.15	11.32	1.95
5	18	3	478.18	477.65	8.45
6	18	3	31.9	36.11	2.21
7	18	3	98.12	88.62	4.16
8	18	3	0.01	2.85	5.17
9	18	3	49.65	45.3	2.74
10	18	3	8.21	-1.35	6.3
1	19	3	34.31	45.16	15.49
2	19	3	6.83	-0.45	4.54
3	19	3	109.06	105.13	5.21
4	19	3	13.11	12.45	1.95
5	19	3	104.09	98.9	4.76
6	19	3	7.79	6.22	2.1
7	19	3	54.34	55.98	3.26
8	19	3	0.29	3.41	5.17
9	19	3	68.61	63.64	2.85

h	k	l	F_c^2	F_o^2	σF_o^2
0	20	3	221.7	203.92	6.15
1	20	3	203.77	182.72	4.54
2	20	3	75.27	83.63	4.05
3	20	3	16.72	15.93	2.06
4	20	3	2.46	4.72	1.99
5	20	3	14.97	19.68	2.55
6	20	3	0.03	-8.55	4.87
7	20	3	0.4	0	5.06
8	20	3	2.4	1.16	2.36
9	20	3	29.72	29.51	2.62
1	21	3	15.71	-5.92	29.41
2	21	3	62.29	57.15	3.11
3	21	3	70.63	75.41	3.75
4	21	3	1.26	-2.96	4.65
5	21	3	10.41	12.11	2.06
6	21	3	14.74	12.79	2.14
7	21	3	16.08	21.33	2.36
8	21	3	4.01	9.34	2.36
0	22	3	0.42	2.1	1.95
1	22	3	189.1	181.24	12.66
2	22	3	5.34	3	4.69
3	22	3	85.5	104.37	5.44
4	22	3	5.53	4.24	2.02
5	22	3	6.87	3.52	4.84
6	22	3	0.18	-1.84	4.8
7	22	3	8.08	5.4	5.4
1	23	3	1.65	0.9	12.78
2	23	3	3.37	5.89	1.99
3	23	3	0.66	24.82	2.55
4	23	3	1.79	-4.65	5.02
5	23	3	2.78	-3.04	5.02
6	23	3	4.93	-0.37	5.32
7	23	3	3.84	4.39	2.4
0	24	3	4.38	7.05	2.06
1	24	3	2.64	35.2	20.08
2	24	3	3.42	4.2	4.87
3	24	3	8.18	6.79	2.17
4	24	3	14.89	15.75	2.25
5	24	3	3.35	-0.26	2.14
6	24	3	6.68	7.39	2.25
1	25	3	142.37	141.09	7.45
2	25	3	10.15	8.06	2.1
3	25	3	5.27	9.49	2.21
4	25	3	0.07	3.26	5.02
5	25	3	17.81	11.7	2.32
0	26	3	37.94	48.33	2.62
1	26	3	42.11	49.06	7.54
2	26	3	0.26	-11.25	5.17
3	26	3	0.02	-5.74	5.25
1	27	3	4.18	3.82	9.09
0	0	4	4213.15	4302.64	17.72
1	0	4	10.43	14.48	1.69
2	0	4	373.96	351.87	6.95
3	0	4	999.19	966.56	10.32
4	0	4	343.83	322.73	7.73
5	0	4	169.5	184.54	7.02
6	0	4	12.81	9.37	2.4
7	0	4	62.95	52.54	2.85
8	0	4	131.73	131.73	6.94
9	0	4	6.55	26.09	2.85
10	0	4	10.83	7.91	2.81
11	0	4	0	-1.26	2.62
12	0	4	20.47	25.4	2.33
1	1	4	9.6	13.17	1.68
2	1	4	141.41	131.47	6.08
3	1	4	117.98	139.86	17.65
4	1	4	165.25	179.06	4.7
5	1	4	126.7	144.41	5.4
6	1	4	54.87	75.14	2.63
7	1	4	146.89	101.81	6.4
8	1	4	13.46	13.24	2.02
9	1	4	435.85	402.4	16.99
10	1	4	18.95	26.49	2.31
11	1	4	17.11	12.29	2.61
12	1	4	124.8	112.31	4.09
0	2	4	0.11	0.34	4.39
1	2	4	140.48	131.39	6.79
2	2	4	21.16	64.42	3.3
3	2	4	5.71	14.61	2.14
4	2	4	0.25	12.6	2.25
5	2	4	8.91	20.58	2.85
6	2	4	7.27	24.45	2.44
7	2	4	38.76	45.93	2.59
8	2	4	4.94	2.77	2.47
9	2	4	18.85	26.21	2.74
10	2	4	156.59	160.28	7.76
11	2	4	6.4	4.47	2.02
12	2	4	3.22	0.87	4.25
1	3	4	0.42	0.05	3.14
2	3	4	745.06	702.15	8.42
3	3	4	223.72	186.81	6.19
4	3	4	167.84	156.6	6.23
5	3	4	97.61	101.98	5.29
6	3	4	525.47	509.41	9.32
7	3	4	1.49	3.97	5.55
8	3	4	0.01	-2.74	5.74
9	3	4	4.62	6.26	2.62
10	3	4	24.35	26.25	2.92
11	3	4	0.11	0.16	5.1
12	3	4	29.66	33.26	1.9

h	k	l	F_c^2	F_o^2	σF_o^2
0	4	4	225.82	195.07	5.67
1	4	4	1.31	12.82	3.99
2	4	4	23.86	38.81	2.02
3	4	4	0.02	23.17	2.1
4	4	4	196.37	216.61	6.72
5	4	4	0.06	-11.14	5.1
6	4	4	164.58	170.62	6.83
7	4	4	1.5	2.89	5.62
8	4	4	19.99	20.28	2.55
9	4	4	0.21	4.76	6.15
10	4	4	198.27	185.43	8.29
11	4	4	38.15	44.35	1.84
1	5	4	145.79	146.54	3.8
2	5	4	216.26	208.04	5.97
3	5	4	332.34	321.36	7.06
4	5	4	7.42	18.82	2.21
5	5	4	12.08	8.21	2.17
6	5	4	131.95	99.81	5.18
7	5	4	59.34	54.64	2.89
8	5	4	22.29	19.08	2.55
9	5	4	255.21	230.05	8.37
10	5	4	89.21	90.23	4.84
11	5	4	25.75	29.76	1.81
0	6	4	31.94	32.77	1.95
1	6	4	0.3	1.74	3.11
2	6	4	81.34	98.11	4.69
3	6	4	61.74	69.83	3.38
4	6	4	446.56	408.28	7.81
5	6	4	109.37	97.44	5.1
6	6	4	1.4	3.34	5.36
7	6	4	0.04	2.44	5.4
8	6	4	78.02	69.45	3.94
9	6	4	0.09	3.41	2.62
10	6	4	3.54	3.6	2.85
11	6	4	28.32	30.05	1.82
1	7	4	101.49	98.04	3.38
2	7	4	534	539.81	7.82
3	7	4	145.43	142.4	5.85
4	7	4	50.74	49.95	2.81
5	7	4	39.98	41.36	2.21
6	7	4	80.78	85.99	4.13
7	7	4	61.8	55.16	2.7
8	7	4	0.17	5.36	5.89
9	7	4	113.49	90.28	4.54
10	7	4	181.86	211.34	8.63
11	7	4	24.74	20.34	1.84
0	8	4	35.97	43.87	2.14
1	8	4	50.99	49.22	2.66
2	8	4	192.17	207.27	1.13
3	8	4	298.22	308.32	7.02
4	8	4	56.36	52.87	2.92
5	8	4	12.16	10.35	2.1
6	8	4	6.59	4.8	4.99
7	8	4	2.23	1.76	5.4
8	8	4	169.24	157.74	7.31
9	8	4	93.16	103.4	5.36
10	8	4	679.98	678.06	12.17
11	8	4	5.1	3.14	2.8
1	9	4	106.1	97.78	3.47
2	9	4	484.97	464.2	7.59
3	9	4	412.02	355.83	7.17
4	9	4	31.54	35.28	2.14
5	9	4	11.69	11.66	2.1
6	9	4	48.47	45.79	2.4
7	9	4	7.66	6.15	2.32
8	9	4	0.11	2.96	5.92
9	9	4	46.67	50.06	2.89
10	9	4	129.13	121.93	8.19
11	9	4	5.07	1.71	4.05
0	10	4	40.39	42.37	2.36
1	10	4	78.35	78.59	2.85
2	10	4	9.06	106.67	3.82
3	10	4	0.01	0.82	4.69
4	10	4	14.04	22.08	2.17
5	10	4	11.34	11.62	2.06
6	10	4	70.6	59.1	2.65
7	10	4	22.63	21.26	2.32
8	10	4	181.65	160.9	7.58
9	10	4	0.51	5.36	6.04
10	10	4	33.29	35.17	2.96
11	10	4	8.34	14.85	1.8
1	11	4	8.56	8.44	3.66
2	11	4	678.73	657.1	8.72
3	11	4	60.99	64.99	3.3
4	11	4	321.44	326.18	7.36
5	11	4	60.7	67.54	3.56
6	11	4	81.26	87.91	4.46
7	11	4	9.12	9	2.36
8	11	4	132.25	122.24	6
9	11	4	4.12	5.29	6.26
10	11	4	87.97	73.62	4.09
0	12	4	317.77	281.9	6.49
1	12	4	56.19	51.15	1.79
2	12	4	220.59	227.61	6.38
3	12	4	9.12	13.72	2.06
4	12	4	598.69	579.91	8.98
5	12	4	3.32	2.44	4.8
6	12	4	58.34	61.65	2.92
7	12	4	3.17	3.64	5.55
8	12	4	46.83	55.42	2.96
9	12	4	0.25	1.42	2.59
10	12	4	33.62	32.17	2.89
1	13	4	4.24	-2.68	6.34
2	13	4	58.04	67.01	3.45
3	13	4	153.06	139.73	5.89
4	13	4	123.26	119.73	5.59
5	13	4	62.36	71.44	3.49
6	13	4	42.77	46.42	2.44
7	13	4	25.72	26.21	2.47
8	13	4	125.51	121.75	6.3
9	13	4	24.84	26.96	2.74
10	13	4	1.28	0.3	6.3
0	14	4	261.39	264.34	6.49
1	14	4	28.34	52.15	15.39
2	14	4	77.97	121.24	5.55
3	14	4	8.8	22.95	2.17
4	14	4	38.09	38.55	2.29
5	14	4	2.35	-3.37	4.87
6	14	4	274.41	273.14	7.54
7	14	4	0.44	-4.61	5.47
8	14	4	230.43	246.68	8.07
9	14	4	66.62	71.92	3.37
1	15	4	213	181.05	4.32
2	15	4	309.68	268.95	6.76
3	15	4	263.33	283.92	7.2
4	15	4	203.4	203.98	6.72
5	15	4	35.3	36	2.25
6	15	4	62.05	57.6	2.62
7	15	4	0.7	-3.49	5.47
8	15	4	56.32	61.91	2.89
9	15	4	5.44	-0.3	6.19
0	16	4	0.4	-1.09	1.91
1	16	4	2.95	0.98	3.29
2	16	4	1.34	4.61	1.91
3	16	4	81.3	86.22	4.24
4	16	4	82.24	79.73	3.86
5	16	4	15.64	20.43	2.17
6	16	4	163.99	161.67	6.86
7	16	4	0.46	-4.84	5.59
8	16	4	142.29	141.67	6.98
9	16	4	15.29	13.35	2.74
1	17	4	5.55	6	3.62
2	17	4	0.26	68.8	2.74
3	17	4	47.33	45.56	2.4
4	17	4	20.13	20.02	2.29
5	17	4	0.9	4.35	4.95
6	17	4	23.73	23.21	2.4
7	17	4	43.52	35.88	2.59
8	17	4	72.6	82.27	4.16
0	18	4	220.68	193.33	6.53
1	18	4	6.31	5.78	4.2
2	18	4	259.18	258.01	7.05
3	18	4	32.86	32.51	2.32
4	18	4	54.36	52.99	2.85
5	18	4	15.78	20.02	2.17
6	18	4	29.44	32.4	2.4
7	18	4	1.27	0.26	5.44
8	18	4	7.78	6.71	2.62
1	19	4	16.21	7.74	9.82
2	19	4	28.94	28.01	2.25
3	19	4	30.4	34.68	2.32
4	19	4	120.3	128.08	8.26
5	19	4	49.97	49.23	2.66
6	19	4	7.95	10.76	2.25
7	19	4	11.26	5.36	5.77
0	20	4	69.89	66.49	3.26
1	20	4	41.93	45.63	2.57
2	20	4	0.01	-0.75	5.1
3	20	4	8.98	7.12	2.25
4	20	4	0.11	-7.72	5.29
5	20	4	1.91	1.95	5.17
6	20	4	25.49	19.91	2.4
1	21	4	1.88	0.46	3.39
2	21	4	36.9	70.23	2.96
3	21	4	2.49	-1.8	5.36
4	21	4	20	20.36	2.32
5	21	4	2.17	1.76	5.36
6	21	4	1.98	-5.74	5.62
0	22	4	21.28	21.11	2.21
1	22	4	2.46	4.34	1.93
2	22	4	129.48	135.7	6.56
3	22	4	28.06	28.5	2.44
4	22	4	3.04	3.82	2.32
5	22	4	34.23	41.73	2.47
1	23	4	0.95	-2.44	3.84
2	23	4	12.43	16.91	2.92
3	23	4	11.62	10.35	2.44
4	23	4	0.03	-12.71	5.62
0	24	4	2.11	-3.82	5.21
1	24	4	3.39	3.66	2.09
2	24	4	4.76	24	3.07
1	1	5	0.58	59.36	21.09
2	1	5	1.55	-0.26	3.62
3	1	5	15.94	16.14	3.41
4	1	5	17.31	17.38	1.81
5	1	5	24.19	34.48	4.91
6	1	5	14.53	15.14	2.98
7	1	5	0.86	-1.58	4.63
8	1	5	43.49	39.22	2.24
9	1	5	41.54	40.61	2.29
10	1	5	0.06	0.94	5.3
0	2	5	278.46	269.69	6.83
1	2	5	805.87	785.42	44.05
2	2	5	26.47	38.85	2.25
3	2	5	5.95	15.15	2.29
4	2	5	0.59	-1.57	5.59
5	2	5	84.3	71.78	3.98
6	2	5	47.97	58.76	3.41
7	2	5	13.87	9.67	2.89
8	2	5	1.93	-8.29	7.05
9	2	5	0.1	5.21	2.96
10	2	5	15.39	15.63	3.26
1	3	5	13.84	65.48	15.04
2	3	5	49.79	54.6	2.81
3	3	5	89.18	94.96	4.69
4	3	5	27.38	37.42	2.59
5	3	5	5.57	4.27	5.81
6	3	5	9.31	19.27	2.66
7	3	5	9.06	0.26	6.56
8	3	5	55.01	44.51	3.07
9	3	5	9.25	1.84	7.05
10	3	5	16.66	6.34	7.57
0	4	5	350.02	322.49	7.51
1	4	5	550.12	525.92	8.77
2	4	5	49.97	75.03	3.6
3	4	5	104.8	113.68	5.63
4	4	5	204.81	208.04	7.5
5	4	5	34.72	41.13	2.59
6	4	5	82.01	93.57	4.54
7	4	5	6.35	3.52	6.34
8	4	5	5.15	0.86	6.49
9	4	5	26.79	35.25	3
1	5	5	314.58	301.75	15.05
2	5	5	155	159.84	6.34
3	5	5	14	14.17	2.29
4	5	5	90.72	95.52	4.76
5	5	5	67.47	65.4	2.93
6	5	5	126.69	128.09	6.19
7	5	5	0.08	3.9	6.45
8	5	5	7.5	8.17	2.81
9	5	5	20.19	22.31	3.07
0	6	5	177.97	170.28	6.49
1	6	5	0.89	56.18	13.72
2	6	5	1.19	0.64	4.99
3	6	5	36.15	39.3	2.4
4	6	5	56.1	60.26	3.22
5	6	5	50.85	55.68	2.59
6	6	5	59.06	61.16	2.85
7	6	5	42.06	54.15	2.96
8	6	5	4.83	4.24	6.3
9	6	5	19.85	26.17	3.07
1	7	5	441.88	412.48	10.46
2	7	5	0.7	4.65	5.02
3	7	5	101.96	103.36	4.76
4	7	5	44.51	40.12	2.47
5	7	5	13.45	22.65	2.62
6	7	5	3.28	2.32	2.55
7	7	5	151.53	155.18	7.13
8	7	5	1.36	3	2.85
9	7	5	25.49	30.97	3.04
0	8	5	18.47	17.66	2.14
1	8	5	126.61	115.77	4.03
2	8	5	1.99	7.84	2.25
3	8	5	8.98	2.21	5.25
4	8	5	0.58	3.6	5.36
5	8	5	198.56	215.57	7.47
6	8	5	32.17	29.02	2.66
7	8	5	1.26	13.98	2.77
8	8	5	21.8	30.75	2.96
9	8	5	0.63	0.6	6.71
1	9	5	9.02	7.74	5.31
2	9	5	59.04	60.94	2.92
3	9	5	12.83	20.62	2.32
4	9	5	27.28	27.11	2.4
5	9	5	188.3	162.74	7.28
6	9	5	22.61	29.73	2.66
7	9	5	110.71	121.4	5.96
8	9	5	39.93	43.95	3.04
9	9	5	13.11	11.77	2.96
0	10	5	0.07	-7.99	4.6
1	10	5	51.8	51.48	2.23
2	10	5	12.86	90.88	4.61
3	10	5	70.81	82.58	3.34
4	10	5	0.16	-4.65	5.32
5	10	5	41.65	41.43	2.59
6	10	5	60.21	65.36	3.52
7	10	5	91.85	106.81	5.1
8	10	5	1.09	2.44	6.67
1	11	5	12.86	11.3	2.87
2	11	5	351.25	347.57	7.99
3	11	5	89.66	86.11	4.2
4	11	5	3.24	5.92	2.29
5	11	5	27.21	26.21	2.51
6	11	5	83.23	102.98	4.46
7	11	5	35.07	49.87	2.92
8	11	5	15.64	21.67	2.89
0	12	5	0.44	3.11	4.95
1	12	5	2.33	2.21	3.55
2	12	5	37.52	38.06	2.4
3	12	5	47.71	59.06	2.66

h	k	l	F_c^2	F_o^2	σF_o^2
4	12	5	0.4	-0.9	5.4
5	12	5	65.47	66.07	3.41
6	12	5	158.68	164.37	7.39
7	12	5	5.05	16.35	2.89
8	12	5	0.34	-7.8	6.52
1	13	5	1.49	-3.19	5.31
2	13	5	13.02	16.65	2.29
3	13	5	161.5	172.25	6.9
4	13	5	17.31	4.39	5.55
5	13	5	20.32	13.95	2.44
6	13	5	2.33	-1.91	5.74
7	13	5	159.52	170.52	8.03
0	14	5	2.48	4.16	4.95
1	14	5	13.47	12.71	7.01
2	14	5	16.6	19.05	2.25
3	14	5	96.86	95.67	4.58
4	14	5	1.18	-6.04	5.47
5	14	5	0.03	-1.46	5.4
6	14	5	0.23	4.46	2.51
7	14	5	0.07	-7.65	6.49
1	15	5	28.84	19.65	1.68
2	15	5	6.46	3.75	5.17
3	15	5	26.29	26.96	2.44
4	15	5	6.46	10.39	2.47
5	15	5	15.05	14.66	2.44
6	15	5	9.56	5.29	6
0	16	5	267.39	258.9	7.5
1	16	5	17.93	23.98	3.17
2	16	5	9.75	10.95	2.29
3	16	5	0.35	26.51	2.62
4	16	5	65.15	68.74	3.37
5	16	5	3.06	-0.9	5.44
6	16	5	5.33	-8.06	6
1	17	5	2.77	-7.76	3.85
2	17	5	0.24	2.7	5.17
3	17	5	142.96	154.04	7.28
4	17	5	0.02	5.1	2.4
5	17	5	0.5	-7.8	5.66
0	18	5	0.03	0	5.29
1	18	5	3.52	0.33	2.11
2	18	5	0.99	-0.6	5.32
3	18	5	91.82	90.3	4.69
4	18	5	1.32	-6.86	5.77
1	19	5	3.27	4.36	4.39
2	19	5	7.01	9.26	2.36
3	19	5	20.49	26.7	2.7
0	20	5	94.54	110.41	5.48
1	20	5	42.64	46.3	2.51
2	20	5	5.7	7.27	2.36
0	0	6	1028.04	965.17	12.26
1	0	6	266.74	247.65	5.73
2	0	6	188.48	187.49	7.77
3	0	6	0.15	-4.5	6.56
4	0	6	95.56	98.11	5.1
5	0	6	26.84	34.05	3.07
6	0	6	0	13.42	3.07
7	0	6	8.83	5.62	3.41
1	1	6	81.47	93.08	7.12
2	1	6	20.81	44.1	15.32
3	1	6	32.84	38.96	2.16
4	1	6	101	107.54	4.18
5	1	6	17.68	14.99	2.15
6	1	6	5.76	10.19	2.88
7	1	6	14.45	16.28	4.09
0	2	6	122.14	118.67	5.55
1	2	6	13.59	10.93	4.95
2	2	6	0.4	2.7	6
3	2	6	12.48	18.15	2.74
4	2	6	30.57	54.26	3.15
5	2	6	7.12	11.14	2.92
6	2	6	15.25	17.28	3.11
7	2	6	4.09	0.49	7.42
1	3	6	29.3	34.32	2.62
2	3	6	18.57	25.53	2.59
3	3	6	17.13	17.43	2.7
4	3	6	127.34	124.07	5.85
5	3	6	23.05	27.9	2.96
6	3	6	3.71	11.21	3.04
0	4	6	95.18	99.72	5.06
1	4	6	20.47	18.21	7.46
2	4	6	20.71	34.46	2.66
3	4	6	2.06	10.57	2.62
4	4	6	8.21	23.1	2.96
5	4	6	13.52	17.36	2.92
6	4	6	27.4	32.88	3.11
1	5	6	3.16	3.39	2.34
2	5	6	41.81	47.51	2.77
3	5	6	9.57	11.44	2.66
4	5	6	69.48	80.77	4.01
5	5	6	15.68	24.52	2.92
6	5	6	19.38	22.31	3.04
0	6	6	93.07	66.11	3.94
1	6	6	11.89	3.97	4.16
2	6	6	35.99	43.61	2.7
3	6	6	8.96	14.21	2.62
4	6	6	69.37	72.75	3.9
5	6	6	9.27	25.95	3
6	6	6	0.16	1.87	2.92
1	7	6	14	23.28	2.91
2	7	6	18.57	20.06	2.55
3	7	6	6.25	2.44	6.04
4	7	6	37.08	55.12	3.07
5	7	6	93.35	91.92	4.16
6	7	6	2.5	15.11	2.96
0	8	6	60.93	63.82	3.19
1	8	6	63.22	58.77	2.25
2	8	6	0.82	4.65	2.47
3	8	6	0.49	6.64	2.7
4	8	6	85.28	95.25	5.18
5	8	6	61.94	71.92	3.49
1	9	6	4.29	9.67	4.86
2	9	6	4.35	3.41	2.51
3	9	6	22.64	24.93	2.81
4	9	6	7.41	25.57	2.89
5	9	6	57.7	62.62	3.37
0	10	6	44.57	42.97	2.7
1	10	6	1.28	1.38	4.02
2	10	6	0.93	4.24	5.77
3	10	6	15.65	21.41	2.74
4	10	6	57.08	83.36	4.46
5	10	6	42	39.78	2.96
1	11	6	5.35	2.47	4.2
2	11	6	1.75	5.66	5.7
3	11	6	31.19	35.92	2.81
4	11	6	100.59	103.17	4.84
0	12	6	76.85	88.24	4.5
1	12	6	3.05	1.43	4.18
2	12	6	10.24	8.77	2.59
3	12	6	24.01	21.9	2.77
1	13	6	20.41	21.42	1.85
2	13	6	0.22	-0.37	6.07
0	14	6	5.79	-1.16	6.07
1	14	6	1.83	4.38	2.39

A3.7 PYRXL

h	k	l	F_c^2	F_o^2	σF_o^2
-1	2	0	6037.18	3512.48	4074.76
0	2	0	704.5	351.51	34.9
-2	3	0	18446.92	16061.99	1776.68
-1	3	0	450.36	538.27	179.58
0	3	0	597.97	742.73	85.22
-3	4	0	3782.28	4301.86	274.17
-2	4	0	148.65	144.12	36.21
-1	4	0	1122.2	1075.21	437.67
0	4	0	6206.84	6078.87	774.36
-4	5	0	1616.76	1788.58	76.52
-3	5	0	789.46	640.12	62.92
-2	5	0	9678.42	7463.89	2415.08
-1	5	0	42.54	54.1	12.06
0	5	0	1312.47	1161.05	101.53
-5	6	0	10.91	48.48	20.77
-4	6	0	1112.74	1075.26	45.46
-3	6	0	991.92	1056.76	216.34
-2	6	0	1767.93	1355.84	379.6
-1	6	0	1260.51	786.76	213.41
0	6	0	3051.84	2599.26	155.19
-6	7	0	20.48	39.83	11.92
-5	7	0	6882.41	6702.21	393.81
-4	7	0	2276.77	2058.01	116.14
-3	7	0	303.57	293.25	30.43
-2	7	0	82.71	121.67	18.99
-1	7	0	2642.96	2378.95	381.04
0	7	0	83.4	83.99	6.85
-7	8	0	2635.78	2555.27	89.19
-6	8	0	2579.8	2763.38	129.15
-5	8	0	1622.48	1676.51	114.92
-4	8	0	401.22	357.49	31.44
-3	8	0	1525.11	1466.44	255.77
-2	8	0	1050.19	1050.89	186.36
-1	8	0	46.26	40.48	5.8
0	8	0	294.13	367.64	18.9
-8	9	0	119.64	118.49	3.54
-7	9	0	1535.7	1644.63	73.69
-6	9	0	7558.61	7662.67	441.11
-5	9	0	311.14	283.49	24.83
-4	9	0	40.09	19.58	6.7
-3	9	0	14.38	1.59	5.94
-2	9	0	506.34	527.07	62.48
-1	9	0	0.56	-2.54	5.95
0	9	0	0.25	-0.24	6.62
-9	10	0	1018.87	984.9	41.24
-8	10	0	1258.25	1194.23	47.85
-7	10	0	12.46	3.13	3.55
-6	10	0	12.81	6.27	4.49
-5	10	0	464.15	614.5	68.47
-4	10	0	59.71	49.61	7
-3	10	0	138.66	122.97	12.9
-2	10	0	235.23	181.4	23.15
-1	10	0	118.87	101.94	15.46
0	10	0	486.84	494.72	36.08
-10	11	0	73.53	60.26	5.1
-9	11	0	205.66	189.74	6.07
-8	11	0	188.46	173.32	13.36
-7	11	0	6.95	2.9	3.47
-6	11	0	234.21	189.63	21.83
-5	11	0	255.36	295.66	39.35
-4	11	0	707.14	661.39	114.23
-3	11	0	2287.38	2051.02	248.79
-2	11	0	162.76	148.57	13.88
-1	11	0	0.51	-10.51	7.27
0	11	0	58.32	47.06	4.15
-11	12	0	2.13	3.19	7.37
-10	12	0	202.73	233.7	7.25
-9	12	0	691.21	656.39	14.77
-8	12	0	8.91	11.91	4.31
-7	12	0	388.85	376.65	48.27
-6	12	0	105.18	99.6	6.96
-5	12	0	245.98	218.28	28.1
-4	12	0	248.14	203.98	29.91
-3	12	0	344.41	293.44	24.02
-2	12	0	7.72	10.28	3.2
-1	12	0	7.68	11.48	3.05
0	12	0	46.24	40.87	2.4
-12	13	0	111.16	99.67	8.17
-11	13	0	104.31	121.36	5.18
-10	13	0	0.38	-4.1	7.47
-9	13	0	606.28	596.97	18.14
-8	13	0	65.57	67.96	9.88
-7	13	0	4.05	9.06	7.2
-6	13	0	114.46	115.29	8.75
-5	13	0	3.88	3.02	3.07
-4	13	0	74.88	75.13	8.42
-3	13	0	1.7	-0.94	4.35
-2	13	0	82.03	88.91	7.05
-1	13	0	396.58	355.6	27.63
0	13	0	13.96	19.42	2.79
-13	14	0	42.83	47.75	4.01
-12	14	0	74.71	53.41	3.08
-11	14	0	11.51	9.2	4.36
-10	14	0	215.64	200.47	6.4
-9	14	0	79.5	90.93	5.69
-8	14	0	10.54	-9.87	7.77
-7	14	0	1.2	-3.26	4.82
-6	14	0	1.38	-5.63	4.24
-5	14	0	47.87	43.9	9.8
-4	14	0	114.68	113.87	14.9
-3	14	0	181.95	145.35	14.37
-2	14	0	261.68	231.02	21.62
-1	14	0	4.27	-0.71	4.68
0	14	0	20.21	19.88	3.15
-14	15	0	3.27	-0.77	8.74
-13	15	0	57.55	37.58	3.32
-12	15	0	7.32	17.05	3.59
-11	15	0	54.26	56.61	5.02
-10	15	0	120.6	113.73	6.61
-9	15	0	118.05	95.1	4.27
-8	15	0	0.02	1.4	4.28
-7	15	0	59.39	66.26	11.58
-6	15	0	107.77	95.5	26.09
-5	15	0	1.09	12.19	3.55
-4	15	0	210.68	193.55	20.36
-3	15	0	204.61	180.94	12.3
-2	15	0	45.77	37.46	3.36
-1	15	0	120.39	138.75	12.25
0	15	0	68.31	60.3	8.29
-15	16	0	0.33	7.29	5.43
-14	16	0	25.98	28.32	3.49
-13	16	0	46.07	37.74	3.53
-12	16	0	1.3	4.1	5.01
-11	16	0	49.01	45.04	7.79
-10	16	0	39.66	28.77	8.46
-9	16	0	0.82	4.44	8.69
-8	16	0	1.11	3.35	6.51
-7	16	0	142.97	143.47	31.27
-6	16	0	9.28	12.38	8.05
-5	16	0	7.61	7.03	7.86
-4	16	0	23.37	21.54	4.64
-3	16	0	1.7	2.77	3.89
-2	16	0	1.34	-2.59	9.32
-1	16	0	51.21	48.01	6.8
-14	17	0	3.2	7.19	5.45
-13	17	0	0	-1.85	7.43
-12	17	0	11.01	12.86	9.29
-11	17	0	64.54	61.1	8.04
-10	17	0	0.13	-8.18	9.13
-9	17	0	37.77	31.64	3.66
-8	17	0	18.51	18.04	8.94
-7	17	0	0.82	6.16	9.22
-6	17	0	10.17	-1.58	9.11
-5	17	0	3.49	-6.72	9.23
-4	17	0	19.78	16.53	4.07
-3	17	0	0.2	-13.18	9.59
-12	18	0	18.14	22.44	5.6
-11	18	0	0.26	3.54	8.92
-10	18	0	3.13	0.6	5.36
-9	18	0	0.38	-11.29	9.84
-8	18	0	111.66	104.26	13.56
-7	18	0	1.79	12.39	5.54
-6	18	0	10.45	5.1	9.73
-1	2	1	1678.04	2002.72	34.35
0	2	1	9117.61	7302.52	118.98
-2	3	1	13850.35	15460.34	413.12
-1	3	1	5.09	6.12	2.41
0	3	1	16694.95	18495.66	808.66
-3	4	1	19457.22	20598.33	442.24
-2	4	1	13931.98	11866.69	615.45
-1	4	1	1420.29	1198.1	251.34
0	4	1	223.6	242.96	12.14
-4	5	1	544.39	533.37	8.51
-3	5	1	679.53	503.62	24.37
-2	5	1	1864.94	1882.14	131.43
-1	5	1	506.16	515.71	93.49
0	5	1	642.5	539.53	32.55
-5	6	1	5624.35	5886.65	178.9
-4	6	1	1899.88	1888.31	57.11
-3	6	1	13.56	12.24	1.52
-2	6	1	140.6	175.53	14.55
-1	6	1	3354.15	2641.06	514.03
0	6	1	913.76	776.07	20.05
-6	7	1	1593.18	1631.17	37.96
-5	7	1	3662.22	3843.04	154.01
-4	7	1	182.06	142.54	4.42
-3	7	1	3483.27	3456.45	190.85
-2	7	1	228.96	187.47	9.03
-1	7	1	36.94	48.17	4.73
0	7	1	1637.7	1743.63	76.23
-7	8	1	124.75	130.19	8.84
-6	8	1	2043.37	1845.2	48.09
-5	8	1	583.72	564.24	26.1
-4	8	1	1533.32	1416.77	61.35
-3	8	1	7.36	-1.28	5.01
-2	8	1	43.12	58.62	5.2
-1	8	1	21.33	11.38	3.72
0	8	1	10.63	8.6	2.17
-8	9	1	7.8	4.78	5.96
-7	9	1	1.79	7.12	6.08
-6	9	1	6642.61	6945.38	266.04
-5	9	1	199.07	176.19	13.75
-4	9	1	29.81	29.36	2.18
-3	9	1	0.68	2.59	2.24
-2	9	1	153.75	162	18.19
-1	9	1	2.21	3.28	5.98
0	9	1	657.62	668.28	32.07
-9	10	1	749.93	732.64	23.96
-8	10	1	107.57	99.7	3.05
-7	10	1	825.2	816.14	34.27
-6	10	1	51.2	35.97	2.23
-5	10	1	87.12	74.74	3.44
-4	10	1	20.06	16.8	4.28
-3	10	1	23.67	43.49	5.37
-2	10	1	14.11	15.65	3.06
-1	10	1	21.35	20.62	8.12
0	10	1	122.65	105.22	6.53
-10	11	1	97.28	89.62	3.03
-9	11	1	0.02	4.22	7.07
-8	11	1	2	-3.8	6.68
-7	11	1	123.13	115.49	10.42
-6	11	1	418.62	428.66	29.08
-5	11	1	153.05	114.54	21.7
-4	11	1	0.16	3.84	3.69
-3	11	1	10.57	10.01	3.79
-2	11	1	484.87	474.38	26.83
-1	11	1	0.58	3.84	5.11
0	11	1	70.53	54.9	2.34
-11	12	1	9.44	8.78	4.33
-10	12	1	2.09	4.75	4.74
-9	12	1	162.12	164.16	5.14
-8	12	1	638.43	614.6	39.36
-7	12	1	75.16	81.74	6.23
-6	12	1	80.96	72.35	6.71
-5	12	1	75.33	78.65	6.77
-4	12	1	33.29	43.54	4.71
-3	12	1	21.47	11.59	4.18
-2	12	1	13.91	11.46	5.66
-1	12	1	0.7	-0.35	4.15
0	12	1	3.51	2.45	3.74
-12	13	1	1.5	-1.08	4.18
-11	13	1	157.51	144.39	4.4
-10	13	1	10.69	3.11	7.35
-9	13	1	10.57	14.37	8.7
-8	13	1	389.77	377.5	13.41
-7	13	1	105.59	89.37	8.28
-6	13	1	7.14	4.16	3.06
-5	13	1	3.25	3.54	3.91
-4	13	1	418.05	353.36	29.58
-3	13	1	122.89	113.81	4.34
-2	13	1	0.12	-0.21	9.16
-1	13	1	36.44	44.03	2.94
0	13	1	4.31	5.06	4.66
-13	14	1	4.72	-2.45	8.37
-12	14	1	17.47	14.49	6.85
-11	14	1	310.88	301.68	17.67
-10	14	1	0.19	-2.76	7.92
-9	14	1	6.92	-2.34	7.74
-8	14	1	15.88	19.74	3.94
-7	14	1	14.93	-6.78	7.99
-6	14	1	74.84	90.93	9.61
-5	14	1	148	106.45	21.35
-4	14	1	9.32	-4.26	5.18
-3	14	1	117.68	106.64	5.42
-2	14	1	13.02	-4.26	12.34
-1	14	1	41.95	26.99	9.89
0	14	1	98.24	101.68	5.76
-14	15	1	0.01	2.49	8.92
-13	15	1	6.92	6.63	8.86
-12	15	1	106.24	88.65	3.73
-11	15	1	5.88	5.92	6.32
-10	15	1	8.2	10.05	8.06
-9	15	1	1.41	-15.04	8.26
-8	15	1	62.88	54.79	6.43
-7	15	1	0.17	-2.14	4.3
-6	15	1	74.74	64.87	20.88
-5	15	1	224.95	159.54	30.09
-4	15	1	0.4	11.05	8.25
-3	15	1	13.48	1.05	8.67
-2	15	1	5.79	-0.5	8.83
-1	15	1	6.21	1.4	9.05
0	15	1	10.73	-10.07	11.26
-15	16	1	28.57	36.12	3.99
-14	16	1	13	12.68	4.09
-13	16	1	83.57	66.64	5.25
-12	16	1	97.87	80.68	4.56
-11	16	1	62.27	61.9	6.8
-10	16	1	92.27	86.56	3.54
-9	16	1	0.02	-8	8.6
-8	16	1	131.71	127.42	23.61
-7	16	1	9.19	11.64	3.2
-6	16	1	1.11	-16.51	8.83

h	k	l	F_c^2	F_o^2	σF_o^2
-5	16	1	28.24	31.56	9.18
-4	16	1	0.26	1.14	5.02
-3	16	1	13.61	28.84	6.52
-2	16	1	0.85	-4.95	9.41
-1	16	1	25.44	24.8	7.38
-14	17	1	8.91	-11.37	9.9
-13	17	1	13.96	9.94	3.47
-12	17	1	69.44	77.43	4.3
-11	17	1	19.49	23.74	6.45
-10	17	1	28	22.1	11.36
-9	17	1	21.16	14.55	5.23
-8	17	1	2.16	-3.62	9.29
-7	17	1	64.16	70.53	10.63
-6	17	1	3.68	5.16	9.17
-5	17	1	0.65	5.32	9.15
-4	17	1	0.06	1.4	9.35
-3	17	1	12.38	18.45	7.6
-12	18	1	1.22	3.88	4.13
-11	18	1	51.89	51.91	10.04
-10	18	1	9.28	17.47	4.2
-9	18	1	24.14	18.12	11.6
-8	18	1	1.84	1.75	7.81
-7	18	1	0.03	-5.2	5.4
-6	18	1	4.5	-16.83	12.69
0	0	2	45822.93	43674.58	891.29
0	1	2	407.94	820.92	12.38
-1	2	2	1597.8	1276.47	15.69
0	2	2	7820.02	8015.77	90.54
-2	3	2	5407.14	4876.05	57.24
-1	3	2	22409.36	27102.78	690.04
0	3	2	3902.84	3865.1	39.58
-3	4	2	7784.52	9099.67	117.25
-2	4	2	3833.29	3488.73	41.5
-1	4	2	8734.9	9136.94	446.71
0	4	2	1681.05	2000.34	33.56
-4	5	2	559.65	566.4	8.85
-3	5	2	1733.64	1683.01	25.62
-2	5	2	1934.15	2050.18	38.59
-1	5	2	5.05	3.48	4.32
0	5	2	1.67	-5.09	3.76
-5	6	2	4375.61	4591.16	80.44
-4	6	2	93.16	102.79	3.11
-3	6	2	312.94	386.01	11.65
-2	6	2	530.13	521.68	19.85
-1	6	2	383.24	333.81	22.43
0	6	2	119.49	91.17	3.25
-6	7	2	914.02	988.49	16.05
-5	7	2	379.94	340.63	7.36
-4	7	2	99.42	143.32	18.14
-3	7	2	642.45	761.23	21.25
-2	7	2	389.33	307.65	11.16
-1	7	2	217.29	236.49	17.19
0	7	2	23.37	30.19	1.57
-7	8	2	931.17	868.66	15.09
-6	8	2	1254.44	1380.86	37.89
-5	8	2	345.83	363.17	7.84
-4	8	2	0.4	-2.62	3.72
-3	8	2	103.61	114.77	3.93
-2	8	2	48.21	61.63	1.96
-1	8	2	573.6	543.71	27.95
0	8	2	37.85	33.2	1.75
-8	9	2	155.92	191.25	6.01
-7	9	2	236.99	238.79	7.02
-6	9	2	266.44	269.15	11.98
-5	9	2	306.45	303.1	11.61
-4	9	2	31.42	41.08	2.05
-3	9	2	107.54	111.86	5.72
-2	9	2	10.99	6.47	2.95
-1	9	2	44.98	40.73	3.18
0	9	2	418.62	416.44	15.37
-9	10	2	262.05	260.21	7.83
-8	10	2	125.86	94.76	2.91
-7	10	2	51.42	47.93	3.76
-6	10	2	59.55	57.52	3.27
-5	10	2	4.49	12.97	3.15
-4	10	2	168.51	171.34	8.92
-3	10	2	5.22	-0.7	6.08
-2	10	2	10.49	18.45	3.13
-1	10	2	16.62	16.05	2.31
0	10	2	72.59	78.73	2.4
-10	11	2	7.82	6.96	2.5
-9	11	2	325.34	314.87	9.12
-8	11	2	415.18	431.08	17.24
-7	11	2	35.02	27.71	2.73
-6	11	2	3.3	2.59	3.44
-5	11	2	120.54	119.46	12.17
-4	11	2	9.05	14.82	4.55
-3	11	2	78.04	75.1	4.76
			F_c^2	F_o^2	σF_o^2
-2	11	2	79.69	77.63	2.8
-1	11	2	8.48	18.73	2.55
0	11	2	92.89	97.42	7.26
-11	12	2	4.63	-5.55	7.43
-10	12	2	212.14	221.3	6.9
-9	12	2	39.19	41.11	3.54
-8	12	2	0.01	-6.14	7.92
-7	12	2	59.51	67.63	2.75
-6	12	2	0.88	-4.81	6.96
-5	12	2	57.6	51.03	4.9
-4	12	2	7.35	11.42	3.14
-3	12	2	37.76	34.81	2.72
-2	12	2	357.84	380.01	14.03
-1	12	2	8.93	10.53	4.74
0	12	2	80.19	84.84	5.17
-12	13	2	12.96	12.41	2.77
-11	13	2	24.02	18.94	3.32
-10	13	2	44.27	45.94	2.78
-9	13	2	311.39	312.31	9.58
-8	13	2	0.86	-1.75	4.32
-7	13	2	117.84	113.72	4.49
-6	13	2	32.62	21.71	2.64
-5	13	2	78.66	60.69	9.54
-4	13	2	2.35	-1.76	9
-3	13	2	7.81	7.84	4.79
-2	13	2	11.23	14.8	3.86
-1	13	2	77.15	67.41	5.55
0	13	2	1.1	-0.39	4.07
-13	14	2	2.36	-5.1	6
-12	14	2	9.38	7.78	5.88
-11	14	2	7.19	11.19	4.28
-10	14	2	173.55	166.04	5.04
-9	14	2	24.59	29.81	3.07
-8	14	2	42.51	40.64	3.22
-7	14	2	11.2	11.91	4.13
-6	14	2	99.16	94.42	3.12
-5	14	2	88.07	73.69	8.41
-4	14	2	6.09	1.03	7.73
-3	14	2	3.98	2.92	7.92
-2	14	2	4.21	8.34	7.99
-1	14	2	0.24	-2.91	9.99
0	14	2	4.74	-1.09	5.29
-14	15	2	3.37	-8.35	11.38
-13	15	2	18.58	15.1	6.59
-12	15	2	4.21	3.51	8.63
-11	15	2	49.82	51.46	3.06
-10	15	2	12.84	16.86	3.47
-9	15	2	124.94	123.32	3.99
-8	15	2	3.61	-2.28	4.48
-7	15	2	7.17	5.74	7.7
-6	15	2	10.23	6.84	3.38
-5	15	2	27.46	19.21	4.28
-4	15	2	57.52	66.4	3.16
-3	15	2	27.22	22.69	3.76
-2	15	2	23.1	19.34	3.93
-1	15	2	2.62	-19.27	9.26
0	15	2	13.12	9.05	4.97
-15	16	2	2.57	3.57	6.49
-14	16	2	1.42	-5.66	10.74
-13	16	2	21.12	7.59	9.3
-12	16	2	1.57	-3.53	9
-11	16	2	22.26	29.78	3.67
-10	16	2	24.04	18.76	6.26
-9	16	2	3.8	9.32	4.71
-8	16	2	6.23	-1.5	8.72
-7	16	2	0.15	0.17	8.65
-6	16	2	4	-7.91	8.85
-5	16	2	39	32.47	5.84
-4	16	2	0.6	-2.36	12.64
-3	16	2	10.48	15.93	3.94
-2	16	2	12.42	10.56	4.18
-1	16	2	0.03	-3.33	5.61
-14	17	2	1.69	-3.97	9.59
-13	17	2	5.79	6.24	5.16
-12	17	2	0.33	-4.5	9.18
-11	17	2	32.85	26.21	4.01
-10	17	2	2.58	2.95	7
-9	17	2	0	-2.75	6.43
-8	17	2	0.01	-3.01	4
-7	17	2	10.82	12.61	9.29
-6	17	2	0.33	1.22	9.12
-5	17	2	5.22	-7.74	9.24
-4	17	2	1.65	-3.51	9.24
-3	17	2	14.56	13.75	4.74
-12	18	2	4.55	-13.76	9.89
-11	18	2	1.01	-4.85	9.76
-10	18	2	6.24	2.26	6.1
-9	18	2	3.14	1.33	9.84
-8	18	2	0.39	6.24	5.32
-7	18	2	0.81	7.92	9.61
-6	18	2	0	5.32	11.86
0	1	3	2942.74	2823.98	143.37
-1	2	3	9198.71	8467.76	110.92
0	2	3	21101.94	22118.29	278.61
-2	3	3	10.98	8	2.23
-1	3	3	1047	1275.15	16.11
0	3	3	455.88	348.43	5.6
-3	4	3	17822.92	19640.13	247.95
-2	4	3	288.72	162.79	10.37
-1	4	3	73.89	59.86	9.87
0	4	3	1608.3	1634.67	17.75
-4	5	3	861.59	907.05	12.52
-3	5	3	4610.39	4675.88	55.46
-2	5	3	7.84	-1.53	4.32
-1	5	3	97.98	76.59	2.35
0	5	3	566.85	534.36	7.47
-5	6	3	13.99	15.35	3.83
-4	6	3	239.37	267.01	6.26
-3	6	3	239.59	258.72	6.05
-2	6	3	155.17	215.42	12.84
-1	6	3	90.5	97.38	3.33
0	6	3	166.39	169.37	4.58
-6	7	3	211.67	226.16	7.7
-5	7	3	441.69	534.14	12.74
-4	7	3	110.13	116.22	3.69
-3	7	3	806.15	778.24	22.59
-2	7	3	23.67	31.61	1.73
-1	7	3	309.42	339.46	7.33
0	7	3	1007.67	1104.45	27.08
-7	8	3	144.89	155.09	4.72
-6	8	3	579.12	558.98	9.8
-5	8	3	371.14	398.51	17.59
-4	8	3	1261.35	1327.07	17.95
-3	8	3	445.33	463.89	12.71
-2	8	3	0.3	-2.15	2.76
-1	8	3	280.75	268.79	8.42
0	8	3	3.16	3.87	3.8
-8	9	3	285.61	286.64	16.32
-7	9	3	130.77	106.33	4.09
-6	9	3	568.11	604.4	13.06
-5	9	3	83.51	70.81	2.93
-4	9	3	16.21	23.84	1.96
-3	9	3	105.79	84.94	2.67
-2	9	3	6.88	-1.35	5.73
-1	9	3	139.31	148.02	4.36
0	9	3	35.31	43.69	3.26
-9	10	3	5.95	-1.62	6.54
-8	10	3	1.39	-5.63	3.31
-7	10	3	1.65	-7.75	6.08
-6	10	3	39.64	30.06	6.23
-5	10	3	25.78	24.88	4.15
-4	10	3	16.44	19.74	2.13
-3	10	3	443.97	428.23	14.49
-2	10	3	0.26	3.98	6.3
-1	10	3	24.9	30.93	3.5
0	10	3	65.04	71.87	2.75
-10	11	3	123.74	116.81	4.3
-9	11	3	0.32	3.85	3.54
-8	11	3	58.05	69.64	2.62
-7	11	3	48.07	51.05	2.4
-6	11	3	81.28	78.46	3.65
-5	11	3	154.11	145.54	11.17
-4	11	3	267.42	252.98	7.64
-3	11	3	9.07	7.78	5.35
-2	11	3	91.43	94.09	4.42
-1	11	3	242.14	230.11	15.8
0	11	3	213.01	225.74	10.98
-11	12	3	1.48	5.96	4.12
-10	12	3	20.21	19.68	2.59
-9	12	3	0.83	-14.26	7.1
-8	12	3	10.93	9.11	3.67
-7	12	3	37.39	30.83	6.29
-6	12	3	3.39	10.31	8.32
-5	12	3	504.92	502.46	41.62
-4	12	3	507.07	496.44	16.32
-3	12	3	1.91	3.6	3.16
-2	12	3	184.32	159.36	8.02
-1	12	3	46.14	50.4	2.81
0	12	3	59.68	52.16	2.48
-12	13	3	5.21	4.3	7.17
-11	13	3	8.03	8.3	4.67
-10	13	3	0.03	-7.56	7.51
-9	13	3	1.69	0.87	5.13
-8	13	3	22.31	15.87	8.73
-7	13	3	31.26	22.7	2.65
-6	13	3	0.11	-4.35	6.59
-5	13	3	44.18	34.23	3.23
-4	13	3	38.47	39.44	2.79
-3	13	3	26.81	18.66	5.62
-2	13	3	105.19	86.24	3.82
-1	13	3	76.06	78.48	3.09
0	13	3	4.32	0.02	7.46
-13	14	3	54.93	58.13	13.57
-12	14	3	2.22	-13.62	8.13
-11	14	3	101.07	103.91	4.32
-10	14	3	9.57	14.29	4.4
-9	14	3	142.34	143.68	4.56
-8	14	3	0.04	-10.03	7.77
-7	14	3	104.71	94.27	4.21
-6	14	3	5.48	2.96	4.24
-5	14	3	2.25	5.25	4.29
-4	14	3	5.99	2.03	4.24
-3	14	3	2.78	1.04	6.36
-2	14	3	2.06	6.26	8.07
-1	14	3	43.5	46.28	4.8
0	14	3	5.09	-0.13	4.52
-14	15	3	0.08	-3.99	6.06
-13	15	3	6.85	2.77	10.2
-12	15	3	24.28	27.98	3.15
-11	15	3	29.7	20.19	2.93
-10	15	3	2.05	2.83	8.08
-9	15	3	5.54	10.04	4.27
-8	15	3	0.27	7.38	4.26
-7	15	3	32.07	29.02	5.55
-6	15	3	1.6	3.49	4.48
-5	15	3	4.45	2.8	8.07
-4	15	3	8.33	7.1	6.45
-3	15	3	18.55	24.01	5.27
-2	15	3	2.6	2.26	4.94
-1	15	3	4.51	3.42	8.91
0	15	3	0.52	2.19	4.84

h	k	l	F_c^2	F_o^2	σF_o^2
-15	16	3	0.09	8.04	9.44
-14	16	3	6.02	-1.79	9.31
-13	16	3	9.1	4.75	5
-12	16	3	9.86	-6.33	9.09
-11	16	3	19.11	19.65	3.23
-10	16	3	2.56	3.44	4.91
-9	16	3	6.55	0.32	6.53
-8	16	3	20.03	19.92	5.12
-7	16	3	0.01	1.7	8.46
-6	16	3	70.98	60.59	9.09
-5	16	3	18.6	1.24	8.86
-4	16	3	1.46	1.01	7.68
-3	16	3	18.18	14.9	5.04
-2	16	3	9.07	14.89	5.31
-1	16	3	4.38	-17.24	10.32
-14	17	3	2.42	-4.66	9.57
-13	17	3	0.57	-5.16	7.71
-12	17	3	5.07	2.7	6
-11	17	3	0.9	-2.33	5.24
-10	17	3	1.9	-10	8.91
-9	17	3	3.74	2.68	4.77
-8	17	3	0.02	2.44	5.39
-7	17	3	9.67	8.74	9.13
-6	17	3	8.75	1.47	15.84
-5	17	3	3.97	5.79	9.25
-4	17	3	0.05	-7.61	9.33
-3	17	3	10.95	23.42	14.9
-11	18	3	2.67	-15.16	9.64
-10	18	3	0.18	0.31	9.67
-9	18	3	0.82	-11.94	9.72
-8	18	3	0.78	4.27	5.57
-7	18	3	27.73	27.49	9.25
0	0	4	628.43	827.83	18.94
0	1	4	1374.2	1283.3	113.39
-1	2	4	840.84	1187.67	16.23
0	2	4	270.65	313.06	38.56
-2	3	4	12750.68	13748	177.01
-1	3	4	1971.28	1610.74	20.02
0	3	4	4147.98	3698.51	38.09
-3	4	4	2.5	-5.57	4.35
-2	4	4	357.51	388.63	7.01
-1	4	4	4682.35	4776.88	56.53
0	4	4	1230.45	1154.37	13.14
-4	5	4	118.38	96.74	4.42
-3	5	4	528.64	532.08	8.6
-2	5	4	551.42	498.29	8.63
-1	5	4	3.15	28.26	10.01
0	5	4	956.85	1119.04	13
-5	6	4	60.06	76.96	2.45
-4	6	4	1937.24	2031.38	25.45
-3	6	4	43.57	54.33	1.87
-2	6	4	190.16	252.77	6.27
-1	6	4	403.18	413.96	7.79
0	6	4	454.1	510.8	7.69
-6	7	4	201.94	188.85	5.78
-5	7	4	319.68	322.44	7.18
-4	7	4	4.84	5.78	6.52
-3	7	4	850.85	848.45	12.49
-2	7	4	2016.48	1932.97	31
-1	7	4	332.7	362.73	7.68
0	7	4	969.95	957.96	12.13
-7	8	4	163.31	178.23	5.54
-6	8	4	8.48	8.44	4.48
-5	8	4	71.88	70.54	3.23
-4	8	4	345.72	352.47	9.79
-3	8	4	8.03	4.65	2.83
-2	8	4	363.14	316.79	9.78
-1	8	4	20.39	28.28	2.64
0	8	4	58.16	46.93	1.81
-8	9	4	15.82	4.62	4.93
-7	9	4	12.58	17.1	3.88
-6	9	4	84.86	71.42	2.41
-5	9	4	37.4	49.17	2.07
-4	9	4	22.84	23.14	3.68
-3	9	4	299.13	316.73	11.52
-2	9	4	14.1	17.99	9.93
-1	9	4	574.35	500.94	12.71
0	9	4	7.19	16.3	3.69
-9	10	4	20.2	17.73	3.21
-8	10	4	42.08	41.73	2.28
-7	10	4	97.45	117.07	3.81
-6	10	4	44.24	43.28	2.2
-5	10	4	34.67	33.79	2.19
-4	10	4	76.2	78.95	2.51
-3	10	4	197.46	201.45	7.89
-2	10	4	119.32	109.62	3.94
-1	10	4	93.96	99.13	3.58
0	10	4	1.13	-1.18	4.62
-10	11	4	0.14	-8.9	7.36
-9	11	4	2.88	-2.92	7.62
-8	11	4	2.47	-3.66	6.72
-7	11	4	34.21	41.84	2.44
-6	11	4	51.55	61.48	2.48
-5	11	4	253.72	247.14	9.54
-4	11	4	15.09	5.4	11.66
-3	11	4	42.71	39.02	2.6
-2	11	4	342.63	354.81	14.41
-1	11	4	1.03	7.29	3.97
0	11	4	145.32	146.34	3.78
-11	12	4	1.2	-6.58	4.1
-10	12	4	2.84	-0.01	6.44
-9	12	4	2.39	0.53	4.02
-8	12	4	6.73	-5.5	7.97
-7	12	4	5.1	1.42	7.13
-6	12	4	436.92	428.86	12.72
-5	12	4	1.97	5.83	4.34
-4	12	4	37.38	38.56	2.69
-3	12	4	204.5	216.56	11.91
-2	12	4	17.82	22.66	4.44
-1	12	4	14.81	16.33	5.29
0	12	4	83.79	75.89	2.58
-12	13	4	0.53	8.02	7.76
-11	13	4	64.51	60.75	3.07
-10	13	4	12.72	17.48	6.29
-9	13	4	4.15	1.92	7.71
-8	13	4	18.78	15.11	2.66
-7	13	4	9.07	2.02	7.51
-6	13	4	8.88	12.64	4.06
-5	13	4	32.5	39.17	2.75
-4	13	4	25.8	28.05	2.73
-3	13	4	10.32	9.38	3.27
-2	13	4	13.34	16.05	4.18
-1	13	4	2.08	-4.3	5.14
0	13	4	3.93	-2.26	6.85
-13	14	4	3.16	7.95	2.91
-12	14	4	5.98	6.9	4.31
-11	14	4	7.04	-2.44	8.19
-10	14	4	2.03	1.24	4.71
-9	14	4	36.86	22.75	6.04
-8	14	4	17.51	13.22	4.32
-7	14	4	83.48	83.41	4.11
-6	14	4	54.73	62.61	2.9
-5	14	4	33.14	30.74	3.8
-4	14	4	8.91	-3.66	7.95
-3	14	4	5.66	7.15	4.36
-2	14	4	0.1	12.09	4.55
-1	14	4	56	58.55	3.83
0	14	4	0.54	6.18	4.61
-14	15	4	6.35	-10.33	13.87
-13	15	4	4	3.43	8.78
-12	15	4	13.27	7.49	4.72
-11	15	4	0.01	-5.49	7.91
-10	15	4	19.4	14.85	10.95
-9	15	4	91.9	83.16	3.45
-8	15	4	5.11	-1.83	8.16
-7	15	4	33.59	30.68	2.91
-6	15	4	11.76	8.13	4.35
-5	15	4	0.69	-11.2	8.17
-4	15	4	16.78	24.58	3.85
-3	15	4	18.91	5.91	8.62
-2	15	4	4.57	-11.02	11.89
-1	15	4	1.39	2.69	4.97
0	15	4	24.78	26.57	3.02
-15	16	4	0.11	3.37	9.81
-14	16	4	0.19	-6.7	5.06
-13	16	4	7.75	7.48	8.9
-12	16	4	0.25	-1.07	4.9
-11	16	4	5.81	6.06	5.38
-10	16	4	2.84	2.02	8.67
-9	16	4	0.33	-0.2	8.41
-8	16	4	10.95	0.1	4.86
-7	16	4	3.6	7.14	8.53
-6	16	4	15.49	29.17	8.13
-5	16	4	2.83	-5.03	7.56
-4	16	4	1.24	-9.4	9.03
-3	16	4	10.13	14.73	3.37
-2	16	4	16.1	10.07	5.36
-1	16	4	6.56	3.39	5.44
-14	17	4	0.03	-1.59	11.83
-13	17	4	0.52	-21.53	9.53
-12	17	4	0.92	7.45	6.21
-11	17	4	1.16	-5.86	6.85
-10	17	4	1.09	-12.34	8.9
-9	17	4	0	1.31	9.11
-8	17	4	31.95	35.67	3.43
-7	17	4	0.53	-3.74	9.36
-6	17	4	1	-12.62	9.34
-5	17	4	25.15	30.93	5.4
-4	17	4	5.67	2.8	6.99
-3	17	4	10.37	-1.41	12.04
-11	18	4	0.06	10.09	9.53
-10	18	4	5.86	9.65	7.73
-9	18	4	0.87	-3.02	6.17
-8	18	4	7.21	-1.78	5.88
-7	18	4	14.02	7.18	10.49
0	1	5	2037.68	1338.63	167.28
-1	2	5	109.92	68.99	10.86
0	2	5	1389.78	997.53	315.11
-2	3	5	290.55	322.34	14.7
-1	3	5	5318.52	5506	64.86
0	3	5	262.99	216.86	6.32
-3	4	5	2594.54	2446.12	172.24
-2	4	5	5230.36	5025.44	62.05
-1	4	5	440.44	440.34	7.68
0	4	5	100.58	64.06	1.82
-4	5	5	171.26	201.42	5.66
-3	5	5	759.47	772.4	11.2
-2	5	5	1924.38	1915.45	23.97
-1	5	5	103.66	171.32	9.56
0	5	5	419.75	400.17	6.55
-5	6	5	19.64	25.91	1.7
-4	6	5	95.33	87.37	2.52
-3	6	5	570.65	585.51	9.56
-2	6	5	590.03	655.02	10.22
-1	6	5	2098.63	2234	27.95
0	6	5	12.88	10.7	2.37
-6	7	5	118.23	124.73	3.91
-5	7	5	256.25	253.26	9.69
-4	7	5	1.53	-8.5	4.85
-3	7	5	241.18	284.02	6.9
-2	7	5	160	132.44	3.85
-1	7	5	4.36	12.52	3.73
0	7	5	12.24	17.96	3.29
-7	8	5	46.58	63.78	2.12
-6	8	5	58.6	73.67	2.28
-5	8	5	52.5	69.4	2.06
-4	8	5	70.7	58.13	2.18
-3	8	5	40.06	45.55	2.28
-2	8	5	315.68	340.02	7.92
-1	8	5	62.38	60.93	2.15
0	8	5	44.3	41.81	2.37
-8	9	5	127.15	140.03	4.25
-7	9	5	165.4	148.32	7.23
-6	9	5	48.6	41.46	2.08
-5	9	5	84.85	88.71	3.66
-4	9	5	420.25	428.55	11.23
-3	9	5	82.56	116.29	3.38
-2	9	5	619.11	570.88	10.69
-1	9	5	223.59	253.26	8.89
0	9	5	35.63	42.1	2.03
-9	10	5	80.05	84.89	2.73
-8	10	5	8.17	2.68	6.31
-7	10	5	16.79	16.45	2.99
-6	10	5	198.96	225.98	7.37
-5	10	5	263.66	237.45	7.3
-4	10	5	46.6	43.45	2.34
-3	10	5	59.9	62.35	4.23
-2	10	5	139.58	144.44	4.18
-1	10	5	364.81	381.95	9.8
0	10	5	413.59	462.44	9.26
-10	11	5	178.68	157.65	5.92
-9	11	5	28.74	23.18	2.54
-8	11	5	170.39	171.45	6.78
-7	11	5	27.55	27.05	2.47
-6	11	5	274.28	246.36	7.37
-5	11	5	9.24	14.21	6.63
-4	11	5	0.09	3.12	3.99
-3	11	5	22.13	19.36	4.41
-2	11	5	115.51	109.41	4.72
-1	11	5	1.02	11.27	4.03
0	11	5	1.9	5.88	3.83
-11	12	5	16.05	12.39	2.73
-10	12	5	268.83	301.27	9.23
-9	12	5	11.81	10.62	6.67
-8	12	5	0.33	-3.99	7.36
-7	12	5	3.37	0.42	7.2
-6	12	5	270.1	260.78	11.99
-5	12	5	197.44	220.45	6.91
-4	12	5	10.23	14.28	3.11
-3	12	5	0.44	-13.14	7.49
-2	12	5	0.49	5.25	2.64
-1	12	5	1.93	4.73	4.21
0	12	5	5.89	8.41	4
-12	13	5	66.44	74.25	3.14
-11	13	5	41.6	44.25	2.95
-10	13	5	18.29	22.03	3.38
-9	13	5	9.3	22.37	2.81
-8	13	5	276.32	298.79	8.94
-7	13	5	166.08	194.68	6.01
-6	13	5	220.89	224.25	6.88
-5	13	5	0.6	9.77	4
-4	13	5	0.05	-18.16	11.12
-3	13	5	92.4	82.08	4.41
-2	13	5	49.16	61.46	2.94
-1	13	5	0.06	-10.86	7.94
0	13	5	0.02	0.55	4
-13	14	5	30.61	30.82	3.14
-12	14	5	0.44	-2.97	11.77
-11	14	5	50.64	53.22	3.04
-10	14	5	1.06	7.06	8.13
-9	14	5	2.2	10.54	8.01
-8	14	5	6.96	13.45	5.1
-7	14	5	7.01	2.7	4.17
-6	14	5	2.76	3.12	4.13
-5	14	5	0.31	-1.02	3.26
-4	14	5	19.2	11.45	11.43
-3	14	5	0.56	-4.36	5.68
-2	14	5	108.37	107.65	4.2
-1	14	5	10.02	11.53	4.69
0	14	5	0.59	0.56	5.61
-14	15	5	4.37	-0.93	10.94
-13	15	5	8.31	2.97	3.75
-12	15	5	4.25	10.38	3.68
-11	15	5	40.12	23.26	4.95
-10	15	5	3.89	-2.19	8.11
-9	15	5	13.2	16.6	3.38
-8	15	5	3.01	2.16	6.74
-7	15	5	0.11	-3.21	4.39
-6	15	5	37.41	41.54	9
-5	15	5	13.9	1.03	8.41

h	k	l	F_c^2	F_o^2	σF_o^2
-4	15	5	1.38	5.24	5.21
-3	15	5	6.79	6.92	4.73
-2	15	5	1.13	1.14	10.38
-1	15	5	1.06	6.69	5.11
0	15	5	3.71	-0.28	8.12
-15	16	5	0.16	-1.31	4.52
-14	16	5	7.86	7.17	5.34
-13	16	5	1.86	-2.85	5
-12	16	5	25.2	23.98	3.31
-11	16	5	5.81	0.53	4.78
-10	16	5	14.52	15.28	5.01
-9	16	5	0.78	-1.61	8.57
-8	16	5	30.72	34.02	3.21
-7	16	5	57.59	47.81	4.17
-6	16	5	0.01	-3.41	8.78
-5	16	5	16.38	18.8	3.71
-4	16	5	4.31	2.8	8.96
-3	16	5	0.11	-5.37	7.57
-2	16	5	4.06	4.27	4.25
-1	16	5	2.5	-2.66	9.8
-13	17	5	4.36	7.79	5.2
-12	17	5	0.03	-0.21	4.95
-11	17	5	1.29	0	9.19
-10	17	5	1.28	-5.49	10.58
-9	17	5	0.02	4.99	5.11
-8	17	5	23.03	28.25	3.44
-7	17	5	8.25	15.03	11.3
-6	17	5	1.64	-2.51	5.18
-5	17	5	8.44	2.1	9.65
-4	17	5	4.85	4.22	4.2
-10	18	5	1.6	13.76	5.96
-9	18	5	26.58	25.7	31.06
-8	18	5	2.7	1.1	17.05
0	0	6	4.86	13.9	2.58
0	1	6	1011.65	774.7	69.74
-1	2	6	33.68	37.53	8.86
0	2	6	3492.81	1717.48	914.48
-2	3	6	1305.63	1053.67	154.56
-1	3	6	227.34	313.5	6.47
0	3	6	13.29	13.75	3.88
-3	4	6	6080.58	4664.49	1170.54
-2	4	6	1107.41	937.3	33.48
-1	4	6	1800.17	1890.21	23.65
0	4	6	8391.75	7220.08	1159.99
-4	5	6	5.76	26.06	11.88
-3	5	6	5246.38	5508.66	65.36
-2	5	6	1679.53	1931.87	24.28
-1	5	6	329.65	401.94	7.73
0	5	6	1187.52	1317.32	15.18
-5	6	6	1161.68	1121.47	19.4
-4	6	6	1154.26	1193.69	16.26
-3	6	6	1747.45	1679.02	21.66
-2	6	6	535.34	536.89	9.17
-1	6	6	0.21	-1.3	4.01
0	6	6	5.46	-4.87	4.35
-6	7	6	667.87	727.22	11.6
-5	7	6	79.04	53.14	1.94
-4	7	6	625.51	614.54	10.25
-3	7	6	269.65	358.05	7.71
-2	7	6	1780.45	2025.46	25.91
-1	7	6	163.7	186.74	5.74
0	7	6	22.49	20.67	1.66
-7	8	6	81.1	89.91	2.92
-6	8	6	0.87	1.08	5.43
-5	8	6	267.36	317.36	7.68
-4	8	6	147.96	147.62	4.53
-3	8	6	316.22	313.09	7.65
-2	8	6	51.75	59.77	2.16
-1	8	6	29.1	32.67	2.11
0	8	6	216.69	211.41	5.79
-8	9	6	6.55	4.59	6.25
-7	9	6	7.22	8.75	5.46
-6	9	6	1.76	-4.31	5.88
-5	9	6	19.34	21.22	2.05
-4	9	6	0.96	-1.52	3.17
-3	9	6	306.6	312.37	13.51
-2	9	6	167.08	186.27	6.89
-1	9	6	42.1	41.92	2.56
0	9	6	2.45	-0.36	5.7
-9	10	6	118.71	122.07	3.95
-8	10	6	238.63	274.18	8.18
-7	10	6	330.42	345.77	11.22
-6	10	6	247.33	247.33	7.45
-5	10	6	88.88	97.64	3.05
-4	10	6	118.43	115.08	6.8
-3	10	6	520.44	497.62	10.83
-2	10	6	437.31	403.8	16.86
-1	10	6	5.79	-1.56	7.27
0	10	6	43.45	44.28	2.36
-10	11	6	122.03	142.76	4.36
-9	11	6	31.58	30.03	2.69
-8	11	6	187.51	173.51	5.36
-7	11	6	10.62	7.23	3.85
-6	11	6	400.49	396.57	12.24
-5	11	6	93.26	101.27	3.21
-4	11	6	1015.76	1121	17.52
-3	11	6	674.45	672.42	13.02
-2	11	6	349.27	353.39	17.16
-1	11	6	0.24	6.82	4.07
0	11	6	166	158.6	5.3
-11	12	6	13.99	8.77	3.38
-10	12	6	26.27	32.19	2.96
-9	12	6	136.32	130.56	3.66
-8	12	6	2.81	1.5	7.48
-7	12	6	92.01	74.29	2.92
-6	12	6	14.8	16.95	3.13
-5	12	6	104.46	98.55	3.05
-4	12	6	0.17	-1.36	4.78
-3	12	6	136.71	130.14	6.84
-2	12	6	9.67	11.58	3.21
-1	12	6	0.01	6.24	4.21
0	12	6	2.77	4.06	4.03
-12	13	6	3.15	-5.11	4.51
-11	13	6	21.09	23.75	6.73
-10	13	6	326.25	339.49	11.58
-9	13	6	428.11	436.64	11.48
-8	13	6	198.83	187.82	5.87
-7	13	6	357.39	378.2	12.51
-6	13	6	16.29	18.38	6.64
-5	13	6	19	10.35	5.78
-4	13	6	32.69	27.9	2.78
-3	13	6	24.1	25.27	2.81
-2	13	6	75.38	80.23	3.09
-1	13	6	21.88	26.85	10.3
0	13	6	80.75	84.8	2.77
-13	14	6	12.15	17.86	3.19
-12	14	6	0	-2.97	8.07
-11	14	6	0.05	-4.41	8.36
-10	14	6	32.65	35.31	3.02
-9	14	6	55.38	67.45	3.12
-8	14	6	83.95	86.47	5.12
-7	14	6	2.74	6.87	4.61
-6	14	6	0.78	2.04	8.31
-5	14	6	51.45	49.14	12.54
-4	14	6	76.48	88	3.16
-3	14	6	25.27	27.41	2.9
-2	14	6	63.9	65.65	3.21
-1	14	6	172.16	182.96	5.93
0	14	6	1.25	-4.31	7.6
-14	15	6	0.66	0.59	9.02
-13	15	6	0.1	-3.86	8.76
-12	15	6	0.31	-16.25	8.59
-11	15	6	5.04	2.29	5.14
-10	15	6	8.84	4.41	4.69
-9	15	6	20.32	20.38	4.41
-8	15	6	9.01	7.41	5.75
-7	15	6	1.63	-0.97	8.05
-6	15	6	51.61	46.92	7.38
-5	15	6	33.28	31.99	4.95
-4	15	6	68.92	81.79	3.75
-3	15	6	2.11	-8.03	8.73
-2	15	6	22.09	14.53	3.98
-1	15	6	71.51	60.48	7.28
0	15	6	18.77	10.82	6.33
-14	16	6	3.46	-5.29	5.41
-13	16	6	7.77	7.54	8.85
-12	16	6	3.21	6.58	8.73
-11	16	6	24.62	26.07	3.28
-10	16	6	7.76	7.82	3.81
-9	16	6	30.32	21.42	8.11
-8	16	6	19.6	12.81	4.6
-7	16	6	1.8	-10.68	9.21
-6	16	6	21.91	15.81	5.08
-5	16	6	16.07	4.74	7.89
-4	16	6	8.86	8.36	6.9
-3	16	6	15.2	14.53	5.43
-2	16	6	6.81	7.93	9.74
-13	17	6	0.13	-4.15	9.62
-12	17	6	1.24	-2.15	9.28
-11	17	6	8.62	3.09	9.28
-10	17	6	0.86	2.61	9.24
-9	17	6	3.72	4.14	9.32
-8	17	6	18.66	25.89	4.86
-7	17	6	40.12	43.89	5.73
-6	17	6	0.15	-7.48	9.63
-5	17	6	58.87	61.06	8.08
-4	17	6	0.82	2.82	5.01
0	1	7	623.55	589.71	40.89
-1	2	7	3471.69	1972.45	1002.37
0	2	7	405.14	318.96	66.05
-2	3	7	852.37	757.87	218.1
-1	3	7	2838.73	2761.15	168.41
0	3	7	189.66	114.13	36.85
-3	4	7	2522.53	1532.25	737.03
-2	4	7	189.48	254.09	36.17
-1	4	7	76.07	80.98	2.42
0	4	7	1313.3	1033.8	218.74
-4	5	7	1820.81	1964.8	24.9
-3	5	7	153.8	169.61	5.27
-2	5	7	164.78	199.2	5.93
-1	5	7	1479.74	1597.27	20.74
0	5	7	1297.93	1234.4	49.76
-5	6	7	687.59	734.06	11.52
-4	6	7	155.27	246.05	6.67
-3	6	7	2089.41	2112.76	26.72
-2	6	7	361.28	272.06	6.89
-1	6	7	80.12	71.41	3.14
0	6	7	161.46	160.01	4.18
-6	7	7	2.96	-2.27	5.35
-5	7	7	335.54	387.06	13.28
-4	7	7	109.24	152.12	4.61
-3	7	7	175.52	154.22	4.76
-2	7	7	27.61	33.52	1.99
-1	7	7	183.06	212.79	6.45
0	7	7	436.04	510.26	9.81
-7	8	7	0.16	-5.16	5.83
-6	8	7	278.39	282.62	13.82
-5	8	7	123.46	119.26	3.42
-4	8	7	484.22	487.73	9.74
-3	8	7	45.72	38.7	2.27
-2	8	7	34.86	31.56	2.14
-1	8	7	563.24	599.94	10.99
0	8	7	29.38	17.09	3.36
-8	9	7	48.59	47.66	2.36
-7	9	7	240.24	198.8	7.35
-6	9	7	43.05	53.05	2.27
-5	9	7	0.53	-0.39	3.27
-4	9	7	819.81	931.27	14.5
-3	9	7	157.9	156.49	6.99
-2	9	7	1792.11	1922.25	25.78
-1	9	7	382.78	376.21	14
0	9	7	3.65	2.27	5.8
-9	10	7	11.23	1.72	7.26
-8	10	7	99.34	109.66	3.11
-7	10	7	4.97	6.26	3.72
-6	10	7	169.77	194.48	6.04
-5	10	7	3.12	3.22	6.49
-4	10	7	183.6	168.03	5.14
-3	10	7	1323.85	1251.78	18.86
-2	10	7	829.12	891.66	15.13
-1	10	7	156.29	131.45	3.79
0	10	7	753.23	812.13	12.49
-10	11	7	175.45	182.62	6.01
-9	11	7	27.26	48.68	2.88
-8	11	7	987.47	1083.05	17.28
-7	11	7	29.3	27.88	4.27
-6	11	7	733.23	686.15	12.91
-5	11	7	10.4	12.7	3.06
-4	11	7	9.39	8.74	3.19
-3	11	7	16.49	0.41	8.05
-2	11	7	9.46	12.66	3.4
-1	11	7	115.44	110.8	3.48
0	11	7	110.51	109.35	3.02
-11	12	7	101.76	93.68	4.42
-10	12	7	1456.9	1461.11	22.19
-9	12	7	4.81	9.92	2.95
-8	12	7	1.01	1.72	4.33
-7	12	7	55.83	68.43	2.98
-6	12	7	20.2	14.23	7.68
-5	12	7	93.67	80.75	2.96
-4	12	7	25.62	35.23	4.22
-3	12	7	22.93	22.79	5.82
-2	12	7	168.63	152.41	4.88
-1	12	7	49.8	42.5	2.85
0	12	7	21.6	27.43	2.47
-12	13	7	120.13	113.28	3.68
-11	13	7	17.08	5.17	5.47
-10	13	7	74.92	72.48	4.64
-9	13	7	16.62	30.04	4.39
-8	13	7	11.12	31.78	3.03
-7	13	7	767.26	802.03	23.45
-6	13	7	187.19	178.23	5.84
-5	13	7	3.84	0.44	7.72
-4	13	7	83.85	92.65	3.27
-3	13	7	32.42	24.72	3.41
-2	13	7	21.07	33.15	5.91
-1	13	7	132.31	126.06	5.09
0	13	7	21.39	23	8.21
-13	14	7	11	7.74	9.51
-12	14	7	6.27	12.17	4.78
-11	14	7	7.15	-3.35	8.24
-10	14	7	8.1	1.9	10.13
-9	14	7	13.57	4.51	7.61
-8	14	7	0.09	-7.48	8.17
-7	14	7	21.51	24.48	6.15
-6	14	7	57.75	67.89	3.02
-5	14	7	18.56	16.67	2.83
-4	14	7	0.64	-6.37	9.53
-3	14	7	1.74	-2.38	3.36
-2	14	7	90.8	100.68	3.55
-1	14	7	2.34	1.18	8.89
0	14	7	0.34	0.71	4.76
-14	15	7	1.69	4.52	5.06
-13	15	7	8.74	11.72	5.12
-12	15	7	0.2	2.41	8.73
-11	15	7	7.4	1.36	8.66
-10	15	7	10.22	12.43	4.74
-9	15	7	5.44	-3.98	8.53
-8	15	7	9.47	16.72	10.47
-7	15	7	30.85	40.5	3.19
-6	15	7	74.79	77.62	10.01
-5	15	7	12.24	8.02	8.66
-4	15	7	9.69	21.47	4.86
-3	15	7	12.87	12.18	3.79
-2	15	7	0.07	-8.91	8.97
-1	15	7	0.1	-6.34	9.39
0	15	7	4.22	0.98	8.34
-14	16	7	7.33	10.32	7.68
-13	16	7	0.76	-21.71	10.03
-12	16	7	0.71	6.23	5

h	k	l	F_c^2	F_o^2	σF_o^2
-11	16	7	0	-4.03	6.11
-10	16	7	5.4	4.16	5.05
-9	16	7	23.32	27.26	3.31
-8	16	7	23.58	17.67	6.21
-7	16	7	50.56	51.37	3.46
-6	16	7	35.63	32.81	9.1
-5	16	7	37.5	45.31	3.46
-4	16	7	6.13	2.04	6.09
-3	16	7	23.35	32.47	6.06
-2	16	7	23.47	15.6	7.11
-12	17	7	19.19	21.08	4.21
-11	17	7	0.01	-4	9.35
-10	17	7	0.05	2.49	9.26
-9	17	7	0.06	8.49	5.15
-8	17	7	0.01	10.45	4.25
-7	17	7	8.47	9.53	5.37
-6	17	7	4.12	10.6	5.53
-5	17	7	0	-17.85	9.95
0	0	8	5122.74	4728.73	97.42
0	1	8	70.11	45.46	5.8
-1	2	8	23.77	23.41	8.99
0	2	8	121.42	104.54	20.06
-2	3	8	695.26	534.5	143.24
-1	3	8	255.1	269.68	10.3
0	3	8	4.72	2.15	1.96
-3	4	8	2578.42	1450.59	830.67
-2	4	8	68.5	72.24	11.3
-1	4	8	3302.2	3495.82	42.38
0	4	8	10.88	0.66	4.24
-4	5	8	563.72	524.64	14.45
-3	5	8	189.79	187.98	5.76
-2	5	8	37.77	35.52	1.85
-1	5	8	426.71	438.78	8.53
0	5	8	303.8	222.33	23.81
-5	6	8	58.4	53.4	2.04
-4	6	8	647.71	694.57	11.12
-3	6	8	7.01	4.07	2.79
-2	6	8	2.07	5.12	2.49
-1	6	8	1078.55	1249.33	17.37
0	6	8	65.5	58.45	1.98
-6	7	8	0.74	-4.4	5.7
-5	7	8	280.91	322.8	8.96
-4	7	8	662.78	701.17	11.46
-3	7	8	39.65	51.4	3.38
-2	7	8	1798.27	2115.68	27.29
-1	7	8	286.51	310.4	8.11
0	7	8	1.71	-0.31	4.8
-7	8	8	105.37	102.97	3.12
-6	8	8	242.26	272.4	11.28
-5	8	8	190.73	211.09	7.92
-4	8	8	52.07	52.54	2.21
-3	8	8	290.31	278.5	7.93
-2	8	8	2.02	3.8	3.3
-1	8	8	156.25	165.81	7.07
0	8	8	48.45	51.57	2.06
-8	9	8	4.04	11.52	3.66
-7	9	8	262.73	245.95	7.66
-8	9	8	126.94	137.68	4.12
-5	9	8	45.6	41.81	2.46
-4	9	8	125.79	115.6	5.03
-3	9	8	206.82	219.06	10.71
-2	9	8	3.62	8.96	4.17
-1	9	8	129.92	150.69	4.57
0	9	8	5.43	-8.59	8.51
-9	10	8	448.95	496.19	15.73
-8	10	8	120.53	135.49	5.49
-7	10	8	619.99	615.12	12.08
-6	10	8	250.82	253.75	7.64
-5	10	8	529.78	627.23	18
-4	10	8	5.62	11.89	4.83
-3	10	8	0.02	-5.3	7.5
-2	10	8	114.84	100.35	3.12
-1	10	8	116.66	117.19	3.71
0	10	8	23.61	11.31	5.7
-10	11	8	56.5	82.2	3.2
-9	11	8	3.18	-9.48	8.09
-8	11	8	12.2	5.14	5.5
-7	11	8	405.06	377.07	10.35
-6	11	8	171	160.42	8.21
-5	11	8	0.24	-16.53	8.57
-4	11	8	87.35	119.66	3.63
-3	11	8	946.56	1008.16	16.68
-2	11	8	23.47	19.62	2.75
-1	11	8	19.73	20.23	11.22
0	11	8	59.25	57.34	2.52
-11	12	8	30.92	44.43	2.97
-10	12	8	9.68	3.06	7.32
-9	12	8	56.46	73.88	3.16
-8	12	8	3.85	6.51	4.53
-7	12	8	120.79	112.89	5.85
-6	12	8	6.7	8.18	4.25
-5	12	8	45.43	43.55	2.82
-4	12	8	115.94	150.62	6.42
-3	12	8	8.36	8.77	4.37
-2	12	8	3.17	-5	7.6
-1	12	8	5.34	5.17	4.23
0	12	8	4.75	5.67	4.18
-12	13	8	12.16	4.79	5.85
-11	13	8	7.01	-9.19	8.3
-10	13	8	236.1	239.88	7.37
-9	13	8	536.31	580.09	13.19
-8	13	8	10.19	7.26	8.59
-7	13	8	133.54	152.13	4.82
-6	13	8	10.71	9.05	4.26
-5	13	8	17.29	16.88	3.27
-4	13	8	13.57	15.84	3.94
-3	13	8	35.47	35.29	2.84
-2	13	8	5.61	1.28	4.4
-1	13	8	21.94	30.98	2.96
0	13	8	81.42	86.6	3.03
-13	14	8	65.4	76.52	3.54
-12	14	8	12.68	3.31	8
-11	14	8	92.21	99.25	3.5
-10	14	8	5.62	-6.12	8.81
-9	14	8	1.6	2.42	5
-8	14	8	159.32	154.84	4.76
-7	14	8	0.57	-1.43	7.99
-6	14	8	28.8	32.41	5.66
-5	14	8	0.05	4.79	7.9
-4	14	8	26.68	33.26	2.93
-3	14	8	6.9	6.72	4.69
-2	14	8	60.65	60.11	3.41
-1	14	8	81.9	87.03	4.17
0	14	8	12.44	4.55	5.38
-14	15	8	0.01	-0.81	9.27
-13	15	8	14.83	15.81	7.33
-12	15	8	16.78	21.65	4.53
-11	15	8	16.14	19.22	3.23
-10	15	8	19.07	26.05	3.2
-9	15	8	71.52	90.05	5.98
-8	15	8	0.09	2.66	8.74
-7	15	8	15.93	15.93	5.66
-6	15	8	60.26	66.76	5.78
-5	15	8	24.53	23.14	6.25
-4	15	8	80.73	82.85	3.55
-3	15	8	31.39	28.94	3.42
-2	15	8	38.39	35.82	3.52
-1	15	8	18.88	21.89	4.91
0	15	8	8.43	4.54	5.52
-13	16	8	0.07	3.88	8.1
-12	16	8	0.79	6.08	5.06
-11	16	8	3.15	10.34	3.85
-10	16	8	26.22	14.25	12.05
-9	16	8	18.93	13.48	7.89
-8	16	8	25.18	30.97	3.39
-7	16	8	1.46	2.82	5.22
-6	16	8	1.86	-3.85	5.98
-5	16	8	0.07	-9.15	9.97
-4	16	8	17.54	25.56	9.43
-3	16	8	13.06	1.03	9.86
-11	17	8	16.98	4.32	7.28
-10	17	8	0.02	1.64	7.95
-9	17	8	16.05	16.17	4.21
-8	17	8	10.02	0.02	9.86
-7	17	8	62.21	71.78	3.85
-6	17	8	15.17	10.47	12.24
0	1	9	35.3	48.81	4.25
-1	2	9	383.57	196.45	116.17
0	2	9	0	-5.3	4.15
-2	3	9	802.34	389.67	149.2
-1	3	9	172.26	148.61	19.85
0	3	9	1095.97	759.42	310.76
-3	4	9	2017.59	1277	710.9
-2	4	9	534.25	412.73	141.02
-1	4	9	3.63	5.05	2.74
0	4	9	77.47	89.13	15.22
-4	5	9	773.45	792.17	12.24
-3	5	9	1068.59	1126.11	15.82
-2	5	9	888.96	649.43	10.69
-1	5	9	18.87	24	5.14
0	5	9	255.48	224.43	39.56
-5	6	9	2044.87	2011.38	36.76
-4	6	9	10.7	3.85	2.28
-3	6	9	66.68	73.4	2.63
-2	6	9	154.11	132.44	4.3
-1	6	9	4.57	13.85	6.26
0	6	9	162.07	176.83	9.17
-6	7	9	58.88	55.34	2.21
-5	7	9	251.01	257.48	7.58
-4	7	9	190.09	226.26	6.79
-3	7	9	588.89	622.58	11.41
-2	7	9	8.73	2.94	6.01
-1	7	9	527.51	560.8	10.66
0	7	9	17.02	17.34	2.09
-7	8	9	77.42	81.66	6.72
-6	8	9	140.38	136.21	3.91
-5	8	9	30.7	28.72	2.16
-4	8	9	104	96.55	3.28
-3	8	9	239.75	236.57	7.18
-2	8	9	56.68	54.86	2.35
-1	8	9	82.61	57.66	2.49
0	8	9	318.24	305.08	7.63
-8	9	9	59.07	54.73	2.65
-7	9	9	23.97	8.95	3.81
-6	9	9	255.88	273.95	8.33
-5	9	9	96.73	86.27	4.82
-4	9	9	2.9	-0.21	6.59
-3	9	9	21.77	30.59	2.39
-2	9	9	42.23	59.32	2.97
-1	9	9	0.23	-0.96	8.59
0	9	9	196.3	177.24	5.81
-9	10	9	14.01	8.15	8.79
-8	10	9	460.45	539.72	11.65
-7	10	9	11.71	20.58	2.61
-6	10	9	187.02	211.09	6.83
-5	10	9	0	0.87	3.89
-4	10	9	7.03	14.73	5.82
-3	10	9	0.83	7.52	8.24
-2	10	9	15.74	23.81	2.65
-1	10	9	8.25	14.22	4.14
0	10	9	664.74	733.69	12.09
-10	11	9	271.15	286.5	8.95
-9	11	9	3.24	6.37	7.86
-8	11	9	496.3	522.58	11.9
-7	11	9	0.89	-5.36	7.63
-6	11	9	174.22	191.59	5.9
-5	11	9	37.06	34.25	2.74
-4	11	9	66.16	63.07	2.87
-3	11	9	13.19	2.81	7.65
-2	11	9	58.57	53.06	2.86
-1	11	9	29.95	25.86	2.74
0	11	9	2.46	-1.9	6.67
-11	12	9	10.33	4.54	3.36
-10	12	9	240.02	246.77	7.27
-9	12	9	46.38	42.3	3.29
-8	12	9	133.27	137.25	4.57
-7	12	9	107.6	142	4.58
-6	12	9	45.29	58.55	2.89
-5	12	9	78.52	82.38	3.01
-4	12	9	4.14	6.37	4.74
-3	12	9	80.49	87.74	3.03
-2	12	9	25.14	19.22	4.98
-1	12	9	18.48	17.5	2.78
0	12	9	60.33	69.39	2.67
-12	13	9	0.88	-15.51	8.48
-11	13	9	79.88	74.18	4.71
-10	13	9	35.23	29.37	2.96
-9	13	9	96.13	85.68	3.25
-8	13	9	50.31	42.66	3.02
-7	13	9	102.23	104.42	3.34
-6	13	9	21.11	16.29	2.77
-5	13	9	16.49	19.59	5.65
-4	13	9	75.33	69.4	3.01
-3	13	9	22.13	14.59	3.36
-2	13	9	0.01	-0.61	7.82
-1	13	9	88.53	104.19	3.67
0	13	9	37.21	29.3	7.17
-13	14	9	19.33	20.34	7.44
-12	14	9	0.12	0.99	6.25
-11	14	9	10.24	11.15	5.03
-10	14	9	18.1	15.93	3.13
-9	14	9	138.27	148.06	6.87
-8	14	9	2.95	-2.24	11.42
-7	14	9	46.06	61.43	3.64
-6	14	9	0.01	0.56	7.99
-5	14	9	5.18	3.33	6.72
-4	14	9	1.14	-4.38	8.34
-3	14	9	39.65	48.77	3.5
-2	14	9	27.86	29.26	9.11
-1	14	9	16.14	18.09	7.05
0	14	9	1.51	3.04	9.55
-14	15	9	13.13	12.57	4.21
-13	15	9	5.55	-1.66	9.15
-12	15	9	10.16	8.3	9.14
-11	15	9	24.01	21.49	8.06
-10	15	9	4.67	10.87	3.74
-9	15	9	5.23	4.06	5
-8	15	9	6.96	4.13	8.75
-7	15	9	15.45	10.81	8.97
-6	15	9	16.1	-2.82	8.98
-5	15	9	0.03	-11.37	8.74
-4	15	9	4.43	2.65	4.98
-3	15	9	0.25	-9.33	9.13
-2	15	9	2.08	4.76	5.27
-1	15	9	0.07	2.97	4.26
-13	16	9	8.44	15.12	5.35
-12	16	9	0	-15.44	9.43
-11	16	9	6.44	0.06	8.31
-10	16	9	0.77	0.37	9.11
-9	16	9	24.21	26.18	10.08
-8	16	9	3.86	3.88	6.56
-7	16	9	11.16	17.95	4.19
-6	16	9	40.8	44.08	10.57
-5	16	9	26.31	29.99	8.88
-4	16	9	6.81	3.39	9.63
-3	16	9	7.31	3.14	9.98
-9	17	9	0	-1.22	6.93
-8	17	9	19.26	10.66	13.19
0	0	10	1073.61	1057.05	25.57
0	1	10	69.88	45.98	2.22
-1	2	10	78.42	104.62	25.45
0	2	10	3.19	-1.94	5.55
-2	3	10	96.23	119.45	30.46
-1	3	10	323.87	267.17	64.86
0	3	10	726.7	472.03	187.89
-3	4	10	55.07	64.27	15.82
-2	4	10	408.72	243.47	115.76
-1	4	10	187.99	217.51	24.99
0	4	10	53.76	62.9	8.76
-4	5	10	10.28	14.8	1.93

h	k	l	F_c^2	F_o^2	σF_o^2
-3	5	10	58.66	69.12	2.3
-2	5	10	100.33	102.39	5.48
-1	5	10	89.16	84.21	2.41
0	5	10	11.55	9.38	1.97
-5	6	10	26.57	26.27	2.1
-4	6	10	502.2	513.41	9.9
-3	6	10	428.07	414.2	8.92
-2	6	10	29.64	16.8	7.11
-1	6	10	128.8	139.65	4.39
0	6	10	93.82	119.99	3.19
-6	7	10	18.36	11.01	4.14
-5	7	10	344.04	326.73	10.14
-4	7	10	323.4	342.8	8.57
-3	7	10	86.37	84.91	2.62
-2	7	10	318.29	349.34	10.56
-1	7	10	2.76	-0.83	5.3
0	7	10	427.27	420.42	8.37
-7	8	10	1.13	0.51	3.72
-6	8	10	21.5	21.31	2.39
-5	8	10	170.09	163.56	5.51
-4	8	10	227.57	227.06	6.99
-3	8	10	6.04	5.52	2.61
-2	8	10	267.27	306.8	8.69
-1	8	10	9.96	3.51	6.91
0	8	10	74.19	81.91	2.82
-8	9	10	16.79	20.58	2.57
-7	9	10	41.33	50.03	2.64
-6	9	10	30.99	26.56	2.52
-5	9	10	244.15	257.93	8.13
-4	9	10	16.44	8.76	7.03
-3	9	10	32.39	22.62	6.58
-2	9	10	6.84	3.37	4.51
-1	9	10	112.44	110.3	3.14
0	9	10	44.03	57.65	2.42
-9	10	10	259.83	248.17	7.89
-8	10	10	2.52	1.54	7.45
-7	10	10	45.25	54.01	3.3
-6	10	10	14.97	20.55	3.31
-5	10	10	607.83	640.33	12.59
-4	10	10	129.57	145.69	4.33
-3	10	10	3.34	3.17	7.23
-2	10	10	27.88	24.16	2.63
-1	10	10	18.86	26.04	2.69
0	10	10	25.84	30.9	5.42
-10	11	10	0.15	-0.04	7.64
-9	11	10	2.48	0.55	3.22
-8	11	10	36.98	34.32	2.77
-7	11	10	127.61	134.65	3.8
-6	11	10	154.4	153.81	4.95
-5	11	10	18.34	22.05	6.6
-4	11	10	15.64	5.01	7.61
-3	11	10	21.37	33.96	2.71
-2	11	10	164	154.96	4.85
-1	11	10	5.13	7.25	4.14
0	11	10	1.98	-1.4	3.08
-11	12	10	0.95	-1.98	9.23
-10	12	10	27.96	30.16	2.85
-9	12	10	42.84	45.09	2.88
-8	12	10	65.33	73.25	3.15
-7	12	10	2.95	8.85	7.73
-6	12	10	1.37	-2.61	7.45
-5	12	10	32.98	34.87	2.76
-4	12	10	70.14	71.92	2.93
-3	12	10	103.25	105.3	3.85
-2	12	10	12.53	10.03	4.63
-1	12	10	3.37	2.14	8
0	12	10	5.69	4.59	4.18
-12	13	10	7.73	5.76	4.89
-11	13	10	0.03	3.95	8.5
-10	13	10	2.86	-2.23	7.8
-9	13	10	2.06	-2.16	8.08
-8	13	10	7.45	11.44	8.11
-7	13	10	6.82	7.23	3.85
-6	13	10	7.56	9.85	4.26
-5	13	10	16.01	30.59	3.53
-4	13	10	3.12	5.26	4.25
-3	13	10	0.68	4.51	4.33
-2	13	10	1.07	2.82	4.65
-1	13	10	3.24	-1.51	8.5
0	13	10	23.51	16.99	6.75
-13	14	10	0.07	-0.64	6.02
-12	14	10	33.06	40.14	3.37
-11	14	10	85.58	88.98	3.57
-10	14	10	1.79	-2.44	8.73
-9	14	10	22.21	25.21	3.18
-8	14	10	33.2	36.08	3.17
-7	14	10	0.47	-3.58	8.31
-6	14	10	16.77	11.16	3.1
-5	14	10	2.48	0.71	9.44
-4	14	10	10.55	12	3.1
-3	14	10	8.61	17.27	4.85
-2	14	10	3	-0.59	8.83
-1	14	10	29.92	37.63	12.73
0	14	10	7.52	6.3	8.14
-14	15	10	0	-12.73	16.67
-13	15	10	2.56	-11.8	9.85
-12	15	10	0.09	1.5	6.22
-11	15	10	43.48	55.84	5.65
-10	15	10	0.51	-0.07	8.72
-9	15	10	33.38	23.76	4.74
-8	15	10	3.41	1.32	8.87
-7	15	10	0.13	-7.48	8.75
-6	15	10	0.05	2.63	4.92
-5	15	10	0.03	-5.06	5.84
-4	15	10	1.72	2.41	5.02
-3	15	10	2.18	3.45	9.26
-2	15	10	0.72	-4.88	10.46
-12	16	10	1.43	-3.41	9.56
-11	16	10	3.86	-3.95	9.61
-10	16	10	18.63	16.48	6.67
-9	16	10	6.38	6.97	3.41
-8	16	10	8.39	15.68	5.33
-7	16	10	0.5	1.58	9.35
-6	16	10	0.71	10.89	9.31
-5	16	10	0.02	9.9	9.56
-4	16	10	4.44	6.9	5.49
0	1	11	263.39	261.43	14.85
-1	2	11	284.64	142.97	74.97
0	2	11	251.07	226.64	48.82
-2	3	11	452.4	262.55	159.73
-1	3	11	98.63	80.45	16.31
0	3	11	7.47	8.78	2.25
-3	4	11	351.69	229.79	110.9
-2	4	11	70.65	66.9	15.05
-1	4	11	6.21	3.36	2.94
0	4	11	6.07	0.32	3.14
-4	5	11	3.13	4.45	5.65
-3	5	11	0.19	-12.16	5.73
-2	5	11	4.64	3.69	4.65
-1	5	11	24.38	35.72	2.06
0	5	11	113.11	119.65	22.85
-5	6	11	13.07	6.18	6.81
-4	6	11	143.24	167.68	8.2
-3	6	11	280.23	271.16	7.81
-2	6	11	18.2	24.02	2.08
-1	6	11	4.37	5.57	3.31
0	6	11	0.85	-3.52	5.48
-6	7	11	748.65	767.01	13.17
-5	7	11	260.01	232.93	8.71
-4	7	11	58.63	60.77	3.92
-3	7	11	53.49	53.22	2.31
-2	7	11	51.16	43.67	2.3
-1	7	11	6.83	7.91	2.67
0	7	11	22.82	33.18	2.16
-7	8	11	11.2	5.38	3.9
-6	8	11	440.47	532.94	14.55
-5	8	11	230.75	245.96	17.17
-4	8	11	164.72	178.37	9.81
-3	8	11	173.84	178.68	5.56
-2	8	11	54.67	69.1	3.05
-1	8	11	2.37	-7.64	7.11
0	8	11	70.07	57.04	2.37
-8	9	11	68.24	83	4.25
-7	9	11	140.97	130.79	4.11
-6	9	11	458.27	479.73	10.98
-5	9	11	169.95	169.85	5.22
-4	9	11	0.14	4.9	6.94
-3	9	11	154.9	142.31	4.4
-2	9	11	198.34	193.75	6.14
-1	9	11	17.63	9.84	3.73
0	9	11	0.32	3.34	4.72
-9	10	11	46.99	54.59	3.21
-8	10	11	0.63	6.19	7.26
-7	10	11	0.54	0.76	4.02
-6	10	11	20.93	22.73	2.6
-5	10	11	162.34	177.08	5.45
-4	10	11	58.69	60.43	3.29
-3	10	11	1.61	7.34	2.99
-2	10	11	0.18	-1.8	4
-1	10	11	0.02	-6.26	7.33
0	10	11	42.71	48.05	2.43
-10	11	11	38.21	31.5	2.96
-9	11	11	18.06	22.51	3.6
-8	11	11	3.87	6.61	7.38
-7	11	11	27.31	26.07	3.92
-6	11	11	13.75	17.45	7.63
-5	11	11	46.17	44.26	2.73
-4	11	11	4.84	-0.09	6.57
-3	11	11	7.44	4.5	4.97
-2	11	11	0.62	-3.24	4.08
-1	11	11	3	0.24	4.16
0	11	11	2.58	3.95	6.64
-11	12	11	37.21	33.14	2.9
-10	12	11	1.29	-1.24	4.35
-9	12	11	1.71	-11.26	7.88
-8	12	11	2.31	1.06	7.57
-7	12	11	29.66	25.95	2.72
-6	12	11	0.39	3.41	4.13
-5	12	11	1.21	5.17	4.05
-4	12	11	47.75	51.76	2.85
-3	12	11	1.07	-7.45	7.74
-2	12	11	9.68	10.1	4.5
-1	12	11	3.44	-0.56	7.98
0	12	11	11.6	0.29	7.33
-12	13	11	24.49	32.03	3.28
-11	13	11	17.3	21.07	3.18
-10	13	11	19.71	13.57	8.57
-9	13	11	54.01	60.74	3.41
-8	13	11	7.05	-14.13	8.02
-7	13	11	2.7	6.21	5.01
-6	13	11	0.15	-4.12	7.87
-5	13	11	1.13	5.35	7.28
-4	13	11	7.11	7.56	7.96
-3	13	11	17.97	14.27	4.66
-2	13	11	1.06	6.07	8.4
-1	13	11	5.95	-6.93	8.8
0	13	11	30.18	28.46	2.89
-13	14	11	0.31	-15.54	10.02
-12	14	11	11.5	18.88	10.92
-11	14	11	38.43	33.82	6.48
-10	14	11	0.72	-3.62	8.79
-9	14	11	33.31	45.22	5.09
-8	14	11	0.39	-8.66	8.42
-7	14	11	1.22	-5.21	9.21
-6	14	11	11.31	-4.15	8.56
-5	14	11	5.94	0.18	8.64
-4	14	11	0.07	-9.08	8.62
-3	14	11	0.87	1.65	8.69
-2	14	11	0.8	5.23	6.83
-1	14	11	0.32	-3.47	9.34
0	14	11	5.62	4.8	4.83
-13	15	11	9.04	10.73	5.46
-12	15	11	0.42	-11.58	8.51
-11	15	11	0.15	8.4	9.19
-10	15	11	1.03	-1.89	9.2
-9	15	11	4.41	8.85	5.98
-8	15	11	0.27	-6.89	8.9
-7	15	11	1.61	4.83	8.79
-6	15	11	0.44	7.3	3.86
-5	15	11	0.41	-0.98	6.96
-4	15	11	0	-2.6	13.41
-3	15	11	0.33	2.16	9.35
-2	15	11	1.45	-3.55	9.63
-11	16	11	3.57	2.26	16.22
-10	16	11	3.85	7.61	4.18
-9	16	11	3.95	5.24	9.51
-8	16	11	11.77	13.07	4.12
-7	16	11	20.99	28.46	4.14
-6	16	11	1.32	-10.34	9.51
0	0	12	5235.17	4322.3	91.21
0	1	12	2.98	0.5	5.23
-1	2	12	78.43	82.19	21.04
0	2	12	45.6	23.61	7.39
-2	3	12	1.55	3.38	5.71
-1	3	12	7.78	11	3.17
0	3	12	7.68	3.24	2.29
-3	4	12	103.7	83.1	21.76
-2	4	12	27.96	33.19	7.67
-1	4	12	20.27	27.08	5.9
0	4	12	12.51	4.16	5.74
-4	5	12	26.24	22.43	5.7
-3	5	12	94.76	95.01	3.04
-2	5	12	45.73	33.89	2.13
-1	5	12	43.27	31.81	2.16
0	5	12	15.45	16.8	4.62
-5	6	12	25.51	20.37	2.38
-4	6	12	32.92	30.18	2.22
-3	6	12	106.6	102.55	3.77
-2	6	12	48.48	43.1	2.25
-1	6	12	8.3	5.81	3.4
0	6	12	89.28	83.72	2.75
-6	7	12	141.41	181.92	5.54
-5	7	12	521.95	519.95	11.08
-4	7	12	0.19	1.39	7.41
-3	7	12	6.61	11.67	3.63
-2	7	12	25.71	25.69	2.4
-1	7	12	0.26	5.78	3.7
0	7	12	34.85	37.41	2.29
-7	8	12	450.85	458.12	16.83
-6	8	12	97.03	113.63	3.37
-5	8	12	31.39	40.57	2.7
-4	8	12	367.9	374.85	14.35
-3	8	12	57.6	67.36	3.07
-2	8	12	15.3	12.85	4.23
-1	8	12	180.45	191.35	6.28
0	8	12	9.24	-4.5	7.7
-8	9	12	39.28	43.09	2.71
-7	9	12	183.1	169.99	8.94
-6	9	12	113.52	121.19	4.16
-5	9	12	9.03	-0.65	7.34
-4	9	12	52.8	47.13	3.77
-3	9	12	23.26	18.43	3.47
-2	9	12	4.85	5.64	7.05
-1	9	12	2.28	6.82	7.23
0	9	12	0.03	3.15	6.29
-9	10	12	3.92	-9.35	7.32
-8	10	12	52.57	45.18	2.73
-7	10	12	109.81	103.81	3.15
-6	10	12	3.87	4.82	4.01
-5	10	12	1.27	-2.03	7.24
-4	10	12	32.99	34.39	2.62
-3	10	12	2.19	-0.82	6.22
-2	10	12	0.13	1.69	3.91
-1	10	12	5.67	-1.35	7.43
0	10	12	0.73	0.9	6.51
-10	11	12	33.86	20.06	9.83
-9	11	12	16.82	14.69	4.15
-8	11	12	46.43	39.18	2.77
-7	11	12	0.7	-5.98	7.46
-6	11	12	101.17	104.98	3.29

h	k	l	F_c^2	F_o^2	σF_o^2
-5	11	12	0	-2.15	6.89
-4	11	12	9.14	-5.42	7.52
-3	11	12	29.6	37.14	2.74
-2	11	12	1.79	-0.58	7.5
-1	11	12	1.79	6.03	7.77
0	11	12	3.37	-0.66	4.06
-11	12	12	0.38	-4.28	11.13
-10	12	12	15.81	-3.12	8.01
-9	12	12	63.88	66.4	5.11
-8	12	12	3.79	-3.97	7.81
-7	12	12	11.16	1.28	10.62
-6	12	12	0.33	-6.53	7.74
-5	12	12	1.57	-3.7	7.71
-4	12	12	3.51	10.68	3.26
-3	12	12	0.01	-3.09	8.9
-2	12	12	6.7	2.65	6.8
-1	12	12	22.87	22.71	3.71
0	12	12	0.1	-5.66	7.36
-12	13	12	27.1	31.7	3.31
-11	13	12	17.25	15.14	4.87
-10	13	12	0.67	-6.93	11.99
-9	13	12	1.75	4.06	4.7
-8	13	12	20.68	24.98	5.7
-7	13	12	10.55	8.13	8.33
-6	13	12	0	0.18	4.54
-5	13	12	1.22	1.46	3.54
-4	13	12	2.19	-3.27	8.43
-3	13	12	22.91	21.29	6.5
-2	13	12	1.59	-2.58	8.65
-1	13	12	11.16	5.9	5.11
0	13	12	3.57	0.23	8.03
-13	14	12	0.01	9.15	5.19
-12	14	12	0.15	-2.08	5.07
-11	14	12	11.89	15.54	12.13
-10	14	12	5.51	7.7	8.96
-9	14	12	13.27	1.31	8.86
-8	14	12	7.42	1.99	4.93
-7	14	12	2.46	3.24	8.55
-6	14	12	1.61	-2.91	4.85
-5	14	12	3.33	-0.29	8.67
-4	14	12	1.38	-18.25	8.96
-3	14	12	10.51	10.88	11.69
-2	14	12	15.32	12.04	4.01
-1	14	12	13.51	21.13	4.15
-12	15	12	5.03	8.1	5.96
-11	15	12	0.44	1.23	9.34
-10	15	12	0	-8.45	9.61
-9	15	12	0.1	-9.93	8.68
-8	15	12	35.7	38.59	3.47
-7	15	12	0.73	-1.79	9.16
-6	15	12	4.68	10.62	5.78
-5	15	12	0.25	-10.16	6.16
-4	15	12	10.18	12.17	5.27
-3	15	12	4.43	-0.04	5.45
0	1	13	357.28	374.3	15.3
-1	2	13	194.81	171.92	56.95
0	2	13	390.02	259.74	69.22
-2	3	13	246.4	158.49	64.66
-1	3	13	0.1	5.19	6.07
0	3	13	139.76	102.72	20.31
-3	4	13	125.34	116.21	27.79
-2	4	13	12.99	4.02	6.12
-1	4	13	8.91	5.81	4.29
0	4	13	22.51	12.25	4.78
-4	5	13	11.46	14.79	2.18
-3	5	13	7.44	14.49	3.4
-2	5	13	0.99	-1.32	3.31
-1	5	13	1.12	4.64	2.6
0	5	13	18.71	5.34	3.72
-5	6	13	68.48	69.83	2.67
-4	6	13	16.29	3.43	3.46
-3	6	13	12.87	5.78	3.77
-2	6	13	13.25	14.97	7.91
-1	6	13	12.29	10.64	4.06
0	6	13	93.9	112.25	2.76
-6	7	13	239.26	252.04	7.83
-5	7	13	189.51	171.68	5.56
-4	7	13	30.64	30.97	2.59
-3	7	13	102.64	93.65	3.23
-2	7	13	1.46	3.71	3.73
-1	7	13	0	-11.37	11.08
0	7	13	86.03	77.24	2.57
-7	8	13	0.06	-4.64	4
-6	8	13	1.83	1.16	4.49
-5	8	13	0.65	3.96	4.1
-4	8	13	11.83	17.49	2.58
-3	8	13	4	1.79	3.79
-2	8	13	8.39	13.84	2.92
-1	8	13	8.24	-8.2	7.17
0	8	13	0.17	-6.45	6.36
-8	9	13	9.07	4.84	7.39
-7	9	13	20.52	39	2.7
-6	9	13	19.26	17.51	3.01
-5	9	13	46.51	54.89	2.77
-4	9	13	29.85	24.87	6.36
-3	9	13	0.23	-2.07	7.13
-2	9	13	16	21.8	2.54
-1	9	13	4.89	7.08	7.35
0	9	13	0.14	0.6	6.52
-9	10	13	23.57	34.83	2.81
-8	10	13	7.59	5.88	7.51
-7	10	13	90.83	103.55	3.36
-6	10	13	3.81	1.24	4.37
-5	10	13	0.79	-2.75	4.01
-4	10	13	16.29	9.41	5.19
-3	10	13	2.43	7.98	4.35
-2	10	13	21.77	15.24	4.18
-1	10	13	0.21	-16.84	7.68
0	10	13	1.42	-2.08	6.71
-10	11	13	24.97	18.74	5.67
-9	11	13	3.69	4.82	4.29
-8	11	13	22.26	16.2	2.76
-7	11	13	1.54	2.79	6.07
-6	11	13	1.89	2.71	4.1
-5	11	13	18.56	9.75	4.23
-4	11	13	0.11	9.63	4.17
-3	11	13	0.21	4.19	7.77
-2	11	13	49.93	45.09	8.05
-1	11	13	3.37	2.66	6.57
0	11	13	0.12	-14.59	7.19
-11	12	13	0.75	-13.44	11.38
-10	12	13	2.23	0.36	5.81
-9	12	13	16.4	17.4	4.74
-8	12	13	111.46	108.22	3.36
-7	12	13	30.02	29.43	2.92
-6	12	13	0.96	-8.41	4.93
-5	12	13	5.67	1.86	4.36
-4	12	13	6.68	0.12	4.36
-3	12	13	9.35	9.42	4.62
-2	12	13	0.84	-6.42	3.62
-1	12	13	0.1	-1.01	4.82
0	12	13	2.84	2.23	7.58
-12	13	13	0.01	-1.01	9
-11	13	13	47.96	43.38	11.59
-10	13	13	0	-9.62	17.56
-9	13	13	0.62	-0.41	8.56
-8	13	13	7.72	-12.12	8.62
-7	13	13	7.11	2.34	8.38
-6	13	13	1.51	1.06	4.65
-5	13	13	6.6	17.15	6.46
-4	13	13	21.28	24.83	3.18
-3	13	13	4.45	-1.06	8.75
-2	13	13	8.24	5.16	5.06
-1	13	13	8.6	3.94	9.12
0	13	13	0.21	-1.74	5.08
-12	14	13	4.11	11.27	6.43
-11	14	13	23.96	38.29	7.79
-10	14	13	0	-0.84	5.18
-9	14	13	3.88	-14.42	9.47
-8	14	13	0.01	-8.43	8.9
-7	14	13	0.09	-2.55	8.84
-6	14	13	4.21	7.23	8.77
-5	14	13	14.92	26.02	3.35
-4	14	13	2.01	-2.22	8.88
-3	14	13	7.56	7.17	4.06
-2	14	13	7.45	6.42	9.43
-10	15	13	0	-5.19	9.62
-9	15	13	4.25	6.57	9.69
-8	15	13	0.86	-20.08	9.63
-7	15	13	0.11	2.42	5.22
-6	15	13	27.43	20.85	11.95
-5	15	13	20.05	15.88	8.17
0	0	14	4476.24	4203.92	90.07
0	1	14	55.68	41.92	3.88
-1	2	14	11.46	2.54	7.03
0	2	14	368.56	218.29	59.35
-2	3	14	158.1	117.68	31.91
-1	3	14	190.88	127.26	44.79
0	3	14	11.11	6.59	3.44
-3	4	14	15.11	10.65	9.74
-2	4	14	28.18	21.11	6.67
-1	4	14	49.2	37.1	8.99
0	4	14	24.99	22.89	8.05
-4	5	14	17.55	15.78	2.99
-3	5	14	6.68	-1.08	7.01
-2	5	14	31.6	28.53	2.47
-1	5	14	11.28	13.91	2.46
0	5	14	129.07	123.48	21.77
-5	6	14	114.82	105.06	3.54
-4	6	14	46.6	56.59	2.79
-3	6	14	86.82	76.81	2.85
-2	6	14	4.09	-3.36	6.93
-1	6	14	6.14	9.56	2.98
0	6	14	82.68	83.72	3.7
-6	7	14	444.83	474.35	20.87
-5	7	14	584.34	643.29	12.95
-4	7	14	0.04	-7.83	7.55
-3	7	14	2.41	4.94	4
-2	7	14	29.44	52.19	4.49
-1	7	14	87.35	75.25	2.82
0	7	14	108.94	107.51	3.24
-7	8	14	14.77	25.61	2.68
-6	8	14	96.87	113.54	8.4
-5	8	14	206.73	210.59	8.03
-4	8	14	141.54	136.56	3.99
-3	8	14	0.52	-4.44	3.95
-2	8	14	0.51	-13.32	7.26
-1	8	14	28.89	18.84	2.74
0	8	14	20.12	25.9	2.33
-8	9	14	10.84	2.76	3.19
-7	9	14	29.92	37.39	4.07
-6	9	14	117.81	98.71	5.08
-5	9	14	0	-6.42	7.5
-4	9	14	30.47	44.74	2.77
-3	9	14	56.89	63.33	2.97
-2	9	14	29.02	27.24	5.47
-1	9	14	149.07	152.13	4.59
0	9	14	3.69	3.28	4.02
-9	10	14	170.61	166.57	7.59
-8	10	14	39.71	44.96	3.17
-7	10	14	14.2	17.91	4.78
-6	10	14	0.27	-5.88	5.94
-5	10	14	17.19	7.82	6.3
-4	10	14	0.88	-8.42	7.56
-3	10	14	5.07	2.12	7.66
-2	10	14	2.91	-5.1	9.83
-1	10	14	0	3.65	4.28
0	10	14	62.78	65.69	2.66
-10	11	14	1.34	-1.97	8.31
-9	11	14	4.52	-4.23	8.35
-8	11	14	129.85	134.27	4.13
-7	11	14	8.93	9.36	3.57
-6	11	14	0.87	6.59	4.22
-5	11	14	7.18	0.39	7.81
-4	11	14	16.46	16.7	3.31
-3	11	14	36.96	25.81	2.89
-2	11	14	1.67	4.45	8.28
-1	11	14	0.08	-0.1	8.3
0	11	14	0.33	-18.25	7.48
-11	12	14	6.01	5.09	11.94
-10	12	14	70.76	82.48	3.49
-9	12	14	21.78	27.42	3.23
-8	12	14	21.92	17.74	5.72
-7	12	14	8.49	7.67	7.41
-6	12	14	15.39	4.11	8.31
-5	12	14	2.57	-2.22	8.35
-4	12	14	20.01	20.6	7.05
-3	12	14	14.99	13.77	4.86
-2	12	14	2.81	-0.14	6.71
-1	12	14	0.01	-5.31	8.92
0	12	14	6.95	10.94	3.27
-12	13	14	0.02	-1.06	9.4
-11	13	14	38.54	49.77	3.61
-10	13	14	0.23	-9.75	9.23
-9	13	14	83.15	104.51	3.85
-8	13	14	4.05	-21.43	8.94
-7	13	14	1.55	-7.03	14.19
-6	13	14	8.62	9.93	3.75
-5	13	14	0.03	-12.38	6.03
-4	13	14	0.12	4.55	3.83
-3	13	14	5.74	10.62	8.56
-2	13	14	1.67	3.87	5.22
-1	13	14	0.82	5.18	5.31
0	13	14	1.75	14.21	16
-11	14	14	0	2.78	9.81
-10	14	14	3.79	-2.78	9.92
-9	14	14	2.04	5.99	5.38
-8	14	14	3.35	5.74	5.26
-7	14	14	3.42	6.1	5.23
-6	14	14	1.66	0.11	5.93
-5	14	14	2.41	9.23	8.12
-4	14	14	12.64	16.72	4.14
-3	14	14	0.21	6.13	9.36
0	1	15	1.13	2.44	3.91
-1	2	15	30.54	23.39	11.02
0	2	15	48.39	30.17	6.49
-2	3	15	194.91	181.37	47.42
-1	3	15	16.53	25.47	15.88
0	3	15	241.56	185.41	44.45
-3	4	15	335.39	214.8	101.96
-2	4	15	220.57	181.3	58.14
-1	4	15	6.08	12.28	2.54
0	4	15	73.18	80.03	13.4
-4	5	15	295.27	314.34	9.47
-3	5	15	86.41	76.61	2.95
-2	5	15	10.7	4.49	3.07
-1	5	15	125.67	140.94	5.54
0	5	15	548.51	367.87	130.37
-5	6	15	86.46	95	4.41
-4	6	15	79.6	99.56	4.67
-3	6	15	378.74	346.78	10.34
-2	6	15	44.77	40.16	2.7
-1	6	15	32.16	36.79	2.75
0	6	15	3.43	4.99	3.98
-6	7	15	158.88	151.7	7.23
-5	7	15	0.97	2.48	7.86
-4	7	15	199.28	244.88	7.6
-3	7	15	62.86	51.01	3.07
-2	7	15	37.01	37.09	2.68
-1	7	15	30.99	36.92	2.75
0	7	15	15	7.38	4.58
-7	8	15	9.49	5.82	5.33
-6	8	15	15.87	13.08	3.25
-5	8	15	0.4	4.36	9.33
-4	8	15	44.67	33.58	2.79
-3	8	15	0.46	-8.84	7.5
-2	8	15	21.34	27.57	4.19
-1	8	15	17.48	23.17	3.35
0	8	15	6.34	3.31	3.98
-8	9	15	84.34	102.78	4.37

h	k	l	F_c^2	F_o^2	σF_o^2
-7	9	15	42.9	55.4	2.92
-6	9	15	19.3	6.69	6.99
-5	9	15	49.34	55.16	2.94
-4	9	15	10.74	3.16	4.24
-3	9	15	73.94	81.42	3.03
-2	9	15	36.16	36.91	2.82
-1	9	15	21.84	21.89	4.34
0	9	15	24.99	23.52	6.94
-9	10	15	2.24	0.04	8.24
-8	10	15	15.49	20.4	3.42
-7	10	15	6.4	-0.93	8.02
-6	10	15	0.2	-1.92	5.6
-5	10	15	11.8	6.03	9.49
-4	10	15	1.9	-11.97	4.28
-3	10	15	1.16	-4.78	7.83
-2	10	15	30.77	32.25	2.91
-1	10	15	4.1	2.99	4.7
0	10	15	3.84	-4.31	4.55
-10	11	15	4.47	-4.23	8.73
-9	11	15	15.11	0.94	11.3
-8	11	15	1.73	-8.63	7.37
-7	11	15	92.58	102.74	3.64
-6	11	15	6.63	3.83	8.34
-5	11	15	5.41	7.53	4.55
-4	11	15	1.01	-5.57	8.25
-3	11	15	0.79	-3.03	8.42
-2	11	15	16.3	20.72	3.14
-1	11	15	2.19	-8.12	8.74
0	11	15	3.18	7.49	3.68
-11	12	15	0.5	7.76	3.94
-10	12	15	31.52	39.29	3.59
-9	12	15	6.25	5.78	9.05
-8	12	15	0.63	-7.17	8.87
-7	12	15	6.7	15.89	3.79
-6	12	15	0.85	-1.17	6.6
-5	12	15	1.02	7.14	8.44
-4	12	15	18.13	12.43	5
-3	12	15	8.69	-2.89	5.07
-2	12	15	6.35	9.34	5.09
-1	12	15	0.44	2.34	3.99
0	12	15	7.24	13.43	4.32
-11	13	15	1.74	-1.86	9.84
-10	13	15	4.99	1.72	4.71
-9	13	15	4.06	4.13	5.38
-8	13	15	29.47	28.17	3.45
-7	13	15	0.41	-20.53	11.72
-6	13	15	0	-6.39	10.96
-5	13	15	41.38	58.68	3.54
-4	13	15	3.22	13.55	5.18
-3	13	15	16.19	17.76	4.15
-2	13	15	22.28	28.47	8.1
-9	14	15	0	-9.26	5.57
-8	14	15	0.22	-6.45	15.07
-7	14	15	28.66	34.04	3.54
-6	14	15	0.06	0.19	9.52
-5	14	15	0.06	2.3	8.69
0	0	16	691.55	531.61	20.45
0	1	16	109.9	132.44	5.89
-1	2	16	46.03	70.42	16.58
0	2	16	273.43	150.78	49.02
-2	3	16	33.51	15.47	7.49
-1	3	16	236.74	169.59	63.55
0	3	16	93.54	66.1	11.68
-3	4	16	248.04	192.55	79.75
-2	4	16	54.1	70.32	16.23
-1	4	16	19.97	18.76	5.65
0	4	16	46.73	35.94	6.07
-4	5	16	6.07	-3.81	7.88
-3	5	16	15.25	23.93	5.79
-2	5	16	94.48	88.65	3.01
-1	5	16	1.06	-5.71	7.49
0	5	16	45.96	41.12	5.91
-5	6	16	86.72	76.85	3.04
-4	6	16	0.33	-4.49	7.76
-3	6	16	68.26	87.87	3.09
-2	6	16	11.48	7.77	4.07
-1	6	16	33.76	26.39	6.45
0	6	16	8.46	-1.28	6.65
-6	7	16	1.06	-4.23	4.93
-5	7	16	42.3	47.99	2.88
-4	7	16	69.84	73.75	3
-3	7	16	13.83	0.19	7.59
-2	7	16	0.05	-14.94	14.06
-1	7	16	1.84	2.47	7.54
0	7	16	75.19	75.34	4.66
-7	8	16	61.85	74.11	3.88
-6	8	16	1.47	6.87	3.23
-5	8	16	3.9	4.18	7.87
-4	8	16	23.46	13.64	4.32
-3	8	16	28.28	34.4	2.81
-2	8	16	69.58	62.42	2.96
-1	8	16	0.96	3.32	7.83
0	8	16	43.2	49.79	2.57
-8	9	16	63.52	64.35	3.08
-7	9	16	0.18	4.41	6.92
-6	9	16	12.49	19.97	2.82
-5	9	16	5.5	3.38	4.4
-4	9	16	13.44	17.65	2.8
-3	9	16	12.1	4.44	5.82
-2	9	16	0.91	-8.06	10.44
-1	9	16	0.87	-23.45	8.19
0	9	16	0.24	-10.39	7.28
-9	10	16	33.81	15.44	4.97
-8	10	16	0.36	-21.5	8.46
-7	10	16	54.07	64.45	4.81
-6	10	16	47.79	48.9	3.14
-5	10	16	9.86	6.03	4.42
-4	10	16	8.86	17.11	3.47
-3	10	16	1.59	10.15	5.35
-2	10	16	1.1	-1.8	15.6
-1	10	16	36.54	32	3.48
0	10	16	14.49	18.16	3.68
-10	11	16	15.46	17.34	3.94
-9	11	16	78.66	91.82	4.38
-8	11	16	37.56	49.94	11.46
-7	11	16	20.52	10.24	4.92
-6	11	16	0.12	-4.04	8.56
-5	11	16	6.4	-9.97	8.09
-4	11	16	13.58	16.63	3.11
-3	11	16	12.35	4.03	8.79
-2	11	16	0.13	-6.94	10.99
-1	11	16	2.66	-0.14	8.13
0	11	16	0.01	-2.37	5.33
-11	12	16	2.82	-7.77	9.55
-10	12	16	6.48	9.85	7.63
-9	12	16	0.02	-2.98	9.33
-8	12	16	21.49	21.38	3.44
-7	12	16	0.99	4.04	8.82
-6	12	16	14.39	20.51	8.68
-5	12	16	4.84	6.46	5.53
-4	12	16	5.07	4.24	9.13
-3	12	16	5.87	9.65	4.01
-2	12	16	28.19	30.18	4.51
-1	12	16	0.59	1.45	9.65
-10	13	16	33.73	44.87	4.86
-9	13	16	26.16	32.05	3.69
-8	13	16	1.36	10.6	9.41
-7	13	16	2.84	12.13	3.99
-6	13	16	1.15	7.73	5.56
-5	13	16	8.52	7.19	5.34
-4	13	16	5.3	-0.85	5.4
-3	13	16	1.66	4.29	7.3
0	1	17	30.37	21.95	2.41
-1	2	17	31.98	19.16	3.46
0	2	17	4.02	0.85	3.69
-2	3	17	198.97	133.66	42.85
-1	3	17	10.08	17.84	4.68
0	3	17	20.52	2.76	8.03
-3	4	17	141.31	119.53	31.51
-2	4	17	10.28	2.95	5.15
-1	4	17	1.3	-5.31	11.49
0	4	17	45.63	58.24	14.14
-4	5	17	6.92	8.57	7.67
-3	5	17	56.45	35.51	3.17
-2	5	17	0.14	-1.47	7.49
-1	5	17	10.86	5.76	7.58
0	5	17	14.09	0.67	4.75
-5	6	17	0.65	0.81	4.2
-4	6	17	7.76	-8.66	7.73
-3	6	17	14.12	6.25	4.24
-2	6	17	43.94	51.43	3.25
-1	6	17	13.98	10.41	3.3
0	6	17	20.46	17.69	2.75
-6	7	17	42.27	44.05	2.89
-5	7	17	25.51	35.06	2.81
-4	7	17	1.63	0	5.39
-3	7	17	40.89	47.71	2.91
-2	7	17	0.05	-4.18	7.88
-1	7	17	29.61	28.65	2.86
0	7	17	107.01	107.25	2.88
-7	8	17	16.6	11.05	6.97
-6	8	17	30.77	39.83	4.39
-5	8	17	0.2	1.91	6.68
-4	8	17	38.79	7.79	8.21
-3	8	17	2.09	-6.87	7.92
-2	8	17	20.96	29.89	2.9
-1	8	17	5.06	6.53	4.36
0	8	17	15.24	15.2	3.18
-8	9	17	0.86	2.2	8.47
-7	9	17	0.07	0.72	3.57
-6	9	17	32.99	22.62	5.91
-5	9	17	0.02	2.47	9.25
-4	9	17	10.22	5.74	8.55
-3	9	17	2.58	-10.36	8.73
-2	9	17	2.4	4.35	9.05
-1	9	17	6.58	10.08	4.68
0	9	17	21.64	31.06	2.8
-9	10	17	4.46	-6.76	8.85
-8	10	17	18.8	19.21	4.44
-7	10	17	0.53	0.45	8.55
-6	10	17	9.38	2.71	8.53
-5	10	17	0.63	0.34	8.37
-4	10	17	0.2	-3.81	8.49
-3	10	17	2.52	1.94	5.31
-2	10	17	0.5	-1.1	8.38
-1	10	17	12.19	7.34	4.99
0	10	17	1.81	5.43	4.85
-10	11	17	0	-1	5.19
-9	11	17	5.04	8.18	5.13
-8	11	17	14.3	18.61	6.69
-7	11	17	0.2	-2.19	8.86
-6	11	17	6.7	-6.94	8.82
-5	11	17	0.54	-2.15	4.94
-4	11	17	0.86	9.58	4.96
-3	11	17	6.01	8.87	15.43
-2	11	17	0.04	6.19	3.89
-1	11	17	1.31	-7.39	9.37
0	11	17	1.52	-4.02	6.19
-10	12	17	0.37	0.81	5.33
-9	12	17	0.24	-17.61	9.6
-8	12	17	0.56	-1.16	11.85
-7	12	17	0.08	-1.34	5.11
-6	12	17	2.35	-1.82	9.17
-5	12	17	30.61	45.04	4.55
-4	12	17	0.74	-0.58	9.22
-3	12	17	2.17	-1.52	8.81
-2	12	17	3.31	-6.55	9.63
0	0	18	519.26	471.5	20.54
0	1	18	37.76	40.69	2.47
-1	2	18	8.11	7.45	7.62
0	2	18	4.86	0.62	5.76
-2	3	18	3.39	2.44	7.65
-1	3	18	0.67	1.66	4.21
0	3	18	4.04	-1.81	6.68
-3	4	18	17.11	7.13	11.64
-2	4	18	1.09	5.8	4.2
-1	4	18	5.86	-4.37	4.57
0	4	18	105.9	94.19	14.68
-4	5	18	74.84	78.64	3.09
-3	5	18	66.2	66.77	2.99
-2	5	18	4.52	12.56	4.28
-1	5	18	3.16	5.8	7.22
0	5	18	73.41	75.97	2.71
-5	6	18	21.76	16.38	6.42
-4	6	18	49.45	60.69	3.02
-3	6	18	34	34.3	3.57
-2	6	18	35.45	31.3	2.91
-1	6	18	43.63	50.19	3.18
0	6	18	120.05	124.29	4.37
-6	7	18	0.35	1.09	7.21
-5	7	18	4.28	-6.29	4.43
-4	7	18	1.18	-9.22	8.08
-3	7	18	23.83	29.47	2.91
-2	7	18	12.81	18.36	5.13
-1	7	18	11.05	21.21	2.9
0	7	18	0.37	-6.52	5.29
-7	8	18	24.88	19.95	4.8
-6	8	18	18.94	11.96	8.44
-5	8	18	43.43	50.62	3.22
-4	8	18	13.27	12.35	3.71
-3	8	18	0.21	-0.01	4.62
-2	8	18	7.11	2.94	4.69
-1	8	18	2.35	1.68	4.62
0	8	18	0.5	-7.29	4.52
-8	9	18	0.08	-9.57	8.59
-7	9	18	4.39	2.98	4.78
-6	9	18	1.49	-11.17	8.57
-5	9	18	12.14	27.69	13.61
-4	9	18	0.98	-12.08	8.53
-3	9	18	0.38	4.03	8.51
-2	9	18	1.12	4.01	5.98
-1	9	18	0.98	1.16	8.01
0	9	18	7.66	5.77	5.4
-9	10	18	11.09	-3.16	9.21
-8	10	18	20.53	20.37	16.2
-7	10	18	19.71	23.17	3.9
-6	10	18	4.16	4.02	8.8
-5	10	18	0.13	-1.34	4.78
-4	10	18	15.5	14.29	5.66
-3	10	18	0.2	-0.58	4.91
-2	10	18	2.89	4.91	8.94
-1	10	18	0	-0.84	9.22
0	10	18	0.12	-5.53	10.09
-10	11	18	0.8	-4.44	16.12
-9	11	18	0.75	-12.62	12.38
-8	11	18	5.39	-3.85	11.3
-7	11	18	2.58	4.94	9.07
-6	11	18	6.48	9.7	5.52
-5	11	18	0.7	-5.02	9.11
-4	11	18	3.44	-1.63	5.19
-3	11	18	13.19	7.99	11.51
-2	11	18	1.75	-5.32	9.34
-7	12	18	0.94	-6.25	7.2
-6	12	18	0.6	6.18	9.24
-5	12	18	1.38	-0.84	9.35
0	1	19	0.64	6.82	3.17
-1	2	19	0.52	-4.3	7.75
0	2	19	4.27	-0.83	4.12
-2	3	19	19.03	-0.78	7.86
-1	3	19	0.9	-0.43	7.71
0	3	19	0.4	-3.78	4.07
-3	4	19	14.12	1.29	4.31
-2	4	19	2.23	-1.67	6.82
-1	4	19	9.39	3.72	8.66
0	4	19	0.02	-8.12	6.96
-4	5	19	0.36	3.92	7.99
-3	5	19	1.38	-9.53	7.95
-2	5	19	59.68	58.9	3.03
-1	5	19	5	5.6	4.39
0	5	19	7.05	-0.12	8.48

h	k	l	F_c^2	F_o^2	σF_o^2
-5	6	19	0.29	-3.01	11.18
-4	6	19	0.12	-1.49	4.37
-3	6	19	33.63	21.53	4.86
-2	6	19	4.17	-1.37	11.44
-1	6	19	0.05	-9.28	8.25
0	6	19	9.93	5.2	4.53
-6	7	19	1.23	0.5	4.76
-5	7	19	26.68	28.58	3.17
-4	7	19	0.42	-14.98	8.43
-3	7	19	1.55	-0.09	8.27
-2	7	19	2.75	-6.63	9.97
-1	7	19	0.34	-0.14	8.43
0	7	19	0.77	5.18	4.66
-7	8	19	0.3	2.03	5.35
-6	8	19	1.56	-2.59	8.53
-5	8	19	0.8	4.98	3.66
-4	8	19	19	15.29	7.07
-3	8	19	7.05	-0.88	9.94
-2	8	19	0.26	0.57	6.16
-1	8	19	9.48	2.78	9.36
0	8	19	3.81	-6.04	7.97
-8	9	19	0.92	0.61	9.02
-7	9	19	6.47	7.18	3.55
-6	9	19	7.44	3.24	4.92
-5	9	19	0	-12.31	8.78
-4	9	19	4.56	-6.53	8.92
-3	9	19	0	-13.63	8.95
-2	9	19	0.01	3.48	4.53
-1	9	19	0.04	-5.14	10.07
0	9	19	0.71	0.01	7.94
-9	10	19	0.1	-0.66	9.29
-8	10	19	0.37	-10.78	9.19
-7	10	19	2.87	-10.26	10.85
-6	10	19	0	-14.97	9.11
-5	10	19	1.78	11.75	5.05
-4	10	19	0.71	-0.19	9.08
-3	10	19	0	0.2	10.06
-2	10	19	2.77	-2.51	9.27
-1	10	19	2.95	-0.17	5.26
-7	11	19	0.04	-4.75	9.5
-6	11	19	3.02	3.43	5.21
-5	11	19	2.54	3.98	5.15
-4	11	19	0.07	1.58	9.65
0	0	20	1.69	-4.82	13.94
0	1	20	0.16	-6.96	9.08
-1	2	20	2.61	-0.99	5.72
0	2	20	4.45	1.34	6.9
-2	3	20	12.26	0.21	8.13
-1	3	20	14.23	9.06	8.06
0	3	20	12.08	-4.29	7.12
-3	4	20	50.67	41.57	12.22
-2	4	20	0.12	-4.03	8.23
-1	4	20	3.63	5.27	4.75
0	4	20	12.97	15.95	4.41
-4	5	20	1.51	-0.36	4.8
-3	5	20	0.34	-16.38	8.41
-2	5	20	8.67	1.15	4.75
-1	5	20	0.38	1.44	5.5
0	5	20	7.99	10.81	3.58
-5	6	20	3.21	0.69	10.3
-4	6	20	8.85	1.88	9.43
-3	6	20	26.6	19.92	5.72
-2	6	20	9.56	-1.08	6.27
-1	6	20	18.05	16.19	7.45
0	6	20	16.64	23.73	2.85
-6	7	20	1.16	0.26	8.2
-5	7	20	0.62	-5.35	8.76
-4	7	20	3.88	4.67	3.76
-3	7	20	11.08	10.53	3.86
-2	7	20	30.39	33.33	3.34
-1	7	20	4.4	8.78	7.98
0	7	20	9.32	10.34	3.73
-7	8	20	8.77	6.72	5.03
-6	8	20	2.31	-2.07	10.99
-5	8	20	11.78	16.72	4.7
-4	8	20	4.93	6.53	9
-3	8	20	10.9	21.97	3.93
-2	8	20	0.92	1.91	9.01
-1	8	20	4.28	1.08	9.08
0	8	20	0.11	-11.56	8.09
-8	9	20	0.01	-21.01	9.13
-7	9	20	0.85	-16.6	11
-6	9	20	0.23	12.12	5.05
-5	9	20	2.26	9.85	5.14
-4	9	20	0.64	-29.45	9.17
-3	9	20	0.58	-3.2	5.13
-2	9	20	1.71	-21	9.34
-1	9	20	0.07	-3.58	9.4
-6	10	20	3.07	-6.8	9.27
-5	10	20	0	-2.62	9.27
-4	10	20	1.28	2.32	11.13
0	1	21	16.44	3.31	5.01
-1	2	21	2.2	5.58	6.99
0	2	21	0.13	1.7	3.64
-2	3	21	15.24	19.3	6.35
-1	3	21	1.14	7.17	9.13
0	3	21	5.75	2.41	7.73
-3	4	21	10.77	1.15	7.12
-2	4	21	16.3	9.5	4.9
-1	4	21	1	6.68	4.95

h	k	l	F_c^2	F_o^2	σF_o^2
0	4	21	6.21	-0.06	5.78
-4	5	21	0.83	-0.11	9
-3	5	21	10.87	1.28	5.27
-2	5	21	9.62	16.43	3.68
-1	5	21	7.38	6.58	9.18
0	5	21	35.98	32.9	5.43
-5	6	21	0.16	9.71	8.89
-4	6	21	2.74	-14.32	9.17
-3	6	21	45.13	51.83	3.49
-2	6	21	10.67	8.11	9.32
-1	6	21	1.81	-2.84	9.44
0	6	21	2.49	-1.98	8.12
-6	7	21	5.03	5.24	5.28
-5	7	21	9.98	4.02	5.28
-4	7	21	18.59	25.14	8.38
-3	7	21	1.43	0.95	9.44
-2	7	21	0.94	-10.4	9.45
-1	7	21	16.38	19.06	6.6
0	7	21	0.38	4.61	7.97
-7	8	21	0.01	0.94	9.33
-6	8	21	8.62	1.75	8.05
-5	8	21	4.33	5.02	9.31
-4	8	21	8.59	4.39	9.55
-3	8	21	0.42	1.85	5.27
-2	8	21	7.77	-3.26	9.73
-1	8	21	0.09	-15.59	9.81
0	0	22	10.97	1.07	5.72
0	1	22	0	-8.62	7.84
-1	2	22	0.43	3.73	5.03
0	2	22	0.07	-7.94	7.83
-2	3	22	6.53	1.57	8.99
-1	3	22	0.01	-7.53	16.17
0	3	22	8.19	2.7	7.97
-3	4	22	0.16	-8.97	13.2
-2	4	22	4.27	9.61	7.79
-1	4	22	5.17	-1.15	5.22
0	4	22	5.29	7.58	8.16
-4	5	22	3.64	-6.38	9.6
-3	5	22	4.2	1.67	6.02
-2	5	22	6.87	11.23	4.09
-1	5	22	0.7	0.21	6.41
0	5	22	1.22	-14.28	8.38
-5	6	22	0.05	0.82	7.5
-4	6	22	0.54	0.82	9.54
-3	6	22	36.83	48.17	3.67
-2	6	22	0.12	-8.87	16.19
-1	6	22	18.85	19.46	4.3
0	6	22	15.73	10.45	5.28
-5	7	22	17.22	8.88	5.87
-4	7	22	17.88	24.59	4.56
-3	7	22	0.25	6.4	9.57
-2	7	22	5.57	4.63	6.79
0	1	23	0	-5.08	9.38
-1	2	23	13.54	-4.56	21.05
0	2	23	5.95	-3.34	5.06
-2	3	23	2.76	1.01	5.31
-1	3	23	7.91	17.6	4.8
0	3	23	5.93	7.07	10.28
-3	4	23	2.62	13.08	8.77
-2	4	23	12.32	9.23	4.2
-1	4	23	0.14	-1.86	9.56
0	4	23	2.35	0.32	5.16
-3	5	23	11.26	15.7	5.54
-2	5	23	0.23	-4.98	7.68

A3.8 BUCIP4

h	k	l	F_c^2	F_o^2	σF_o^2
1	0	0	5275.4	5265.08	77.96
2	0	0	2094.25	2076.07	38.41
3	0	0	132.13	151.42	10.28
4	0	0	12.51	10.85	14.56
5	0	0	2.42	-29.22	52.19
-5	1	0	11.92	-22.65	24.4
-4	1	0	0.76	-29.6	13.63
-3	1	0	7.59	12.15	18.5
-2	1	0	856.86	810.18	35.4
-1	1	0	1143	1092.42	22.44
0	1	0	97.97	123.95	4.55
1	1	0	446.76	467.38	15.95
2	1	0	403.79	437.01	16.27
3	1	0	286.37	299.06	11.91
4	1	0	70.46	43.79	18.55
5	1	0	0.19	-7.14	24.4
-5	2	0	3.58	-22.14	24.57
-4	2	0	2.87	4.42	21.9
-3	2	0	0.77	-0.14	23.41
-2	2	0	101.25	92.35	13.49
-1	2	0	35.05	17.75	8.78
0	2	0	62.49	62.58	7.12
1	2	0	128.19	134.12	7.58
2	2	0	10.32	-24.39	15.12
3	2	0	354.97	340.35	13.84
4	2	0	0.56	8.7	15.29
5	2	0	0.03	3.13	18.55
-4	3	0	9.94	-9.77	22.35
-3	3	0	0.41	-7.54	20.17
-2	3	0	57.63	48.81	7.97
-1	3	0	1524.04	1459.66	28.25
0	3	0	17.38	9.72	9.38
1	3	0	62.7	57.82	13.54
2	3	0	117.74	105.43	8.28
3	3	0	10.98	17.01	13.96
4	3	0	14.35	4.82	21.88
5	3	0	1.03	-18.05	28.93
-4	4	0	28.2	25.68	22.94
-3	4	0	118.35	123.99	10.8
-2	4	0	75.9	65.57	8.86
-1	4	0	85.7	89.5	7.09
0	4	0	189.94	185.51	14.99
1	4	0	108.41	105.56	7.4
2	4	0	167.21	148.29	9.91
3	4	0	17.43	12.93	13.9
4	4	0	0.02	-0.36	24.21
-4	5	0	0.13	-19.89	23.14
-3	5	0	0.72	-8.37	13.23
-2	5	0	399.22	398.81	15.88
-1	5	0	5.75	5.4	15.67
0	5	0	168.3	180.97	8.82
1	5	0	2.9	9.21	7.9
2	5	0	0.26	-19.77	20.31
3	5	0	0.41	-1.75	22.75
4	5	0	3.69	26.57	15.7
-4	6	0	53.37	50.65	31.09
-3	6	0	3.94	-25.31	21.29
-2	6	0	5.62	3.56	21.96
-1	6	0	83.48	106.8	9.36
0	6	0	10.57	-8.85	16.84
1	6	0	62.66	72	9.43
2	6	0	336.42	345.1	14.41
3	6	0	29.43	31.4	11.97
4	6	0	0.17	9.84	16.76
-3	7	0	0.11	7.27	21.13
-2	7	0	8.39	27.4	29.58
-1	7	0	24.03	42.69	15.79
0	7	0	35.13	22.65	12.04
1	7	0	68.96	79.55	15.99
2	7	0	120.51	127.31	12.48
3	7	0	1.72	-1.92	24.03
-3	8	0	0.29	-27.04	22.23
-2	8	0	9.69	10.39	13.1
-1	8	0	0.02	10.1	19.07
0	8	0	30.1	1.25	19.78
1	8	0	19.44	10.87	13.18
2	8	0	15.98	3.87	14.24
3	8	0	41.73	40.26	12.62
-2	9	0	27.31	39.32	10.99
-1	9	0	5.04	10.94	19.35
0	9	0	2.8	0.62	20.52
1	9	0	8.58	9.1	13.75
2	9	0	9.32	4.67	14.74
-1	10	0	19.04	18.86	21.8
0	10	0	0.05	-33.93	21.66
1	10	0	3.66	-12.1	22.36
2	10	0	0.97	5.67	12.69
-1	-10	1	0.83	-5.19	14.51
0	-10	1	0.56	3.03	13.93
1	-10	1	5.4	9.91	21.98
-2	-9	1	0.09	-8.85	22.97
-1	-9	1	48.23	51.51	10.95
0	-9	1	0.05	-16.35	20.21
1	-9	1	19.69	20.02	13.29
2	-9	1	4.21	-17.19	21.68
-3	-8	1	5	24.9	15.34
-2	-8	1	4	1.08	22.18
-1	-8	1	57.35	48.15	14.79
0	-8	1	22.31	23	19.49
1	-8	1	12.2	10.5	12.78
2	-8	1	0.08	17.94	20.53
3	-8	1	4.93	-3.3	21.9
-3	-7	1	0	-7.38	24.92
-2	-7	1	83.99	90.28	11.31
-1	-7	1	25.66	30.74	22.96
0	-7	1	1.2	-7.19	36.7
1	-7	1	0.55	-0.99	19.28
2	-7	1	0.58	-15.41	20.46
3	-7	1	8.02	-5.07	22.46
-4	-6	1	0.34	-11.09	39.21
-3	-6	1	276.53	285.32	13.46
-2	-6	1	760.02	780.88	28.07
-1	-6	1	69.49	66.53	9.57
0	-6	1	335.9	351.12	13.33
1	-6	1	34.39	40.52	9.18
2	-6	1	63.58	78.88	10.03
3	-6	1	72.88	59.18	11.12
4	-6	1	4.48	-16.35	22.86
-4	-5	1	3.14	-44.54	25.53
-3	-5	1	26.47	20.88	22.51
-2	-5	1	36.01	22.74	12.95
-1	-5	1	2.25	4.56	15.69
0	-5	1	70.2	70.03	7.72
1	-5	1	2564.63	2616.4	46.34
2	-5	1	106.14	103	9.86
3	-5	1	31.45	25.36	10.41
4	-5	1	35.55	29.29	35.5
-4	-4	1	5.81	-6.64	23.56
-3	-4	1	34.82	15.8	13.78
-2	-4	1	321.94	301.54	11.71
-1	-4	1	336.83	382.97	14
0	-4	1	383.13	372.31	14.18
1	-4	1	431.92	395.28	14.54
2	-4	1	801.35	717.79	49.79
3	-4	1	91.04	96.19	10.83
4	-4	1	144.01	117.63	16.95
-4	-3	1	17.52	-1.78	13.72
-3	-3	1	4.62	-21.69	20.74
-2	-3	1	166.21	165.03	8.89
-1	-3	1	67.66	53.64	7.05
0	-3	1	804.94	749.57	19.43
1	-3	1	89.3	86.55	6.95
2	-3	1	87.03	76.41	8.52
3	-3	1	18.79	12.48	12.92
4	-3	1	18.74	3.22	11.3
-5	-2	1	0.15	2.29	24.23
-4	-2	1	7.89	-28.21	21.79
-3	-2	1	12.08	1.8	16.3
-2	-2	1	18.23	15.01	7.57
-1	-2	1	128.21	121.81	7.41
0	-2	1	1398.58	1260.09	23.72
1	-2	1	297.24	324.5	12.4
2	-2	1	2.21	-15.12	15.09
3	-2	1	2.52	12.88	26.32
4	-2	1	3.03	15.96	21.81
5	-2	1	4.03	-0.2	24.4
-5	-1	1	0.13	9.75	23.83
-4	-1	1	72.81	81.19	16.24
-3	-1	1	155.1	173.99	10.39
-2	-1	1	12.15	-0.9	8.66
-1	-1	1	409.04	418.69	36.35
0	-1	1	52.87	27.4	4.29
1	-1	1	2141.64	1996.56	33.82
2	-1	1	56.29	40.82	18.05
3	-1	1	78.65	66.79	10.1
4	-1	1	52.52	27.6	14.68
5	-1	1	1.31	5.84	24.21
-5	0	1	0.08	-1.85	26.02
-4	0	1	23.01	4.95	22
-3	0	1	19.56	0.96	12.03
-2	0	1	198.09	210.74	8.46
-1	0	1	1570.66	1413.56	27.43
1	0	1	3851.72	3503.24	53.6
2	0	1	842	838.7	21.73
3	0	1	4.81	37.76	9.88
4	0	1	7.57	-37.36	23.14
5	0	1	8.61	0.98	24.78
-5	1	1	9.47	-0.67	23.94
-4	1	1	7.1	-1.8	21.89
-3	1	1	73.29	82.78	10.03
-2	1	1	292.35	321.93	17.35
-1	1	1	3607.29	3615.48	55.52
0	1	1	561.86	536.53	17.25
1	1	1	242.89	245.23	8.9
2	1	1	6.38	1.85	9.24
3	1	1	60.34	82.37	10.2
4	1	1	14.95	-15.82	26.07
5	1	1	0.01	-6.28	24.82
-5	2	1	1.04	-0.62	23.85
-4	2	1	0.77	3.29	31.79
-3	2	1	14.66	6.6	19.71
-2	2	1	7.59	9.88	14.7
-1	2	1	0.19	-10.89	14.22
0	2	1	484.55	488.3	14.68
1	2	1	38.53	7.38	15.13
2	2	1	516.44	501.08	19.8
3	2	1	513.89	500.92	24.17
4	2	1	13.6	10.91	13.94
5	2	1	1.58	4.16	15.11
-4	3	1	2.28	-2.33	21.46
-3	3	1	29.47	-19.22	20.45
-2	3	1	0	-22.93	15.28
-1	3	1	125.72	108.36	17.4
0	3	1	61.95	55	6.98
1	3	1	385.16	368.8	13.71
2	3	1	153.85	173.56	9.02
3	3	1	36.82	46.27	11.31
4	3	1	5.69	-25.95	39.61
5	3	1	0.18	-42.09	25.79
-4	4	1	55.43	61.08	15.84
-3	4	1	11.31	-29.42	26.37
-2	4	1	21.56	27.52	8.46
-1	4	1	24.54	38.2	21.11
0	4	1	9.43	-7.88	8.38
1	4	1	49.93	63.32	7.27
2	4	1	22.26	24.16	11.71
3	4	1	2.85	11.71	23.45
4	4	1	0.69	10.44	24.78
-4	5	1	51.44	63.81	11.83
-3	5	1	167	179.97	11.06
-2	5	1	0.07	-24.36	18.51
-1	5	1	2117.95	2223.04	40.73
0	5	1	848.69	839.71	22.3
1	5	1	679.61	621.39	21.7
2	5	1	43.66	16.4	32.94
3	5	1	20.51	-1.72	14.77
4	5	1	41.75	-17.02	26.86
-4	6	1	1.81	21.98	22.7
-3	6	1	7.63	5.41	20.7
-2	6	1	6.9	16.02	19.24
-1	6	1	11.34	20.37	11.26
0	6	1	2.13	15.34	10.67
1	6	1	12.77	14.59	15.29
2	6	1	718.24	716.78	29.88
3	6	1	177.35	143.53	12.99
4	6	1	4.88	-5.88	17.66
-3	7	1	0.08	2.88	13.7
-2	7	1	1.22	-11.94	19.93
-1	7	1	236.89	235.88	10.92
0	7	1	4.3	-1.33	19.04
1	7	1	13.14	37.43	22.81
2	7	1	14.53	11.1	21.39
3	7	1	1.38	18.29	24.17
4	7	1	0.88	17.15	14.43
-3	8	1	6.65	-13.97	22.02
-2	8	1	14.02	23.5	16.65
-1	8	1	5.54	-16.97	20.2
0	8	1	233.46	237.93	11.27
1	8	1	34.04	18.98	18.45
2	8	1	6.59	3.67	22.65
3	8	1	0.41	3.58	15.75
-2	9	1	3.5	-50.04	21.87
-1	9	1	9.72	-0.46	35.7
0	9	1	5.91	-9.84	13.35
1	9	1	1.04	11.03	46.73
2	9	1	35.75	51.3	15.59
-2	10	1	3.38	-27.29	23.72
-1	10	1	11.29	-1.27	21.8
0	10	1	0.01	-27.21	26.92
1	10	1	0.29	-43.83	32.39
2	10	1	7.64	21.19	24.46
-1	-10	2	0.86	26.67	32.59
0	-10	2	21.95	-11.23	31.89
1	-10	2	61.22	63.28	16.24
-2	-9	2	0.02	-66.28	32.89
-1	-9	2	7.94	26.58	29.08
0	-9	2	20.81	34.19	14.94
1	-9	2	5.1	14.74	14.74
2	-9	2	27.72	-18.05	31.19
-3	-8	2	3.31	8.72	34.7
-2	-8	2	5.79	15.74	30.58
-1	-8	2	57.84	61.37	14.74
0	-8	2	9.23	18.65	27.48
1	-8	2	2.59	10.13	28.08
2	-8	2	4.25	18.45	14.94
3	-8	2	2.59	38.31	16.24
-3	-7	2	3.38	19.55	31.39
-2	-7	2	63.45	36.8	15.54
-1	-7	2	2.83	-20.56	28.08
0	-7	2	0.75	-14.14	26.97
1	-7	2	33.54	53.35	13.74
2	-7	2	16.92	-61.97	29.28
3	-7	2	5.07	-42.02	32.49
-4	-6	2	0.32	16.65	34.4
-3	-6	2	351.16	357.99	20.16
-2	-6	2	683.72	737.54	36.51
-1	-6	2	2.2	-11.13	25.57
0	-6	2	34.2	5.52	24.37
1	-6	2	1.45	2.41	25.67
2	-6	2	96.63	90.45	14.64
3	-6	2	3.48	-10.73	30.28

h	k	l	F_c^2	F_o^2	σF_o^2
4	-6	2	0.75	24.17	34.9
-4	-5	2	15.27	-23.77	33.99
-3	-5	2	203.96	217.5	16.65
-2	-5	2	10.38	-11.93	27.78
-1	-5	2	20.62	13.04	22.86
0	-5	2	4.24	-7.52	21.36
1	-5	2	17.85	2.11	11.53
2	-5	2	0.02	15.84	13.64
3	-5	2	293.51	315.57	18.35
4	-5	2	12.65	-8.32	33.59
-4	-4	2	23.32	23.67	31.79
-3	-4	2	24.35	-16.24	29.98
-2	-4	2	21.78	4.41	25.07
-1	-4	2	345.79	331.42	18.55
0	-4	2	2534.98	2567.6	61.37
1	-4	2	225.31	222.01	12.74
2	-4	2	44.52	51.64	12.94
3	-4	2	32.87	57.66	15.44
4	-4	2	1.93	11.53	34.09
-4	-3	2	19.09	2.21	30.08
-3	-3	2	52.56	72.3	14.04
-2	-3	2	2.82	5.62	10.93
-1	-3	2	0	-24.37	18.85
0	-3	2	63.46	77.11	9.73
1	-3	2	265.96	251.3	14.64
2	-3	2	26.79	10.73	23.67
3	-3	2	251.7	249.49	17.05
4	-3	2	24.11	29.08	33.69
-5	-2	2	11.17	23.97	31.29
-4	-2	2	3	11.73	27.58
-3	-2	2	7.47	19.35	13.04
-2	-2	2	76	82.83	10.13
-1	-2	2	23.92	15.94	9.63
0	-2	2	2.81	-16.35	17.55
1	-2	2	255.23	250.49	15.64
2	-2	2	250.85	235.75	12.63
3	-2	2	48.38	51.04	15.24
4	-2	2	2.39	9.73	33.69
5	-2	2	0.2	22.26	37.2
-5	-1	2	0.53	-25.37	31.89
-4	-1	2	0.2	-30.89	30.18
-3	-1	2	18.55	-32.89	26.97
-2	-1	2	6.69	25.27	9.33
-1	-1	2	1289.81	1338.3	35.8
0	-1	2	567.5	509.21	18.05
1	-1	2	997.73	947.52	30.28
2	-1	2	136.68	157.94	11.43
3	-1	2	17.39	46.53	15.04
4	-1	2	2.8	11.73	16.75
5	-1	2	0.34	-27.28	36.4
-5	0	2	0.01	-45.02	32.29
-4	0	2	51.54	27.98	30.08
-3	0	2	64.47	67.79	13.54
-2	0	2	618.83	630.85	27.18
-1	0	2	611.2	595.65	23.26
1	0	2	4919.9	4746.33	100.48
2	0	2	14.48	19.85	10.53
3	0	2	189.79	185.51	15.84
4	0	2	0.41	-37.9	32.99
5	0	2	6.85	-41.31	36.6
-5	1	2	1.09	-43.42	32.69
-4	1	2	13.25	-0.6	29.78
-3	1	2	399.96	370.83	19.05
-2	1	2	85.57	86.74	10.13
-1	1	2	22701.0	21007.7	424.68
0	1	2	2374.8	2210.92	47.83
1	1	2	5763.96	6012.44	125.75
2	1	2	22.59	22.66	10.23
3	1	2	2.88	-8.02	29.28
4	1	2	4.32	-25.37	32.99
5	1	2	11.33	-23.48	37.1
-5	2	2	0.34	-20.26	32.89
-4	2	2	3.35	-1.3	29.18
-3	2	2	75.44	108.6	13.74
-2	2	2	14.64	23.06	9.93
-1	2	2	0.2	3.61	19.25
0	2	2	1872.21	1816.83	43.22
1	2	2	572.77	564.46	26.97
2	2	2	43.17	22.96	24.07
3	2	2	95.84	96.57	14.64
4	2	2	0.64	-10.33	31.89
5	2	2	0.45	8.22	36.3
-4	3	2	1.68	23.36	14.84
-3	3	2	25.85	44.92	13.74
-2	3	2	54.19	61.37	10.43
-1	3	2	59.15	31.69	9.53
0	3	2	174.39	175.29	10.73
1	3	2	734.02	703.95	28.98
2	3	2	194.74	207.57	13.74
3	3	2	0.34	-4.21	34.6
4	3	2	1.99	15.64	33.79
5	3	2	16.38	36.8	19.75
-4	4	2	34.15	18.15	30.79
-3	4	2	0.26	23.36	27.98
-2	4	2	64.42	56.46	11.83
-1	4	2	63.83	69.29	9.83
0	4	2	1.81	-38.51	19.05
1	4	2	5.1	0.6	21.26
2	4	2	111.11	123.44	14.64
3	4	2	71.23	78.62	18.05
4	4	2	16.24	15.94	19.75
-4	5	2	4.43	-22.76	31.39
-3	5	2	8.23	-16.35	29.08
-2	5	2	157.76	155.43	13.74
-1	5	2	90.45	85.24	11.43
0	5	2	260.59	240.97	11.93
1	5	2	0.12	5.01	23.57
2	5	2	0.05	19.75	15.24
3	5	2	5.57	16.45	17.35
4	5	2	6.86	-25.67	39.91
-4	6	2	3.06	15.84	30.99
-3	6	2	79.39	57.86	15.04
-2	6	2	217.8	242.07	15.64
-1	6	2	32.97	35.8	12.63
0	6	2	443.13	470.7	25.27
1	6	2	4	7.92	26.17
2	6	2	8.92	1.1	32.29
3	6	2	13.54	26.77	35
4	6	2	6.79	-27.78	40.11
-3	7	2	12.44	9.23	28.98
-2	7	2	79.5	90.45	14.74
-1	7	2	35.98	72.5	13.54
0	7	2	137.82	162.75	14.44
1	7	2	2241.08	2240.6	64.38
2	7	2	905.19	892.97	44.22
3	7	2	3.15	34.4	35
4	7	2	43.42	16.95	41.82
-3	8	2	0.1	-18.95	30.99
-2	8	2	0.14	12.33	27.78
-1	8	2	59.39	-3.81	29.18
0	8	2	0.44	-16.04	27.48
1	8	2	109.47	111.81	15.84
2	8	2	13.84	1.1	16.85
3	**8**	**2**	**2.75**	**-22.06**	**36**
-2	9	2	1.05	15.34	15.04
-1	9	2	6.45	13.54	28.28
0	9	2	17.05	22.56	14.74
1	9	2	0.11	-46.23	31.89
2	9	2	15.68	11.53	17.25
-2	10	2	6.27	-2.81	32.79
-1	10	2	0.32	15.54	29.48
0	10	2	17.74	43.32	15.34
1	10	2	0.18	19.85	16.24
2	10	2	2.81	-55.95	34.7
-1	-10	3	0.45	25.57	15.84
0	-10	3	0.18	0	30.08
1	-10	3	16.77	-20.76	31.99
-2	-9	3	7.79	-53.35	32.59
-1	-9	3	35.05	61.47	15.24
0	-9	3	115.3	107.6	15.54
1	-9	3	33.6	39.41	15.24
2	-9	3	17.07	12.13	32.39
-3	-8	3	5.32	-5.31	34.4
-2	-8	3	164.17	171.17	16.35
-1	-8	3	0.09	22.36	27.48
0	-8	3	8.39	18.95	27.38
1	-8	3	31.07	42.82	14.44
2	-8	3	8.25	-43.42	29.08
3	-8	3	52.6	72.6	16.85
-3	-7	3	6.34	-6.32	31.59
-2	-7	3	64.92	64.88	15.04
-1	-7	3	5.95	7.42	13.84
0	-7	3	8.54	17.45	13.54
1	-7	3	0.42	1.1	27.28
2	-7	3	12.17	28.08	28.28
3	-7	3	6.07	29.58	15.64
-4	-6	3	1.32	9.53	17.05
-3	-6	3	4.05	-19.25	31.19
-2	-6	3	29.25	31.69	14.44
-1	-6	3	6.23	-49.44	26.07
0	-6	3	15.36	-7.92	24.77
1	-6	3	123.13	108.2	13.84
2	-6	3	20.93	1.8	28.78
3	-6	3	25.43	-0.7	31.49
4	-6	3	18.03	15.34	33.99
-4	-5	3	77.7	100.58	17.45
-3	-5	3	934.27	863.59	43.42
-2	-5	3	126.81	121.14	14.44
-1	-5	3	38.65	45.33	11.33
0	-5	3	0.04	-34.09	20.86
1	-5	3	286.83	268.34	15.04
2	-5	3	235.9	221.01	15.34
3	-5	3	98.11	107.4	16.35
4	-5	3	15.93	-22.56	33.69
-4	-4	3	4.52	-34.7	31.89
-3	-4	3	46.59	34.4	14.74
-2	-4	3	12.05	2.21	24.77
-1	-4	3	374.05	339.74	16.85
0	-4	3	6425.21	7192.4	152.42
1	-4	3	1028.46	1180.01	36.9
2	-4	3	223.85	234.85	14.54
3	-4	3	5.68	9.93	30.58
4	-4	3	9.2	-9.33	33.79
-4	-3	3	88.43	78.72	15.94
-3	-3	3	0.05	3.71	27.38
-2	-3	3	8.64	-23.97	22.26
-1	-3	3	30.47	6.12	19.05
0	-3	3	1387.71	1389.24	38.01
1	-3	3	311.47	329.81	18.65
2	-3	3	4.25	6.92	23.36
3	-3	3	50.79	67.59	15.44
4	-3	3	0.01	-5.82	32.59
-5	-2	3	0.05	22.36	31.19
-4	-2	3	6.2	1.3	28.28
-3	-2	3	15.72	18.05	25.77
-2	-2	3	69.17	65.48	10.13
-1	-2	3	337.21	311.96	16.75
0	-2	3	723.75	661.93	24.97
1	-2	3	378.17	389.18	20.06
2	-2	3	64.79	68.69	11.23
3	-2	3	0.74	10.63	30.18
4	-2	3	4.63	22.76	16.65
5	-2	3	10.03	-22.36	36.8
-5	-1	3	0.03	-24.67	32.99
-4	-1	3	84.47	27.78	29.68
-3	-1	3	56.11	68.59	13.14
-2	-1	3	97.81	101.28	9.93
-1	-1	3	4951.76	4926.13	104.69
0	-1	3	626.62	564.56	20.16
1	-1	3	233.43	237.16	12.84
2	-1	3	45.15	36.2	10.93
3	-1	3	1.19	24.67	14.74
4	-1	3	0.94	-27.07	16.75
5	-1	3	3.48	22.06	18.75
-5	0	3	3.57	26.17	31.39
-4	0	3	2.59	-28.78	29.48
-3	0	3	42.59	7.62	26.87
-2	0	3	48.59	64.18	9.63
-1	0	3	884.43	864.19	27.88
0	0	3	48.77	-1026.74	27.28
1	0	3	2280.62	2244.81	52.65
2	0	3	111.37	109.1	11.03
3	0	3	55.46	68.09	14.84
4	0	3	1.24	-5.31	32.29
5	0	3	0.95	19.85	36.1
-5	1	3	2.29	-9.02	30.89
-4	1	3	25.66	34.6	14.94
-3	1	3	54.77	53.55	13.44
-2	1	3	1895.7	1907.78	49.34
-1	1	3	14609.3	14121.2	287.29
0	1	3	41.72	37.1	6.72
1	1	3	1420.69	1488.52	39.41
2	1	3	190.87	198.05	11.53
3	1	3	52.64	52.04	14.74
4	1	3	56.89	27.38	16.85
5	1	3	1.77	15.34	35
-5	2	3	2.75	0	32.59
-4	2	3	0.22	-61.57	30.89
-3	2	3	8.21	24.27	13.34
-2	2	3	9.47	-19.15	20.06
-1	2	3	369.84	333.32	18.25
0	2	3	55.78	34.5	8.72
1	2	3	335.14	287.19	16.35
2	2	3	2401.56	2689.04	65.58
3	2	3	63.27	69.59	14.24
4	2	3	34.69	16.45	33.09
5	2	3	0.29	-31.19	36.8
-4	3	3	0.03	-10.83	29.98
-3	3	3	47.31	64.98	13.84
-2	3	3	0.63	-5.92	21.06
-1	3	3	421.04	383.36	20.06
0	3	3	7.05	16.14	19.55
1	3	3	88.63	79.52	10.93
2	3	3	17.53	22.16	24.57
3	3	3	129.69	117.83	17.75
4	3	3	12.45	-1.4	31.19
5	3	3	62.5	71.4	19.85
-4	4	3	19.15	30.79	15.34
-3	4	3	8.56	3.41	27.26
-2	4	3	118.71	121.03	12.23
-1	4	3	15.82	3.81	19.25
0	4	3	11.16	-12.74	18.95
1	4	3	8.73	7.02	10.43
2	4	3	76.44	67.39	14.34
3	4	3	68.49	101.18	18.05
4	4	3	36.86	21.06	39.81
-4	5	3	14.42	27.68	29.88
-3	5	3	0.09	15.74	13.64
-2	5	3	11.99	6.32	25.67
-1	5	3	110.65	118.73	11.43
0	5	3	6.41	-33.99	20.26
1	5	3	4.97	14.64	23.77
2	5	3	31.81	24.77	31.39
3	5	3	10.17	-33.29	35.4
4	5	3	0.01	-27.98	38.61
-4	6	3	6.2	-2.81	31.79
-3	6	3	0.17	-18.05	28.98
-2	6	3	638.73	644.98	34.4
-1	6	3	100.04	114.12	13.14
0	6	3	102.9	97.77	12.43
1	6	3	0.02	-5.11	27.28
2	6	3	127.9	136.08	16.85
3	6	3	10.21	8.42	18.05
4	6	3	0.71	-2.61	41.11
-3	7	3	24.03	-10.03	29.78
-2	7	3	41.57	39.81	14.54
-1	7	3	10.06	10.53	26.47
0	7	3	197.8	208.28	15.04
1	7	3	313.82	288.9	18.65
2	7	3	484.46	483.84	27.07

h	k	l	F_c^2	F_o^2	σF_o^2
3	7	3	18.61	-14.44	36.3
4	7	3	1.69	-56.26	42.52
-3	8	3	2.95	24.97	29.98
-2	8	3	31.8	13.14	28.68
-1	8	3	0.08	-28.98	27.88
0	8	3	31.58	17.85	28.18
1	8	3	235.75	214.29	17.05
2	8	3	2.03	10.73	16.35
3	8	3	1.68	-32.99	37.5
-2	9	3	2.54	-10.03	29.18
-1	9	3	13.01	24.67	28.18
0	9	3	55.69	50.94	15.14
1	9	3	30.59	35.8	15.94
2	9	3	8.52	2.51	33.79
3	9	3	3.84	18.85	37.6
-2	10	3	0	-3.71	31.69
-1	10	3	1.01	4.21	30.58
0	10	3	6.23	24.37	15.34
1	10	3	13.32	21.26	31.49
2	10	3	6.84	6.52	17.65
-1	-10	4	0.07	-24.57	31.19
0	-10	4	4.4	-9.73	31.89
1	-10	4	0	25.57	30.99
-2	-9	4	0.14	10.43	30.99
-1	-9	4	35.19	50.64	15.24
0	-9	4	26.03	41.41	15.14
1	-9	4	86.4	83.53	15.94
2	-9	4	3.82	7.02	30.99
-3	-8	4	15.15	-9.83	33.19
-2	-8	4	5.29	12.23	31.09
-1	-8	4	6.9	-17.95	28.58
0	-8	4	0.91	0.6	28.38
1	-8	4	39.93	22.86	29.18
2	-8	4	2.58	3.81	30.79
3	-8	4	3.3	-17.15	33.29
-3	-7	4	21.88	26.57	31.19
-2	-7	4	20.71	-18.15	29.58
-1	-7	4	1.59	-24.27	28.28
0	-7	4	10.48	-20.96	26.57
1	-7	4	0.21	8.92	26.97
2	-7	4	0.43	-22.36	28.88
3	-7	4	50.51	61.77	17.05
-4	-6	4	2.86	-0.9	34.7
-3	-6	4	31.85	5.11	30.79
-2	-6	4	3.01	-22.36	28.58
-1	-6	4	36.67	65.18	13.04
0	-6	4	34.41	4.81	25.67
1	-6	4	106.03	137.48	14.04
2	-6	4	1.55	19.05	14.04
3	-6	4	4.36	5.82	31.29
4	-6	4	3.45	4.61	33.49
-4	-5	4	0.02	25.87	33.19
-3	-5	4	67.16	63.68	15.84
-2	-5	4	0	4.11	26.47
-1	-5	4	1.54	23.16	11.53
0	-5	4	57.45	11.43	22.36
1	-5	4	289.8	323.8	16.55
2	-5	4	16.09	7.22	27.88
3	-5	4	38.91	15.74	30.99
4	-5	4	14.19	11.83	35.2
-4	-4	4	155.1	165.06	16.55
-3	-4	4	17.29	19.55	14.44
-2	-4	4	12.28	15.74	24.97
-1	-4	4	20.03	24.27	9.83
0	-4	4	554.41	614	26.67
1	-4	4	3.1	17.55	9.93
2	-4	4	587.42	570.68	31.19
3	-4	4	74.12	59.46	15.74
4	-4	4	85.99	96.17	17.65
-4	-3	4	5.26	8.82	29.78
-3	-3	4	134.85	146	14.74
-2	-3	4	2.48	-4.31	21.76
-1	-3	4	832.36	795.6	28.48
0	-3	4	8.08	15.94	9.02
1	-3	4	700.45	649.7	27.18
2	-3	4	267.08	276.87	14.34
3	-3	4	153.63	157.84	16.24
4	-3	4	32.51	47.93	17.05
-5	-2	4	1.4	-4.71	32.09
-4	-2	4	38.11	-41.41	29.28
-3	-2	4	29.78	6.62	26.77
-2	-2	4	119.58	108.1	10.53
-1	-2	4	60.01	44.72	9.43
0	-2	4	666.8	599.66	24.57
1	-2	4	6.06	-22.96	20.06
2	-2	4	1.36	-63.58	22.76
3	-2	4	40.04	39.01	15.44
4	-2	4	36.75	-1.7	17.45
5	-2	4	15.76	13.04	37.8
-5	-1	4	3.31	14.64	31.19
-4	-1	4	1.51	-0.7	28.08
-3	-1	4	17.23	-0.9	26.37
-2	-1	4	14.81	-25.47	19.55
-1	-1	4	46.63	36.6	9.33
0	-1	4	40.2	13.84	16.24
1	-1	4	188.98	202.26	11.33
2	-1	4	17.79	19.75	10.93
3	-1	4	48.12	53.45	15.24
4	-1	4	0.97	0.7	33.09
5	-1	4	1.53	41.82	18.45
-5	0	4	18.81	1.91	32.39
-4	0	4	87.79	65.28	15.24
-3	0	4	50.54	56.96	13.14
-2	0	4	278.68	275.26	15.64
-1	0	4	374.33	384.56	20.66
0	0	4	736.98	-1151.29	34.29
1	0	4	297.96	301.43	16.14
2	0	4	108.06	107.6	11.13
3	0	4	85.97	90.85	15.34
4	0	4	13.61	-10.03	32.49
5	0	4	0.16	4.61	36.7
-5	1	4	0.27	20.06	32.29
-4	1	4	18.31	-0.7	28.78
-3	1	4	59.56	68.29	13.74
-2	1	4	805.24	809.54	30.18
-1	1	4	15395.9	14914.9	303.44
0	1	4	9779.19	9065.79	184.81
1	1	4	0.42	17.35	21.06
2	1	4	897.92	971.69	33.89
3	1	4	100.95	75.91	15.04
4	1	4	10.22	-57.96	33.19
5	1	4	6.88	-5.41	36.7
-5	2	4	3.59	-29.68	32.99
-4	2	4	7.27	13.14	28.88
-3	2	4	0.07	14.44	13.34
-2	2	4	76.62	75.11	10.43
-1	2	4	1928.78	1850.12	48.23
0	2	4	3377.84	3283.49	71.9
1	2	4	2063.91	2082.36	51.54
2	2	4	57.15	67.39	11.43
3	2	4	347.54	378.55	20.86
4	2	4	27.3	15.64	16.55
5	2	4	2.7	-35	36.3
-4	3	4	3.02	-17.35	30.08
-3	3	4	26.89	35	13.64
-2	3	4	31.78	18.45	21.06
-1	3	4	13.28	-14.84	18.95
0	3	4	158.3	150.02	10.73
1	3	4	579.46	572.48	27.38
2	3	4	451.86	453.35	21.86
3	3	4	8	2.11	32.89
4	3	4	13.52	24.97	31.39
-4	4	4	4.43	-35.1	29.68
-3	4	4	0.52	21.76	27.48
-2	4	4	63.31	62.87	12.03
-1	4	4	9.78	-5.52	19.45
0	4	4	57.68	49.14	9.83
1	4	4	84.82	72.2	11.23
2	4	4	3.25	14.74	29.28
3	4	4	10.07	-0.5	35.4
4	4	4	63.37	68.99	20.26
-4	5	4	0	-0.8	30.18
-3	5	4	16.01	5.72	27.98
-2	5	4	0.82	6.32	25.27
-1	5	4	34.95	36.2	10.93
0	5	4	1.26	4.71	20.46
1	5	4	12.79	-4.71	24.67
2	5	4	118.66	131.66	16.45
3	5	4	29.16	13.64	35.9
4	5	4	4.03	24.87	40.51
-4	6	4	1.02	-49.14	31.79
-3	6	4	1.07	6.72	14.14
-2	6	4	3.32	-19.45	27.38
-1	6	4	143.4	141.99	13.54
0	6	4	143.04	123.34	12.94
1	6	4	34.69	54.65	13.94
2	6	4	0.64	-9.33	32.39
3	6	4	33.64	-45.12	36.3
4	6	4	20.46	29.38	40.01
-3	7	4	12.07	-0.7	29.88
-2	7	4	26.99	21.66	27.68
-1	7	4	375.59	378.05	20.56
0	7	4	12.99	6.22	26.87
1	7	4	998.73	1003.18	42.52
2	7	4	220.97	219.91	17.95
3	7	4	21.15	-26.57	37.4
4	7	4	15.91	-38.41	43.72
-3	8	4	5.06	21.46	29.98
-2	8	4	29.67	-6.52	30.08
-1	8	4	14.29	3.21	27.78
0	8	4	465.08	500.48	27.18
1	8	4	512.27	533.68	29.18
2	8	4	18.1	-5.72	33.79
3	8	4	35.14	27.78	19.65
-2	9	4	11.44	-7.42	30.58
-1	9	4	34.19	-66.99	31.79
0	9	4	31.43	22.96	29.68
1	9	4	0.02	13.24	31.89
2	9	4	3.79	14.74	33.89
3	9	4	0.21	-61.27	40.81
-2	10	4	0	-4.71	31.49
-1	10	4	7.11	0	30.79
0	10	4	0.94	3.31	30.89
1	10	4	2.23	12.74	32.49
2	10	4	6.78	-7.32	36.2
-1	-10	5	0.86	-44.32	32.79
0	-10	5	3.59	-4.41	32.39
1	-10	5	0.49	-38.91	32.59
-2	-9	5	0.13	31.99	15.84
-1	-9	5	0.1	8.92	28.98
0	-9	5	1.3	-7.82	28.28
1	-9	5	0.04	-33.19	31.29
2	-9	5	0.02	32.19	15.74
-3	-8	5	16.01	14.54	33.09
-2	-8	5	8.23	-6.22	29.78
-1	-8	5	153.41	119.63	15.64
0	-8	5	77.15	52.55	14.24
1	-8	5	9.15	25.17	14.54
2	-8	5	15.98	-28.98	30.99
3	-8	5	51.49	29.18	33.59
-3	-7	5	85.02	105.09	16.24
-2	-7	5	24.53	-19.85	29.88
-1	-7	5	55.06	53.05	13.84
0	-7	5	26.78	15.64	27.58
1	-7	5	20.33	15.34	13.74
2	-7	5	0.43	-34.5	28.98
3	-7	5	97.82	94.48	17.05
-4	-6	5	16.45	34.09	17.25
-3	-6	5	0.21	-0.7	30.18
-2	-6	5	0.55	-14.44	28.58
-1	-6	5	9.6	-34.19	25.77
0	-6	5	6.92	2.51	25.57
1	-6	5	0.66	-21.86	26.87
2	-6	5	19.28	27.88	28.68
3	-6	5	2.15	-32.49	31.39
4	-6	5	22.11	-9.23	35.5
-4	-5	5	143.97	167.88	17.25
-3	-5	5	171.68	166.06	16.35
-2	-5	5	0.36	-33.79	27.58
-1	-5	5	187.48	174.28	13.04
0	-5	5	123.35	127.75	12.03
1	-5	5	34.27	17.15	12.23
2	-5	5	88.73	109	14.64
3	-5	5	30.39	16.75	16.04
4	-5	5	11.35	-26.37	35.5
-4	-4	5	63.04	63.28	16.04
-3	-4	5	31.16	15.84	14.24
-2	-4	5	19.03	26.67	12.53
-1	-4	5	7.84	10.63	20.06
0	-4	5	91.78	94.96	9.93
1	-4	5	429.1	463.88	23.77
2	-4	5	278.81	303.24	17.65
3	-4	5	44.18	12.74	31.69
4	-4	5	3.1	-8.72	33.99
-4	-3	5	0.23	25.37	29.28
-3	-3	5	0.06	-23.97	26.87
-2	-3	5	58.38	49.94	11.43
-1	-3	5	15.85	15.54	18.85
0	-3	5	3.11	-24.97	18.35
1	-3	5	515.72	516.13	25.47
2	-3	5	122.41	141.19	13.24
3	-3	5	127.12	103.09	16.35
4	-3	5	14.97	9.02	34.5
-4	-2	5	5.72	-3.51	29.08
-3	-2	5	23.36	10.43	26.47
-2	-2	5	104.13	102.78	10.33
-1	-2	5	2.36	-32.59	18.45
0	-2	5	296.33	287.6	15.54
1	-2	5	9.48	-28.08	19.75
2	-2	5	337.3	371.63	20.26
3	-2	5	127.13	121.34	16.45
4	-2	5	0.51	-2.81	32.09
-5	-1	5	0	19.35	31.69
-4	-1	5	0.51	-79.52	29.98
-3	-1	5	7.81	2.51	26.37
-2	-1	5	36.73	21.16	9.73
-1	-1	5	420.35	427.18	22.66
0	-1	5	891.59	834.91	27.18
1	-1	5	256.27	260.62	13.84
2	-1	5	8.1	-24.27	22.16
3	-1	5	51.23	64.48	15.54
4	-1	5	6.18	27.88	16.95
5	-1	5	108.94	140.19	19.85
-5	0	5	5.51	10.03	32.19
-4	0	5	44.81	48.33	14.94
-3	0	5	4.78	-17.55	26.87
-2	0	5	37.2	45.53	9.53
-1	0	5	344.7	356.99	19.05
0	0	5	2425.95	1914.7	45.93
1	0	5	248.6	257.91	14.64
2	0	5	6.9	-0.6	21.76
3	0	5	15.08	10.63	30.38
4	0	5	0.01	10.13	32.69
5	0	5	4.6	35.4	18.55
-5	1	5	35.44	26.87	33.59
-4	1	5	13.43	-15.74	30.08
-3	1	5	5.08	18.55	13.04
-2	1	5	103.56	90.25	10.13
-1	1	5	301.2	315.27	17.05
0	1	5	1242.8	1202.83	32.09
1	1	5	584.81	620.92	26.87
2	1	5	14.14	35.3	10.63
3	1	5	28.5	58.16	14.94
4	1	5	20.52	26.07	16.55
5	1	5	25.65	-12.74	37.3
-5	2	5	1.3	-8.52	17.25
-4	2	5	2.25	7.02	28.98
-3	2	5	165.03	156.13	14.44
-2	2	5	5255.21	5201.29	114.32
-1	2	5	4787.1	4627.91	99.98

h	k	l	F_c^2	F_o^2	σF_o^2
0	2	5	26.98	3.81	19.35
1	2	5	21.05	-3.61	22.66
2	2	5	0.76	-24.77	22.96
3	2	5	99.92	92.15	15.44
4	2	5	24	43.82	16.14
5	2	5	15.93	-7.32	37.3
-4	3	5	13.68	-29.88	29.08
-3	3	5	1.14	-30.68	27.48
-2	3	5	5.52	-3.41	21.76
-1	3	5	276.17	274.36	15.34
0	3	5	127.82	115.92	10.33
1	3	5	5623.03	5925.9	127.05
2	3	5	1198.49	1338.5	43.62
3	3	5	160.14	169.37	17.15
4	3	5	1.52	-26.57	33.39
-4	4	5	0.23	-22.96	29.28
-3	4	5	0.66	14.94	13.64
-2	4	5	1.6	16.85	23.26
-1	4	5	0.09	-7.52	19.55
0	4	5	239.19	228.63	11.23
1	4	5	159.77	181	12.13
2	4	5	251.98	236.55	16.45
3	4	5	26.72	33.99	18.05
4	4	5	40.92	49.64	19.45
-4	5	5	0.64	-31.89	30.48
-3	5	5	51.78	46.33	13.94
-2	5	5	12.73	5.92	25.97
-1	5	5	60.86	80.22	11.33
0	5	5	36.05	1	21.46
1	5	5	7.57	-10.23	24.37
2	5	5	6.77	29.68	15.94
3	5	5	58.06	73.6	18.35
4	5	5	0.09	-38.61	41.01
-4	6	5	1.42	12.84	15.94
-3	6	5	25.86	25.97	14.74
-2	6	5	24.96	17.05	13.34
-1	6	5	1.56	-39.51	25.97
0	6	5	153.03	176.29	13.44
1	6	5	36.2	24.17	14.14
2	6	5	0.16	-76.71	33.59
3	6	5	0.05	6.82	36.4
4	6	5	1.25	23.36	41.31
-3	7	5	6.87	-39.41	28.98
-2	7	5	21.62	24.97	13.94
-1	7	5	82.6	77.31	14.04
0	7	5	81.45	94.86	13.94
1	7	5	48.72	72.5	15.24
2	7	5	30.48	18.85	32.69
3	7	5	27.12	-51.64	38.71
4	7	5	0.03	32.79	42.52
-3	8	5	18.27	19.65	15.34
-2	8	5	1.99	14.54	27.88
-1	8	5	154.85	129.06	15.64
0	8	5	292.78	283.18	16.95
1	8	5	8.56	22.06	15.54
2	8	5	0.63	2.21	32.99
3	8	5	7.37	5.92	36.7
-2	9	5	0.71	-56.16	31.19
-1	9	5	5.56	24.57	29.18
0	9	5	6.6	22.06	15.04
1	9	5	2.14	-11.03	31.09
2	9	5	3.23	-15.54	33.19
3	9	5	13.54	-63.98	40.41
-2	10	5	1.95	-4.61	32.69
-1	10	5	0.69	-48.63	31.39
0	10	5	9.27	-57.76	30.99
1	10	5	4.92	-6.82	32.59
2	10	5	2.36	15.74	35.2
-1	-10	6	0.08	-21.56	32.39
0	-10	6	5.07	24.57	15.54
-2	-9	6	3.84	22.46	31.19
-1	-9	6	5.43	5.21	15.44
0	-9	6	74.23	81.83	15.84
1	-9	6	28.17	36	15.54
2	-9	6	6.06	21.76	31.19
-3	-8	6	10.97	-19.35	34.09
-2	-8	6	15.23	18.25	30.48
-1	-8	6	113.23	120.13	15.24
0	-8	6	5.39	-8.22	28.88
1	-8	6	5.87	-56.16	29.68
2	-8	6	0.01	-15.94	30.79
3	-8	6	9.39	27.88	17.15
-3	-7	6	62.17	93.66	16.55
-2	-7	6	5.55	27.28	28.48
-1	-7	6	70.98	27.28	28.58
0	-7	6	9.2	-5.41	13.84
1	-7	6	21.17	-3.91	13.84
2	-7	6	39.39	16.55	15.34
3	-7	6	49.88	57.46	16.85
-4	-6	6	4.53	-13.74	17.35
-3	-6	6	8.42	-16.45	29.88
-2	-6	6	10.47	-20.26	28.68
-1	-6	6	32.7	41.11	13.34
0	-6	6	49.37	63.98	12.84
1	-6	6	8.35	0.5	27.18
2	-6	6	0.28	-28.48	29.28
3	-6	6	54.62	40.41	16.55
4	-6	6	2.24	-27.98	35.8
-4	-5	6	79.12	77.31	16.65
-3	-5	6	192	155.23	16.35
-2	-5	6	17.45	-3.21	13.74
-1	-5	6	117.64	119.23	12.74
0	-5	6	6.38	-37.3	23.16
1	-5	6	9.81	18.35	12.43
2	-5	6	10.51	30.38	14.04
3	-5	6	64.41	60.17	16.04
4	-5	6	2.55	-12.13	35.4
-4	-4	6	175.14	190.93	17.45
-3	-4	6	48.29	25.27	28.68
-2	-4	6	7.94	-20.96	26.07
-1	-4	6	37.19	36.2	10.53
0	-4	6	16.17	-3.11	20.16
1	-4	6	84.8	81.22	11.53
2	-4	6	25.63	21.46	28.06
3	-4	6	7.55	26.07	30.89
4	-4	6	1	31.39	34.19
-4	-3	6	1.3	-10.03	14.94
-3	-3	6	23.22	27.98	13.74
-2	-3	6	61.76	71.6	11.63
-1	-3	6	2480.8	2513.46	60.77
0	-3	6	913.65	871.61	29.98
1	-3	6	941.15	982.12	33.09
2	-3	6	73.1	79.12	13.24
3	-3	6	144.83	138.78	16.55
4	-3	6	2.3	18.95	34.6
-4	-2	6	29.01	16.65	29.98
-3	-2	6	23.67	43.42	13.04
-2	-2	6	5.04	9.43	10.33
-1	-2	6	117.78	111.71	9.43
0	-2	6	910.6	894.27	29.68
1	-2	6	71.99	58.96	10.03
2	-2	6	555.73	602.47	30.99
3	-2	6	165.02	162.75	16.85
4	-2	6	13.39	-20.16	34.6
-5	-1	6	14.54	-58.66	34.19
-4	-1	6	3.38	-25.17	29.08
-3	-1	6	0	-29.48	26.27
-2	-1	6	25.37	6.32	19.96
-1	-1	6	338.81	331.82	17.65
0	-1	6	168.1	179.3	10.53
1	-1	6	396.93	415.55	22.36
2	-1	6	29.12	20.26	23.06
3	-1	6	91.14	77.11	15.74
4	-1	6	0.26	-18.85	33.59
5	-1	6	62.73	62.47	20.46
-5	0	6	8.28	36.6	16.35
-4	0	6	11.11	-9.73	27.88
-3	0	6	18.31	6.92	25.67
-2	0	6	397.04	375.44	20.26
-1	0	6	98.86	100.88	9.63
0	0	6	278.58	-1281.55	38.61
1	0	6	0.08	-5.92	21.46
2	0	6	15.81	18.55	11.03
3	0	6	22.21	-20.76	30.58
4	0	6	18.6	27.58	17.15
5	0	6	13.75	11.03	36.8
-5	1	6	36.91	11.93	33.49
-4	1	6	31.01	7.62	29.76
-3	1	6	0.36	9.73	13.04
-2	1	6	74.53	77.21	9.93
-1	1	6	0.44	-10.23	19.25
0	1	6	49.52	48.33	9.13
1	1	6	126.83	134.17	11.33
2	1	6	247.97	253.3	14.04
3	1	6	8.17	-48.03	30.28
4	1	6	9.81	-29.58	32.19
5	1	6	1.51	0	36.6
-5	2	6	1.29	21.06	17.15
-4	2	6	0.81	-37.5	29.18
-3	2	6	7.03	-24.27	26.97
-2	2	6	585.42	619.31	28.28
-1	2	6	471.67	516.43	23.77
0	2	6	6.89	-5.52	20.16
1	2	6	106.23	96.87	11.13
2	2	6	419.31	612.8	31.19
3	2	6	150.56	168.67	15.84
4	2	6	89.24	111.61	17.15
5	2	6	20.03	8.52	19.15
-4	3	6	0.13	2.51	14.74
-3	3	6	26.51	23.77	13.54
-2	3	6	638.11	642.58	29.78
-1	3	6	111.3	107.7	9.73
0	3	6	2027.79	2051.28	50.64
1	3	6	365.53	366.21	19.15
2	3	6	645.75	668.85	33.99
3	3	6	74.02	53.75	16.85
4	3	6	4.5	29.68	33.09
-4	4	6	1.74	-49.34	31.09
-3	4	6	25.64	11.63	27.98
-2	4	6	159.34	159.14	12.84
-1	4	6	314.65	351.57	18.85
0	4	6	239.55	258.11	13.54
1	4	6	563.01	587.33	28.68
2	4	6	163.8	184.21	16.14
3	4	6	0.47	-23.57	35.6
4	4	6	71.26	84.83	19.45
-4	5	6	3.27	-19.75	29.98
-3	5	6	1.32	22.96	28.08
-2	5	6	27.26	14.84	26.77
-1	5	6	13.97	9.73	22.16
0	5	6	85.16	79.42	10.73
1	5	6	116.7	124.54	13.24
2	5	6	28.29	28.58	16.45
3	5	6	1.37	0.6	36.6
4	5	6	2.79	28.38	40.01
-4	6	6	5.27	22.26	15.74
-3	6	6	13.54	18.95	28.28
-2	6	6	11.1	26.27	13.54
-1	6	6	1.4	7.62	24.97
0	6	6	6.79	17.15	12.63
1	6	6	0.61	-23.57	28.68
2	6	6	8.27	28.98	32.89
3	6	6	1.32	-1.3	36.6
4	6	6	7.54	26.07	41.51
-3	7	6	64.38	45.83	15.64
-2	7	6	95.03	86.94	14.84
-1	7	6	1.29	11.63	26.67
0	7	6	0.83	-3.51	13.84
1	7	6	92.53	97.17	15.54
2	7	6	78.01	79.32	17.35
3	7	6	56.36	46.93	19.25
4	7	6	1.6	-26.37	43.92
-3	8	6	0.34	-22.36	29.88
-2	8	6	80.08	81.22	15.64
-1	8	6	0.37	-14.24	28.38
0	8	6	1662.63	1623.59	54.25
1	8	6	999.08	1006.38	45.53
2	8	6	10.33	12.23	33.49
3	8	6	35.45	26.27	39.81
-2	9	6	0	10.73	29.28
-1	9	6	0.19	-24.57	29.08
0	9	6	14.34	34.09	14.94
1	9	6	55.03	65.18	16.35
2	9	6	2.53	-33.49	34.6
-2	10	6	6.87	-13.04	31.79
-1	10	6	6.86	26.07	15.34
0	10	6	7.18	9.93	29.18
1	10	6	2.66	10.23	32.69
2	10	6	0.67	11.03	35.4
0	-10	7	0.03	34.8	16.04
-2	-9	7	6.66	23.77	31.49
-1	-9	7	8.57	13.44	29.58
0	-9	7	23.81	36.7	14.84
1	-9	7	0.24	-23.57	29.18
2	-9	7	0.84	-33.99	32.49
-3	-8	7	10.5	-25.27	35.5
-2	-8	7	34.76	1.6	15.74
-1	-8	7	65.83	72.5	15.14
0	-8	7	198.42	180.24	15.44
1	-8	7	70.29	70.6	14.84
2	-8	7	0.13	-26.77	31.09
-3	-7	7	0.24	8.82	16.04
-2	-7	7	154.11	133.47	15.54
-1	-7	7	19.98	18.45	28.38
0	-7	7	5.89	26.07	13.34
1	-7	7	50.82	49.34	14.34
2	-7	7	85.01	86.94	15.74
3	-7	7	305.58	320.39	19.75
-3	-6	7	24.5	25.87	30.58
-2	-6	7	0.06	-38.51	27.98
-1	-6	7	2.73	-40.11	27.28
0	-6	7	32.83	37.6	13.04
1	-6	7	1.07	17.45	13.34
2	-6	7	19.94	15.74	28.88
3	-6	7	1.81	-37.5	31.69
-4	-5	7	0.71	-17.45	31.69
-3	-5	7	14.38	-17.95	28.98
-2	-5	7	9.97	0.5	26.27
-1	-5	7	3.08	17.45	11.93
0	-5	7	81.68	70.9	11.93
1	-5	7	4.53	3.41	12.63
2	-5	7	6.61	21.66	14.14
3	-5	7	46.48	73.4	15.94
4	-5	7	1.92	12.23	33.89
-4	-4	7	276.71	317.58	18.65
-3	-4	7	58.69	45.83	14.64
-2	-4	7	32.6	24.57	24.97
-1	-4	7	21.14	14.84	21.66
0	-4	7	237.96	233.75	13.64
1	-4	7	53.36	57.36	11.43
2	-4	7	116.32	119.23	14.14
3	-4	7	36.08	6.92	31.39
4	-4	7	1.49	-40.01	33.89
-4	-3	7	1.24	-18.45	28.78
-3	-3	7	2.1	0.6	26.97
-2	-3	7	96.29	95.56	12.03
-1	-3	7	1166.69	1172.24	36.4
0	-3	7	635.6	656.92	26.57
1	-3	7	81.03	85.64	10.43
2	-3	7	5.68	24.77	13.04
3	-3	7	0.77	-15.14	32.49
4	-3	7	7.36	-69.89	34.09
-4	-2	7	60.53	53.05	14.84
-3	-2	7	24.96	46.43	13.44
-2	-2	7	835.3	900.99	33.09
-1	-2	7	1345.43	1420.43	39.51
0	-2	7	17.71	-6.42	18.85
1	-2	7	51.54	18.75	20.26
2	-2	7	3.5	6.72	24.67
3	-2	7	4.99	-2.71	31.19

h	k	l	F_c^2	F_o^2	σF_o^2
4	-2	7	14.89	11.73	34.19
-4	-1	7	6.97	10.03	28.68
-3	-1	7	17.57	4.11	27.07
-2	-1	7	6.69	15.04	19.85
-1	-1	7	352.91	343.35	18.45
0	-1	7	54.29	59.36	9.63
1	-1	7	330.48	330.21	17.95
2	-1	7	181.61	176.99	12.63
3	-1	7	51	38.71	15.64
4	-1	7	50.44	72	17.35
5	-1	7	56.66	22.46	40.61
-5	0	7	0.85	27.07	32.99
-4	0	7	0.22	23.87	27.18
-3	0	7	19.49	9.23	25.47
-2	0	7	4.04	5.21	19.65
-1	0	7	432.06	422.57	22.56
0	0	7	727.23	714.98	26.97
1	0	7	65.66	62.57	10.53
2	0	7	221.71	223.82	14.24
3	0	7	3.12	-26.27	30.28
4	0	7	59.72	-16.75	33.69
5	0	7	54.42	5.62	38.21
-5	1	7	1.69	11.23	32.99
-4	1	7	0.01	14.74	28.08
-3	1	7	66.06	56.86	13.34
-2	1	7	82.41	65.98	10.13
-1	1	7	27.66	-21.26	18.75
0	1	7	212.97	203.76	10.73
1	1	7	111.75	115.62	10.93
2	1	7	32.75	8.02	23.67
3	1	7	3.88	-22.66	29.88
4	1	7	0.02	6.42	16.65
5	1	7	3.99	25.87	36.3
-4	2	7	0.45	-3.51	14.64
-3	2	7	111.08	109.5	14.04
-2	2	7	1618.62	1742.62	48.13
-1	2	7	1268.83	1324.46	37
0	2	7	1159.07	1107.77	33.49
1	2	7	305.57	326.6	18.25
2	2	7	435.25	488.15	26.27
3	2	7	105.06	90.35	15.74
4	2	7	157.67	184.81	17.65
5	2	7	0.08	-77.72	38.51
-4	3	7	0.73	18.55	29.18
-3	3	7	63.35	70.8	13.84
-2	3	7	264.74	247.48	13.14
-1	3	7	0.77	0.2	9.13
0	3	7	11.72	5.62	19.35
1	3	7	780.64	862.79	31.79
2	3	7	705.8	840.23	36.2
3	3	7	25.07	-21.26	33.59
4	3	7	39.55	46.03	17.45
-4	4	7	35.39	26.07	15.44
-3	4	7	28.03	-7.72	27.78
-2	4	7	10.2	4.91	24.27
-1	4	7	55.65	59.67	9.83
0	4	7	515.65	557.34	26.07
1	4	7	85.33	120.53	11.93
2	4	7	327	337.03	19.15
3	4	7	4.24	16.24	34.6
4	4	7	49.92	78.42	19.05
-4	5	7	6.56	16.85	29.68
-3	5	7	0.02	20.06	27.78
-2	5	7	4.54	14.34	12.84
-1	5	7	32.87	22.16	22.56
0	5	7	25.76	38.3	10.93
1	5	7	13.38	27.68	12.94
2	5	7	0.17	20.36	32.09
3	5	7	2.79	18.35	36.7
4	5	7	12.33	-30.89	38.81
-4	6	7	0.01	9.83	30.18
-3	6	7	1.55	-33.99	27.18
-2	6	7	3.08	-8.32	25.87
-1	6	7	2.4	7.72	25.07
0	6	7	49.69	47.23	13.04
1	6	7	164.1	150.82	15.24
2	6	7	34.72	68.09	16.75
3	6	7	36.71	33.99	18.85
4	6	7	1.3	6.12	41.41
-3	7	7	37.49	60.07	15.24
-2	7	7	16.56	25.77	14.04
-1	7	7	8.44	-15.14	27.38
0	7	7	25.27	22.38	28.08
1	7	7	47.95	64.18	15.24
2	7	7	81.01	65.48	17.35
3	7	7	0.38	-22.96	37.9
-3	8	7	46.09	52.55	16.14
-2	8	7	57.74	50.34	14.94
-1	8	7	31.27	-5.21	28.38
0	8	7	53.43	63.68	14.34
1	8	7	46.27	26.47	31.09
2	8	7	58.51	50.54	17.15
3	8	7	1	11.03	19.25
-2	9	7	25.52	8.22	29.88
-1	9	7	269.11	284.59	17.55
0	9	7	387.63	426.68	21.16
1	9	7	39.64	56.76	16.35
2	9	7	14.42	-2.61	17.65
-2	10	7	0.01	-28.98	32.59
-1	10	7	6.49	10.33	29.78
0	10	7	0.7	19.05	29.98
1	10	7	0.13	-43.42	33.99
2	10	7	20.46	31.49	34.7
-2	-9	8	5.09	-13.04	33.09
-1	-9	8	2.96	6.92	28.48
0	-9	8	2.33	18.35	28.18
1	-9	8	0.27	7.82	15.34
2	-9	8	0.46	-20.16	17.35
-2	-8	8	6.28	2.51	30.08
-1	-8	8	38.99	45.63	14.54
0	-8	8	32.39	-10.93	28.48
1	-8	8	0.19	16.85	14.64
2	-8	8	10.22	-19.15	30.46
-3	-7	8	19.23	18.95	31.09
-2	-7	8	211.49	207.98	16.24
-1	-7	8	1.83	25.57	27.88
0	-7	8	37.72	-15.64	28.18
1	-7	8	8.41	-16.35	27.18
2	-7	8	3.77	7.32	28.78
3	-7	8	5.49	7.82	32.99
-3	-6	8	0.01	18.65	29.18
-2	-6	8	71.32	74.81	14.64
-1	-6	8	15.1	14.74	25.87
0	-6	8	178.07	182.1	14.04
1	-6	8	46.46	44.52	13.64
2	-6	8	485.58	474.61	25.47
3	-6	8	107.19	131.56	17.15
-4	-5	8	0	15.04	30.99
-3	-5	8	25.71	27.58	28.08
-2	-5	8	9.1	27.68	13.14
-1	-5	8	112.8	100.68	12.94
0	-5	8	3.55	7.82	23.57
1	-5	8	52.16	53.95	13.24
2	-5	8	19.09	-4.61	29.48
3	-5	8	23.98	17.65	15.84
4	-5	8	1.82	-35.6	35.5
-4	-4	8	10.77	28.18	30.28
-3	-4	8	1.18	-28.38	27.98
-2	-4	8	34.12	15.54	12.94
-1	-4	8	101.7	111.91	11.53
0	-4	8	14.66	-12.74	21.36
1	-4	8	1.79	17.25	11.63
2	-4	8	60.3	55.55	14.54
3	-4	8	0.28	-16.14	29.98
4	-4	8	8.87	-80.62	34.9
-4	-3	8	68.64	65.48	15.34
-3	-3	8	5.71	0.6	26.57
-2	-3	8	59.59	81.93	12.03
-1	-3	8	5.13	-24.07	19.45
0	-3	8	59.28	47.83	9.73
1	-3	8	2.49	-0.3	20.76
2	-3	8	25.72	28.36	13.54
3	-3	8	23.46	13.74	31.19
4	-3	8	0.01	1.5	34.9
-4	-2	8	4.45	14.94	28.68
-3	-2	8	1.54	22.96	25.67
-2	-2	8	402.46	457.37	24.27
-1	-2	8	838.32	899.89	30.88
0	-2	8	379.91	314.67	16.75
1	-2	8	43.02	40.81	9.93
2	-2	8	912.27	988.23	38.11
3	-2	8	0.62	18.85	15.54
4	-2	8	87.23	93.36	17.65
-4	-1	8	8.02	-16.65	28.98
-3	-1	8	27.3	42.32	13.14
-2	-1	8	11.36	3.51	20.46
-1	-1	8	360.82	385.77	21.36
0	-1	8	5.41	-2.81	18.55
1	-1	8	21.85	8.42	19.65
2	-1	8	22.35	-4.21	24.07
3	-1	8	20.64	33.09	15.54
4	-1	8	5.72	-27.38	32.89
-4	0	8	0.73	4.91	27.88
-3	0	8	103.71	93.36	13.44
-2	0	8	70.19	69.39	10.43
-1	0	8	5.86	-7.22	17.85
0	0	8	0.56	-363.81	23.57
1	0	8	27.47	8.92	10.13
2	0	8	60	54.95	11.73
3	0	8	0.05	-63.28	31.89
4	0	8	8.93	4.21	33.59
5	0	8	0.58	-8.42	39.31
-4	1	8	5.04	35.7	14.34
-3	1	8	21.37	-2.61	28.27
-2	1	8	25.64	26.97	10.13
-1	1	8	25.75	-36.7	18.65
0	1	8	2.8	1.8	9.63
1	1	8	2.61	-52.24	21.16
2	1	8	6.5	1.4	23.87
3	1	8	0.19	10.33	30.68
4	1	8	20.83	8.42	31.79
5	1	8	8.08	25.27	38.31
-4	2	8	0.01	-18.25	28.98
-3	2	8	110.09	114.42	13.94
-2	2	8	1029.33	796.4	31.79
-1	2	8	382.1	363.51	19.55
0	2	8	1359.98	1447.91	39.31
1	2	8	8.23	-30.48	21.36
2	2	8	77.51	75.51	12.84
3	2	8	5.05	1	30.58
4	2	8	12.51	22.26	33.89
-4	3	8	8.81	27.28	14.84
-3	3	8	460.54	408.13	22.66
-2	3	8	876.18	858.48	34.4
-1	3	8	1.24	-1.1	9.13
0	3	8	128.83	100.08	10.03
1	3	8	627.44	592.94	28.68
2	3	8	115.78	115.32	14.64
3	3	8	171.32	190.73	17.65
4	3	8	82.34	77.72	17.95
-4	4	8	2.74	-11.83	28.98
-3	4	8	0.04	1.8	27.48
-2	4	8	18.31	16.55	23.87
-1	4	8	134.09	141.29	10.83
0	4	8	1261.7	1288.67	38.41
1	4	8	240.42	256.41	13.34
2	4	8	55.71	64.88	15.74
3	4	8	17.41	-69.99	36.3
4	4	8	11.18	20.96	35.7
-4	5	8	5.99	-15.84	31.09
-3	5	8	18.57	-15.04	28.18
-2	5	8	72.18	96.27	13.14
-1	5	8	29.99	25.97	11.63
0	5	8	0.58	20.56	22.26
1	5	8	371.03	389.68	19.75
2	5	8	11.93	-40.51	33.49
3	5	8	109.94	98.87	19.05
4	5	8	37.99	30.38	39.31
-4	6	8	13.75	-8.92	31.39
-3	6	8	28.14	-5.01	29.38
-2	6	8	3.62	-1.1	26.77
-1	6	8	39.96	18.25	26.17
0	6	8	46.28	48.13	13.04
1	6	8	4.58	10.53	14.34
2	6	8	17.68	20.16	17.05
3	6	8	9.5	6.32	36.1
4	6	8	1	-14.14	41.72
-3	7	8	0.69	10.33	14.94
-2	7	8	1.45	-7.22	26.77
-1	7	8	59.25	57.06	13.94
0	7	8	20.91	14.24	13.94
1	7	8	13.16	-25.97	30.79
2	7	8	8.9	-5.52	16.95
3	7	8	28.64	-20.06	38.01
-3	8	8	28.72	38.61	15.14
-2	8	8	2.67	-1.4	27.98
-1	8	8	2.49	2.01	26.87
0	8	8	0.17	-43.32	28.08
1	8	8	96.58	86.14	16.04
2	8	8	38.95	22.96	17.55
3	8	8	19.77	13.74	37.5
-2	9	8	2.43	-1.5	15.44
-1	9	8	161.72	217.5	16.75
0	9	8	206.31	189.22	16.75
1	9	8	10.81	23.97	30.48
2	9	8	0.02	6.92	17.95
-1	10	8	33.11	33.29	15.94
0	10	8	31.79	23.26	32.29
1	10	8	11.01	6.82	33.29
2	10	8	24.46	57.66	19.35
-1	-9	9	2.02	12.23	30.48
0	-9	9	7.9	16.14	28.48
1	-9	9	9.47	-39.51	32.29
-2	-8	9	23.73	12.63	30.28
-1	-8	9	1.68	4.21	14.64
0	-8	9	16.69	26.87	28.08
1	-8	9	1.29	26.27	14.84
2	-8	9	10.37	9.33	30.38
-3	-7	9	28.49	14.94	31.19
-2	-7	9	3.09	-25.47	28.68
-1	-7	9	227.11	206.37	15.44
0	-7	9	208.74	205.77	15.34
1	-7	9	0.28	-23.67	27.98
2	-7	9	79.16	91.55	15.64
3	-7	9	12.83	20.46	16.75
-3	-6	9	113.94	106.59	16.04
-2	-6	9	2.88	8.72	13.74
-1	-6	9	52.35	48.23	13.24
0	-6	9	157.43	172.08	14.24
1	-6	9	8.21	-3.01	27.07
2	-6	9	288.44	314.77	17.55
3	-6	9	105.89	104.99	17.25
-4	-5	9	1.67	-20.76	31.19
-3	-5	9	0.12	17.35	27.38
-2	-5	9	68.08	70.5	13.54
-1	-5	9	16.89	7.62	24.67
0	-5	9	46.75	41.21	12.33
1	-5	9	11.75	27.78	12.94
2	-5	9	11.27	18.05	14.54
3	-5	9	1.12	-5.72	30.89
4	-5	9	0.01	8.22	17.65
-4	-4	9	28.9	26.27	15.64
-3	-4	9	1.87	-15.94	14.14
-2	-4	9	15.96	42.02	12.63
-1	-4	9	1.36	-13.64	23.06
0	-4	9	0	2.51	21.86
1	-4	9	20.97	2.71	24.77
2	-4	9	3.69	23.77	28.18
3	-4	9	11.53	-13.94	31.39
4	-4	9	0	-13.84	17.55

h	k	l	F_c^2	F_o^2	σF_o^2
-4	-3	9	19.34	-15.94	29.48
-3	-3	9	2.11	-38.21	26.07
-2	-3	9	0.09	26.07	14.34
-1	-3	9	3.8	-20.16	20.46
0	-3	9	21.29	16.95	19.35
1	-3	9	27.5	17.85	22.36
2	-3	9	26.76	49.64	13.74
3	-3	9	0.56	-48.43	31.69
4	-3	9	0.71	-4.71	34.29
-4	-2	9	0.13	14.54	28.68
-3	-2	9	0.94	-6.42	25.17
-2	-2	9	1.15	27.28	11.03
-1	-2	9	136.19	143.4	10.23
0	-2	9	0.13	-8.22	18.65
1	-2	9	126.97	111.51	10.73
2	-2	9	72.74	100.68	13.54
3	-2	9	5.38	18.75	15.64
4	-2	9	12.78	-21.96	34.6
-4	-1	9	4.59	2.01	14.44
-3	-1	9	106.49	107.5	13.44
-2	-1	9	0.16	-4.01	20.96
-1	-1	9	1352.14	1401.88	39.41
0	-1	9	111.57	111.41	9.73
1	-1	9	2249.45	2506.24	60.37
2	-1	9	458.6	488.95	26.77
3	-1	9	42.12	39.21	15.94
4	-1	9	2.69	-52.85	34.29
-4	0	9	49.19	10.23	29.48
-3	0	9	28.49	12.94	25.17
-2	0	9	511.96	514.82	26.97
-1	0	9	968.17	1027.84	31.89
0	0	9	45.78	18.85	19.45
1	0	9	15.59	-15.74	20.26
2	0	9	181.99	189.32	13.34
3	0	9	12.09	-37.8	31.59
4	0	9	311.15	312.87	20.06
-4	1	9	2.9	-5.92	28.38
-3	1	9	69.42	79.62	13.34
-2	1	9	356.07	339.14	16.65
-1	1	9	1.12	-1.6	17.65
0	1	9	349.05	330.21	18.15
1	1	9	0.1	-45.63	20.86
2	1	9	22.35	-1.91	25.27
3	1	9	7.34	41.51	15.64
4	1	9	1.06	-7.22	34.19
-4	2	9	0.68	-14.84	28.58
-3	2	9	50.9	40.81	13.54
-2	2	9	19.29	21.96	10.63
-1	2	9	389	333.02	18.05
0	2	9	29.78	11.93	9.53
1	2	9	557.32	575.29	27.18
2	2	9	6.44	23.77	25.47
3	2	9	28.89	16.24	32.59
4	2	9	14.79	44.52	17.15
-4	3	9	28.77	44.92	14.94
-3	3	9	915.42	883.54	40.11
-2	3	9	1588.28	1580.07	46.93
-1	3	9	219.79	220.51	13.34
0	3	9	18.57	8.12	19.35
1	3	9	933.05	896.58	33.39
2	3	9	35.06	33.29	14.54
3	3	9	400.62	414.95	26.07
4	3	9	0.14	-48.13	35.7
-4	4	9	0.05	4.01	28.68
-3	4	9	16.58	29.88	13.64
-2	4	9	24.26	20.76	24.77
-1	4	9	114.3	96.47	11.13
0	4	9	477.36	523.35	26.57
1	4	9	1685.23	1877.6	51.94
2	4	9	20.96	30.18	15.64
3	4	9	39.38	29.58	35.2
4	4	9	1.6	-5.52	18.65
-4	5	9	4.06	-9.33	30.58
-3	5	9	48.81	53.55	14.34
-2	5	9	0	-10.03	26.47
-1	5	9	1.5	1.2	11.73
0	5	9	403.08	430.49	21.96
1	5	9	351.39	420.66	21.36
2	5	9	9.31	6.72	33.19
3	5	9	9.1	-1.3	35.5
4	5	9	1	37.4	39.51
-4	6	9	0.18	17.15	30.18
-3	6	9	0.91	-16.65	28.08
-2	6	9	0.9	16.45	25.97
-1	6	9	0.44	5.82	12.94
0	6	9	0.72	9.43	26.17
1	6	9	14.89	20.86	29.98
2	6	9	4.51	29.48	33.39
3	6	9	45.82	-3.91	19.35
4	6	9	13.99	-60.37	41.92
-3	7	9	8.07	-44.52	30.48
-2	7	9	0.03	-47.73	27.88
-1	7	9	17.86	18.05	13.84
0	7	9	5.74	25.27	27.28
1	7	9	16.5	17.75	30.38
2	7	9	94.47	68.49	17.65
3	7	9	0.02	25.07	19.35
-3	8	9	0.21	9.63	31.19
-2	8	9	0.09	-11.93	14.54
-1	8	9	0.01	10.73	27.38
0	8	9	3.56	-5.11	29.18
1	8	9	102.25	108	16.35
2	8	9	0.9	13.24	33.29
3	8	9	17.91	-2.61	38.21
-2	9	9	25.05	30.99	15.44
-1	9	9	249.34	255.71	17.35
0	9	9	101.67	100.58	16.24
1	9	9	3.28	12.13	32.39
2	9	9	5.35	4.71	17.75
-1	10	9	30.7	3.51	32.19
0	10	9	20.61	11.73	32.89
1	10	9	1.93	2.31	16.85
2	10	9	43.6	63.58	19.55
-1	-9	10	0.04	23.26	28.68
0	-9	10	2.34	7.92	30.08
1	-9	10	5.92	40.61	15.94
-2	-8	10	3.29	-13.84	30.68
-1	-8	10	0.69	34.5	14.24
0	-8	10	0.37	-25.27	29.58
1	-8	10	3.57	24.57	29.58
2	-8	10	17.57	10.53	31.79
-3	-7	10	2.26	28.78	30.48
-2	-7	10	26.94	6.12	29.68
-1	-7	10	149.29	168.77	15.54
0	-7	10	3.39	23.46	26.57
1	-7	10	17.4	9.02	28.48
2	-7	10	1.55	-44.92	30.48
3	-7	10	0.36	18.85	16.65
-3	-6	10	76.28	70.19	16.14
-2	-6	10	15.03	11.03	27.07
-1	-6	10	17.56	21.86	13.34
0	-6	10	104.51	125.35	13.64
1	-6	10	32.15	-55.95	27.98
2	-6	10	387.74	404.82	20.26
3	-6	10	27.25	-47.43	32.89
-4	-5	10	6.33	-11.13	32.09
-3	-5	10	0.24	10.33	27.28
-2	-5	10	5.87	-25.67	26.97
-1	-5	10	17.25	-9.53	25.87
0	-5	10	130.72	143	13.24
1	-5	10	102.3	114.32	13.84
2	-5	10	51.4	64.68	14.34
3	-5	10	1.55	-51.34	31.79
4	-5	10	2.58	-15.74	36.3
-4	-4	10	5.18	-44.82	31.89
-3	-4	10	0.5	-13.64	26.97
-2	-4	10	5	-18.05	26.17
-1	-4	10	7.81	18.85	23.57
0	-4	10	0.82	3.51	22.36
1	-4	10	10.91	-8.92	25.87
2	-4	10	61.69	90.85	14.74
3	-4	10	5.43	21.16	31.49
4	-4	10	0	0	33.39
-4	-3	10	40.66	56.76	15.14
-3	-3	10	31.79	35.6	14.04
-2	-3	10	126.04	145.1	13.14
-1	-3	10	112.32	136.28	11.33
0	-3	10	35.96	18.85	20.96
1	-3	10	174.5	151.52	12.83
2	-3	10	0.77	-35.5	28.28
3	-3	10	0.07	12.03	30.38
4	-3	10	0.05	-1.6	34.5
-4	-2	10	0.35	5.41	28.18
-3	-2	10	121.42	121.74	13.94
-2	-2	10	533.39	649.4	30.99
-1	-2	10	44.17	33.49	9.63
0	-2	10	313.42	336.93	17.15
1	-2	10	213.84	224.92	13.14
2	-2	10	20.78	12.03	13.74
3	-2	10	10.36	-30.18	31.69
4	-2	10	31.11	-48.13	35.1
-4	-1	10	26.09	-11.33	28.18
-3	-1	10	5.45	13.14	25.97
-2	-1	10	0.09	19.45	21.96
-1	-1	10	328.94	332.32	18.25
0	-1	10	298.47	329.01	18.45
1	-1	10	2041.14	2391.02	58.76
2	-1	10	73.83	87.24	13.84
3	-1	10	72.05	89.75	16.14
4	-1	10	0.04	-38.21	34.29
-4	0	10	15.18	16.85	14.54
-3	0	10	0.12	14.94	26.17
-2	0	10	228.83	221.81	13.14
-1	0	10	48.36	58.56	9.23
0	0	10	17.21	-3421.87	82.83
1	0	10	6.4	-5.11	21.06
2	0	10	0.04	29.28	12.94
3	0	10	0.68	-25.27	32.09
4	0	10	0.81	27.48	17.15
-4	1	10	30.69	-31.89	30.08
-3	1	10	6.25	20.56	12.84
-2	1	10	1.67	0	21.36
-1	1	10	18.8	-14.14	18.55
0	1	10	595.01	642.98	26.07
1	1	10	57.3	51.34	10.43
2	1	10	84.56	106.8	13.74
3	1	10	100.9	125.05	16.55
4	1	10	264.85	284.49	19.65
-4	2	10	18.01	-12.84	28.28
-3	2	10	0.12	-32.89	27.38
-2	2	10	5.57	25.07	11.03
-1	2	10	136.03	138.78	9.83
0	2	10	20.38	12.43	19.65
1	2	10	48.09	46.83	10.83
2	2	10	0.2	14.14	13.64
3	2	10	3.68	26.17	31.99
4	2	10	26.74	-39.31	34.9
-4	3	10	3.82	-10.03	29.28
-3	3	10	9.74	-15.44	28.18
-2	3	10	106.72	116.22	12.43
-1	3	10	64.48	50.44	9.83
0	3	10	46.18	54.25	9.73
1	3	10	60.2	67.19	11.23
2	3	10	78.35	51.44	15.14
3	3	10	52.4	64.88	16.95
4	3	10	5.28	18.35	34.7
-4	4	10	157.7	106.7	16.85
-3	4	10	449.09	393.89	18.45
-2	4	10	1.53	-53.95	25.27
-1	4	10	139.82	145.7	11.73
0	4	10	140.45	162.55	11.33
1	4	10	71.78	90.05	13.04
2	4	10	207.67	182	16.85
3	4	10	40.04	-16.04	35.1
4	4	10	29.08	80.32	18.45
-4	5	10	43.89	40.01	15.64
-3	5	10	1.02	6.92	14.04
-2	5	10	22.74	20.96	26.27
-1	5	10	224.79	231.94	13.74
0	5	10	501.63	586.32	29.98
1	5	10	1.65	17.55	13.84
2	5	10	53.16	69.59	16.75
3	5	10	70.84	72.2	18.35
4	5	10	28.74	-11.03	40.21
-4	6	10	4.07	18.35	15.74
-3	6	10	8.62	-17.65	29.58
-2	6	10	7.02	22.16	26.17
-1	6	10	0.84	-4.11	26.17
0	6	10	83.2	88.55	13.64
1	6	10	20.5	21.46	30.18
2	6	10	2.09	27.88	32.89
3	6	10	0.21	25.97	37
4	6	10	16.76	18.95	41.01
-3	7	10	0.18	-18.45	29.78
-2	7	10	0.99	7.42	27.48
-1	7	10	0.36	2.41	27.28
0	7	10	19.12	8.92	28.88
1	7	10	1.04	15.44	15.34
2	7	10	0.08	-39.11	33.69
3	7	10	0.55	-18.15	38.41
-3	8	10	17.6	-16.85	30.48
-2	8	10	8.4	35.7	14.54
-1	8	10	29.81	22.96	27.68
0	8	10	21.73	6.52	29.48
1	8	10	0.05	-25.47	15.94
2	8	10	30.87	0.7	34.9
3	8	10	0.12	-34.8	38.51
-2	9	10	1.89	0.9	15.34
-1	9	10	62.07	75.81	15.34
0	9	10	206.78	190.03	17.65
1	9	10	7.93	-29.08	33.29
2	9	10	35.21	-15.14	35.5
-1	10	10	84.39	99.27	16.85
0	10	10	56.41	38.01	16.35
1	10	10	19.67	7.82	32.89
-1	-9	11	4.39	13.64	33.09
0	-9	11	11.7	12.53	30.89
1	-9	11	0.19	-1.8	31.39
-2	-8	11	0.16	-7.12	30.36
-1	-8	11	9.69	-17.05	15.04
0	-8	11	1.52	-14.94	28.38
1	-8	11	0.6	-48.13	30.08
2	-8	11	0.4	-44.62	31.99
-3	-7	11	22.47	28.48	31.69
-2	-7	11	8.52	3.21	28.88
-1	-7	11	221.16	187.62	15.94
0	-7	11	27.12	-33.19	29.48
1	-7	11	14.99	-48.03	30.18
2	-7	11	8.64	8.52	15.64
3	-7	11	1.14	9.23	33.19
-3	-6	11	1.91	10.03	28.88
-2	-6	11	2.2	-4.91	26.87
-1	-6	11	109.8	97.37	14.34
0	-6	11	15.65	38.71	13.04
1	-6	11	129.44	95.06	14.84
2	-6	11	123.73	125.85	16.45
3	-6	11	11.32	-42.72	32.59
-3	-5	11	5.77	-22.16	28.58
-2	-5	11	107.61	113.31	14.54
-1	-5	11	93.68	87.14	13.44
0	-5	11	235.92	223.82	14.64
1	-5	11	14.29	18.65	13.64
2	-5	11	0.54	-15.84	29.58
3	-5	11	7.16	8.42	32.19
-4	-4	11	15.5	-18.55	30.88
-3	-4	11	36.96	0.7	29.28
-2	-4	11	23.56	46.03	12.94
-1	-4	11	1.19	-16.04	24.17
0	-4	11	19.74	21.76	11.93
1	-4	11	96.6	109.2	13.84

h	k	l	F_c^2	F_o^2	σF_o^2
2	-4	11	4.6	20.46	27.88
3	-4	11	1.78	-13.34	31.59
4	-4	11	13.38	-28.18	34.4
-4	-3	11	14.05	-8.32	30.68
-3	-3	11	0.62	-14.34	26.67
-2	-3	11	3.11	14.44	24.97
-1	-3	11	14.53	24.57	10.93
0	-3	11	18.04	20.86	10.53
1	-3	11	0.69	-0.2	12.03
2	-3	11	82.97	74.31	14.84
3	-3	11	0.94	-3.31	30.48
4	-3	11	9.29	30.89	17.35
-4	-2	11	6.17	-4.01	28.58
-3	-2	11	0.01	-5.52	12.84
-2	-2	11	117.51	140.29	12.53
-1	-2	11	315.81	365.01	19.05
0	-2	11	112.46	107.3	10.13
1	-2	11	9.17	1	11.03
2	-2	11	73.21	70.9	14.34
3	-2	11	1.06	22.06	30.68
4	-2	11	33.37	48.43	17.75
-4	-1	11	10.04	-30.99	28.88
-3	-1	11	186.63	226.33	14.84
-2	-1	11	700.4	690.21	31.99
-1	-1	11	135.69	134.27	10.13
0	-1	11	361.22	378.85	19.65
1	-1	11	13.09	-12.84	21.86
2	-1	11	14.62	12.84	27.58
3	-1	11	0.22	-9.93	31.59
4	-1	11	8.84	-44.42	35
-4	0	11	25.66	9.83	29.38
-3	0	11	141.44	143.4	14.04
-2	0	11	598.09	646.29	30.99
-1	0	11	494.96	477.42	23.87
0	0	11	3014.37	3195.94	73.9
1	0	11	425.15	524.55	26.87
2	0	11	94.67	96.07	14.04
3	0	11	12.3	33.09	15.94
4	0	11	171.03	171.47	18.55
-4	1	11	34.97	24.37	29.08
-3	1	11	25.63	42.12	13.14
-2	1	11	186.46	172.48	12.43
-1	1	11	6.09	5.82	18.65
0	1	11	53.49	40.61	9.43
1	1	11	296.83	302.94	16.35
2	1	11	12.75	15.84	13.64
3	1	11	149.14	137.78	17.05
4	1	11	172.76	183.21	18.85
-4	2	11	20.66	40.61	15.04
-3	2	11	124.04	121.64	14.04
-2	2	11	0.39	22.56	11.33
-1	2	11	61.05	49.74	9.63
0	2	11	10.39	-9.02	19.15
1	2	11	17.76	0.7	21.76
2	2	11	0.69	7.82	28.58
3	2	11	59.4	65.98	16.75
4	2	11	0.96	23.46	34.7
-4	3	11	35.17	53.95	14.94
-3	3	11	256.18	261.22	15.34
-2	3	11	1.5	23.26	24.27
-1	3	11	74.14	45.02	10.53
0	3	11	1.66	-17.65	19.85
1	3	11	72.2	58.76	11.43
2	3	11	23.43	32.39	14.94
3	3	11	35.02	33.39	33.79
4	3	11	5.61	-32.69	35.6
-4	4	11	5.25	-6.52	30.08
-3	4	11	148.95	135.88	15.04
-2	4	11	4.46	10.03	25.27
-1	4	11	11.69	17.85	11.13
0	4	11	136.72	119.23	11.93
1	4	11	98.05	133.67	13.54
2	4	11	282.27	289.6	18.05
3	4	11	1.15	-20.76	35
4	4	11	9.57	-42.12	38.21
-4	5	11	2.33	13.04	30.28
-3	5	11	31.06	37	14.14
-2	5	11	3.18	-17.15	26.07
-1	5	11	9.25	-2.81	24.97
0	5	11	7.86	-22.86	24.57
1	5	11	5.45	11.13	14.14
2	5	11	2.74	11.33	16.65
3	5	11	33.04	-20.96	36.9
4	5	11	11.42	0.8	39.81
-4	6	11	5.42	22.26	32.29
-3	6	11	3.26	26.17	28.68
-2	6	11	0.09	12.03	13.24
-1	6	11	8.03	8.52	26.07
0	6	11	55.21	45.83	13.94
1	6	11	93.68	108.4	15.54
2	6	11	25.84	44.12	16.85
3	6	11	138.61	92.96	19.85
4	6	11	11.1	-2.81	42.32
-3	7	11	3.57	-4.31	14.84
-2	7	11	0.42	8.92	26.37
-1	7	11	15.86	-20.56	27.58
0	7	11	135.15	129.76	14.94
1	7	11	0.01	31.69	15.14
2	7	11	7.9	-14.14	33.59
3	7	11	12.73	14.44	39.01

h	k	l	F_c^2	F_o^2	σF_o^2
-3	8	11	1.02	26.07	30.28
-2	8	11	4.76	-5.31	28.68
-1	8	11	19.54	-2.81	28.88
0	8	11	3.85	-35.5	28.68
1	8	11	20.32	37.3	15.74
2	8	11	0.94	-20.36	34.9
3	8	11	20.77	12.33	39.01
-2	9	11	0.22	1.7	29.28
-1	9	11	4.66	-17.95	28.98
0	9	11	1.76	-7.52	30.48
1	9	11	0.56	21.66	31.49
2	9	11	11.21	11.93	35.7
-1	10	11	263.35	296.92	20.66
0	10	11	25.19	-5.11	31.59
1	10	11	0.26	-13.14	34.5
0	-9	12	4.06	16.55	30.18
-2	-8	12	0.11	20.96	15.54
-1	-8	12	0.15	-10.73	15.14
0	-8	12	7.01	-11.33	28.68
1	-8	12	5.01	-20.16	30.48
2	-8	12	10.96	18.85	16.45
-2	-7	12	1.57	9.02	29.38
-1	-7	12	14.64	-19.96	27.88
0	-7	12	0.54	-6.42	27.07
1	-7	12	5.38	16.24	29.18
2	-7	12	0.99	15.54	30.28
-3	-6	12	14.98	6.02	15.24
-2	-6	12	354.22	331.52	17.75
-1	-6	12	33.24	-5.21	26.77
0	-6	12	11.65	20.66	27.38
1	-6	12	0.09	-3.31	27.58
2	-6	12	4	0.6	15.14
3	-6	12	8.13	8.62	33.39
-3	-5	12	45.35	54.65	15.04
-2	-5	12	10.6	-28.98	26.77
-1	-5	12	539.19	562.26	31.79
0	-5	12	47.01	56.66	13.14
1	-5	12	2315.81	2384.7	66.38
2	-5	12	598.65	553.23	30.28
3	-5	12	3.99	-50.44	33.29
-4	-4	12	14.14	13.44	15.54
-3	-4	12	17.65	16.65	27.18
-2	-4	12	7.74	-13.14	26.27
-1	-4	12	261.01	237.56	14.54
0	-4	12	11.79	-10.53	24.87
1	-4	12	91.22	78.92	13.94
2	-4	12	0	21.96	29.08
3	-4	12	12.94	50.84	15.94
4	-4	12	15.49	23.46	36.4
-4	-3	12	0.64	-9.43	28.78
-3	-3	12	3.45	-94.56	27.88
-2	-3	12	7.1	9.23	24.27
-1	-3	12	4.21	-29.88	23.16
0	-3	12	70	62.77	11.63
1	-3	12	61.42	65.18	12.84
2	-3	12	0.24	12.94	28.58
3	-3	12	1.71	26.27	30.18
4	-3	12	8.19	7.72	35.9
-4	-2	12	0.87	16.85	14.54
-3	-2	12	16.72	-14.04	26.57
-2	-2	12	10.44	4.51	24.77
-1	-2	12	16.8	17.65	10.53
0	-2	12	368.82	364.21	19.15
1	-2	12	10.12	9.33	23.16
2	-2	12	19.63	33.89	14.34
3	-2	12	7.82	20.86	31.89
4	-2	12	5.59	-11.33	35.5
-4	-1	12	14.04	-0.8	28.78
-3	-1	12	115.14	113.92	13.84
-2	-1	12	151.13	161.55	13.04
-1	-1	12	34.69	5.62	20.16
0	-1	12	372.95	368.32	19.85
1	-1	12	121.06	150.62	11.93
2	-1	12	83.76	80.02	14.64
3	-1	12	54.7	30.89	16.35
4	-1	12	16.47	14.54	17.65
-4	0	12	0.18	10.13	28.38
-3	0	12	11.86	-26.17	26.47
-2	0	12	60.94	82.43	11.93
-1	0	12	942.38	1051.71	34.4
0	0	12	92.79	-4116.49	99.68
1	0	12	23.48	-2.51	22.36
2	0	12	82.49	89.25	14.34
3	0	12	10.29	2.31	32.29
4	0	12	0.19	17.75	34.8
-4	1	12	0.13	-4.71	29.58
-3	1	12	172.46	171.37	14.54
-2	1	12	226.23	237.96	13.54
-1	1	12	104.82	106.8	10.03
0	1	12	0.01	-5.92	19.05
1	1	12	2.29	-51.24	22.26
2	1	12	4.08	15.04	28.58
3	1	12	293.01	333.72	20.16
4	1	12	41.46	17.45	18.35
-4	2	12	5.65	25.17	28.38
-3	2	12	1.57	-9.23	13.44
-2	2	12	48.86	11.43	24.07
-1	2	12	350.27	349.27	19.75
0	2	12	1.82	2.61	9.63
1	2	12	62.49	64.28	11.43

h	k	l	F_c^2	F_o^2	σF_o^2
2	2	12	10.57	2.81	28.88
3	2	12	196.74	195.74	17.55
4	2	12	48.89	9.33	36.1
-4	3	12	2.03	-4.81	28.98
-3	3	12	85.76	74.51	13.84
-2	3	12	3.72	-1.4	24.47
-1	3	12	0.3	4.71	21.26
0	3	12	9	4.61	20.56
1	3	12	13.7	18.05	12.33
2	3	12	0.32	2.31	30.58
3	3	12	37.41	26.47	33.99
4	3	12	28.33	18.65	18.75
-4	4	12	206.92	214.99	16.55
-3	4	12	171	169.77	15.24
-2	4	12	0.01	-32.39	25.37
-1	4	12	194.18	214.99	13.14
0	4	12	102.46	93.16	12.33
1	4	12	9.37	25.57	27.18
2	4	12	127.78	136.58	16.95
3	4	12	5.93	7.82	34.19
4	4	12	4.11	14.04	37.5
-4	5	12	13.5	13.64	15.54
-3	5	12	13.66	18.35	27.48
-2	5	12	81.44	84.53	13.84
-1	5	12	88.89	76.41	13.24
0	5	12	593.34	684.29	33.59
1	5	12	70.03	60.97	15.04
2	5	12	13.84	29.38	16.95
3	5	12	78.55	9.73	37.3
4	5	12	3.2	-0.9	19.96
-3	6	12	20.59	-40.41	29.28
-2	6	12	4.84	-10.63	26.67
-1	6	12	0.79	8.22	26.47
0	6	12	71.12	50.14	14.14
1	6	12	52.71	44.82	15.44
2	6	12	82.8	82.83	17.05
3	6	12	76.78	48.33	19.65
4	6	12	0.43	35.1	42.72
-3	7	12	0.48	27.48	28.38
-2	7	12	0.34	-14.04	27.48
-1	7	12	22.45	14.64	13.54
0	7	12	8.79	24.67	28.78
1	7	12	1.62	-53.85	30.89
2	7	12	74.2	28.28	34.5
3	7	12	7.91	-8.22	40.11
-3	8	12	4.23	-12.74	30.79
-2	8	12	2.11	-50.64	30.18
-1	8	12	1.63	23.77	27.68
0	8	12	5.3	-16.75	29.18
1	8	12	58.08	0	32.29
2	8	12	0.1	-49.94	35.5
3	8	12	0.39	-14.34	39.11
-2	9	12	0.43	17.35	29.58
-1	9	12	1.06	-49.84	30.99
0	9	12	2.32	-28.28	31.59
1	9	12	1.46	20.46	32.49
2	9	12	1.43	-56.76	36.9
-1	10	12	27.56	34.29	16.35
0	10	12	0.56	-9.53	32.19
1	10	12	6.67	31.09	32.89
-1	-8	13	7.93	26.77	27.58
0	-8	13	1.03	-20.16	29.28
1	-8	13	13.08	35.7	15.44
-2	-7	13	0.17	0.8	29.58
-1	-7	13	3.55	-17.55	29.28
0	-7	13	1.74	9.53	14.24
1	-7	13	16.63	23.87	29.58
2	-7	13	6.23	14.14	15.64
-3	-6	13	4.5	26.47	30.89
-2	-6	13	79.7	69.39	15.24
-1	-6	13	27.87	19.05	26.27
0	-6	13	2.68	3.81	13.64
1	-6	13	24.2	24.17	14.64
2	-6	13	5.09	-44.62	31.39
3	-6	13	10.28	-12.33	33.49
-3	-5	13	14.79	34.09	14.64
-2	-5	13	0.15	2.81	26.97
-1	-5	13	10.62	-0.6	26.37
0	-5	13	8.02	-14.44	27.28
1	-5	13	18.24	13.94	27.68
2	-5	13	101.49	99.98	15.74
3	-5	13	44.32	41.82	16.75
-4	-4	13	0	24.17	29.98
-3	-4	13	21.67	40.91	14.24
-2	-4	13	25.69	22.86	26.27
-1	-4	13	255.01	268.94	15.74
0	-4	13	0.04	-7.02	25.27
1	-4	13	122.34	98.57	14.44
2	-4	13	30.76	-11.73	29.88
3	-4	13	0.05	28.87	31.19
4	-4	13	10.85	26.37	18.65
-4	-3	13	0.24	-21.96	30.46
-3	-3	13	3.46	5.62	26.87
-2	-3	13	5.05	15.54	12.43
-1	-3	13	8.93	3.91	24.27
0	-3	13	408.69	400.61	21.26
1	-3	13	91.99	89.25	13.34
2	-3	13	93.72	107.1	15.24
3	-3	13	11.13	12.43	31.59
4	-3	13	26.91	-16.55	36

h	k	l	F_c^2	F_o^2	σF_o^2
-4	-2	13	0.21	-22.66	29.08
-3	-2	13	22.21	-28.38	26.97
-2	-2	13	13.68	-28.28	25.77
-1	-2	13	1.93	-2.71	21.86
0	-2	13	41.02	-4.81	21.86
1	-2	13	14.61	-5.21	25.27
2	-2	13	5.75	15.04	28.78
3	-2	13	33.77	32.39	16.14
4	-2	13	12.7	13.34	34.19
-4	-1	13	12.01	-18.75	29.48
-3	-1	13	38.41	15.84	27.68
-2	-1	13	0.75	6.92	24.07
-1	-1	13	18.14	11.23	20.86
0	-1	13	2.19	-3.01	20.36
1	-1	13	1.07	-12.33	23.46
2	-1	13	23.12	51.94	14.44
3	-1	13	48.36	54.95	16.65
4	-1	13	6.92	21.76	35.5
-4	0	13	44.07	18.65	15.14
-3	0	13	66.62	61.07	13.54
-2	0	13	272.24	285.29	15.54
-1	0	13	522.78	478.72	25.37
0	0	13	2696.27	2914.46	69.89
1	0	13	902.29	1098.54	37.8
2	0	13	2.2	-20.76	28.88
3	0	13	80.46	55.05	16.55
4	0	13	0.19	-34.7	35.1
-4	1	13	40.25	42.62	14.84
-3	1	13	167.72	158.04	14.04
-2	1	13	317.46	302.24	16.35
-1	1	13	156.55	166.06	11.33
0	1	13	18.42	22.16	9.83
1	1	13	21.03	6.72	24.07
2	1	13	2.76	-13.04	29.68
3	1	13	423.92	495.07	26.67
4	1	13	102.96	124.75	18.85
-4	2	13	9.64	12.84	14.94
-3	2	13	2.78	1.8	26.97
-2	2	13	34.66	49.94	12.03
-1	2	13	0.1	2.81	20.36
0	2	13	14.19	-0.3	20.66
1	2	13	0	5.62	12.03
2	2	13	4.49	-10.43	30.28
3	2	13	19.22	30.58	34.09
4	2	13	1.41	-34.8	35.8
-4	3	13	13.91	-14.04	30.18
-3	3	13	17.02	1.3	27.18
-2	3	13	3.9	-25.77	24.67
-1	3	13	151.43	153.02	12.13
0	3	13	0.42	-26.88	22.06
1	3	13	0.32	1.1	12.84
2	3	13	32.53	52.65	15.74
3	3	13	0.35	-41.11	33.69
4	3	13	1.63	-53.55	36.5
-4	4	13	119.32	103.59	16.55
-3	4	13	156.44	141.79	15.24
-2	4	13	0.87	8.72	25.57
-1	4	13	1.43	11.73	11.93
0	4	13	0.45	-38.11	24.57
1	4	13	13.11	-3.61	27.48
2	4	13	20.65	-14.94	33.09
3	4	13	1.1	-11.23	34.9
4	4	13	0.35	-11.73	36.5
-4	5	13	17.33	-26.17	32.29
-3	5	13	0.18	-8.02	28.08
-2	5	13	5.86	-30.58	27.58
-1	5	13	0.21	-12.53	25.87
0	5	13	293.62	309.86	17.35
1	5	13	31.04	13.44	29.58
2	5	13	6.65	15.64	34.19
3	5	13	0.51	-4.41	18.35
4	5	13	14.12	30.99	39.61
-3	6	13	0.43	-14.04	27.78
-2	6	13	68.33	63.17	14.44
-1	6	13	326.56	359.09	21.26
0	6	13	1.42	-21.26	27.38
1	6	13	28.94	29.68	15.54
2	6	13	0.19	20.96	33.19
3	6	13	0.02	-19.96	19.35
-3	7	13	0.99	2.61	30.18
-2	7	13	13.69	6.42	28.18
-1	7	13	4.98	-8.32	27.28
0	7	13	0.21	-9.13	28.68
1	7	13	30.2	10.53	16.14
2	7	13	193.34	145.4	18.75
3	7	13	13.53	22.36	39.61
-3	8	13	7.18	3.21	16.24
-2	8	13	6.23	13.54	27.88
-1	8	13	42.81	30.79	14.64
0	8	13	9.27	-32.89	30.58
1	8	13	84.27	86.24	16.55
2	8	13	1.05	4.71	35.7
3	8	13	0.77	17.15	39.81
-2	9	13	35.31	35.3	15.94
-1	9	13	0.29	7.22	29.18
0	9	13	0.28	-16.45	15.64
1	9	13	4.09	6.42	32.39
2	9	13	11.48	-17.45	18.35
-1	10	13	37.43	19.96	32.99
0	10	13	1.97	7.02	30.18
1	10	13	7.1	-29.78	34.29
-1	-8	14	2.34	25.87	29.88
0	-8	14	2.27	-23.36	29.38
1	-8	14	6.97	0	31.49
-2	-7	14	12.33	15.64	29.78
-1	-7	14	16.09	0.8	28.88
0	-7	14	31.4	48.13	14.54
1	-7	14	0.4	-24.57	30.18
2	-7	14	25.6	1.7	32.19
-3	-6	14	16.27	18.95	15.54
-2	-6	14	5.53	5.31	14.44
-1	-6	14	2.27	7.72	26.17
0	-6	14	0.47	-2.91	13.64
1	-6	14	8.43	-7.72	28.98
2	-6	14	15.84	22.66	15.44
3	-6	14	5.9	15.44	32.19
-3	-5	14	47.68	58.66	15.24
-2	-5	14	19.43	26.67	13.84
-1	-5	14	5.4	2.51	26.17
0	-5	14	11.41	15.14	25.77
1	-5	14	220.96	221.71	16.14
2	-5	14	108.54	90.35	16.14
3	-5	14	0.01	17.55	31.39
-3	-4	14	0.27	-57.26	28.68
-2	-4	14	335.23	324.2	16.95
-1	-4	14	5	11.23	25.87
0	-4	14	1015.33	1070.56	41.92
1	-4	14	536.83	521.34	27.07
2	-4	14	42.59	59.56	15.14
3	-4	14	23.07	3.91	33.09
-4	-3	14	11.41	9.93	30.68
-3	-3	14	0.01	-3.61	26.87
-2	-3	14	19.67	21.26	12.94
-1	-3	14	63.16	62.67	12.63
0	-3	14	30.16	29.68	12.23
1	-3	14	30.65	28.08	13.34
2	-3	14	0.93	25.07	14.64
3	-3	14	5.36	12.94	32.19
4	-3	14	0.21	12.63	18.25
-4	-2	14	0.03	-0.8	29.28
-3	-2	14	9.34	15.54	13.54
-2	-2	14	2.8	8.02	12.53
-1	-2	14	63.53	76.01	12.03
0	-2	14	25.07	6.92	23.26
1	-2	14	78.94	90.25	13.14
2	-2	14	0.07	44.32	14.54
3	-2	14	0.74	-16.95	31.69
4	-2	14	3.25	-22.26	37.1
-4	-1	14	0.51	-37.7	28.48
-3	-1	14	37.79	3.31	26.97
-2	-1	14	90.59	108.2	12.53
-1	-1	14	45.57	31.59	11.43
0	-1	14	0.63	-13.14	22.06
1	-1	14	48.92	43.62	12.74
2	-1	14	19.03	2.11	14.84
3	-1	14	7.83	27.28	32.09
4	-1	14	1.76	-50.54	36.2
-4	0	14	6.78	-24.67	28.58
-3	0	14	14.11	5.21	13.64
-2	0	14	26.78	6.02	24.07
-1	0	14	52.49	9.93	23.97
0	0	14	38.91	-1347.53	47.53
1	0	14	147.24	149.21	13.14
2	0	14	3.02	12.33	29.08
3	0	14	21.82	-2.41	16.85
4	0	14	4.13	21.96	35.4
-4	1	14	50.64	21.26	29.58
-3	1	14	7.48	-16.55	25.57
-2	1	14	187.01	193.33	13.64
-1	1	14	663.55	766.02	31.99
0	1	14	39.43	20.16	22.36
1	1	14	258.93	286.09	15.54
2	1	14	14.07	-4.91	29.88
3	1	14	43.8	42.42	17.25
4	1	14	0.03	-30.68	36.3
-4	2	14	4.45	18.15	28.68
-3	2	14	96.79	100.88	14.04
-2	2	14	19.83	-3.11	24.57
-1	2	14	7.11	19.05	21.96
0	2	14	267.45	269.35	14.54
1	2	14	8.54	-41.92	26.17
2	2	14	774.42	798.81	39.91
3	2	14	793.15	820.17	44.02
4	2	14	6.49	9.83	35.4
-4	3	14	0.44	-4.21	29.38
-3	3	14	40.98	-12.63	28.38
-2	3	14	9.5	9.63	12.43
-1	3	14	62.53	73.4	11.93
0	3	14	2.12	-53.95	23.77
1	3	14	75.79	71.9	13.84
2	3	14	23.59	14.94	16.04
3	3	14	4.72	31.39	33.99
4	3	14	5.74	4.21	38.31
-4	4	14	1.95	1.7	30.48
-3	4	14	0.42	13.24	26.97
-2	4	14	0.14	12.94	12.74
-1	4	14	125.76	116.62	13.04
0	4	14	75.14	100.78	12.84
1	4	14	15.35	39.81	14.24
2	4	14	39.67	-12.63	33.69
3	4	14	15.21	-5.52	35
4	4	14	2.16	24.07	38.71
-4	5	14	198.22	159.24	17.75
-3	5	14	11.63	-5.92	28.18
-2	5	14	58.67	57.86	13.64
-1	5	14	81.07	89.35	13.44
0	5	14	98.54	123.64	14.04
1	5	14	14.42	17.55	30.38
2	5	14	18.84	7.72	33.49
3	5	14	0.04	-29.88	36.8
4	5	14	11.97	23.46	39.81
-3	6	14	3.98	10.33	28.18
-2	6	14	7.88	-7.32	26.87
-1	6	14	293.01	293.11	16.85
0	6	14	6.41	-2.71	28.48
1	6	14	43.4	49.94	15.54
2	6	14	176.51	148.71	18.45
3	6	14	1.02	21.56	18.95
-3	7	14	3.16	7.72	28.68
-2	7	14	0.03	11.73	27.38
-1	7	14	127.47	123.64	15.14
0	7	14	22.86	-8.02	28.68
1	7	14	0.04	16.35	15.74
2	7	14	11.67	-35.3	34.29
3	7	14	6.13	15.24	39.01
-2	8	14	17.92	-26.77	29.28
-1	8	14	25.34	23.36	28.08
0	8	14	3.07	19.15	14.94
1	8	14	4.02	28.98	31.79
2	8	14	4.71	-6.22	18.05
3	8	14	0.44	0.9	40.41
-2	9	14	0.69	31.39	31.89
-1	9	14	0.72	-42.72	30.18
0	9	14	24.01	2.31	31.29
1	9	14	0.55	12.23	31.79
2	9	14	4.52	11.53	36.3
-1	10	14	14.62	2.71	32.39
0	10	14	0.77	10.73	31.99
1	10	14	3.1	-0.9	34.19
-1	-8	15	1.15	19.25	30.28
0	-8	15	8.72	7.02	15.64
1	-8	15	11.55	21.26	31.59
-2	-7	15	0.43	-11.63	30.48
-1	-7	15	0.55	-5.62	14.64
0	-7	15	6.15	-3.21	27.38
1	-7	15	19.09	2.41	30.58
2	-7	15	2.49	-31.39	31.69
-2	-6	15	33.4	21.86	14.84
-1	-6	15	7.71	10.33	27.98
0	-6	15	63.16	66.58	14.34
1	-6	15	2.15	-18.35	29.26
2	-6	15	13.68	-7.32	30.79
-3	-5	15	11.19	-15.64	30.38
-2	-5	15	2.01	-29.48	27.56
-1	-5	15	14.45	15.84	26.07
0	-5	15	2.5	6.92	26.17
1	-5	15	6.01	-23.67	28.78
2	-5	15	54.69	45.63	16.14
3	-5	15	0.41	8.62	31.79
-3	-4	15	45.84	32.09	15.04
-2	-4	15	29.69	52.95	13.54
-1	-4	15	145.83	126.55	14.14
0	-4	15	1995.2	2106.53	61.07
1	-4	15	50.47	8.22	28.48
2	-4	15	81.02	75.91	15.54
3	-4	15	7.81	-18.35	33.59
-4	-3	15	0.4	-18.55	30.79
-3	-3	15	9.11	2.21	27.88
-2	-3	15	163.21	172.38	14.04
-1	-3	15	72.44	57.86	12.94
0	-3	15	3.58	-57.86	25.87
1	-3	15	23.29	32.69	13.74
2	-3	15	33.62	23.67	14.94
3	-3	15	61.33	56.36	17.15
4	-3	15	17.06	14.74	37.4
-4	-2	15	0.11	7.12	15.04
-3	-2	15	1.29	-11.33	25.97
-2	-2	15	24.54	30.08	12.63
-1	-2	15	54.62	41.01	12.13
0	-2	15	2.91	5.62	12.03
1	-2	15	314.44	299.03	16.04
2	-2	15	32.7	53.65	14.84
3	-2	15	0.09	-1.8	16.55
4	-2	15	0.18	24.67	35.2
-4	-1	15	0.6	14.74	28.38
-3	-1	15	1.37	-3.41	26.47
-2	-1	15	2.32	-19.15	25.07
-1	-1	15	32.41	-23.87	23.46
0	-1	15	10.83	-3.51	23.06
1	-1	15	154.83	148.31	14.04
2	-1	15	42.02	44.02	15.14
3	-1	15	14.33	8.72	32.59
4	-1	15	10.14	2.51	36.7
-4	0	15	61.29	69.79	15.44
-3	0	15	222.53	222.21	15.64
-2	0	15	23.25	-3.71	25.47
-1	0	15	55.76	73.9	11.63
0	0	15	45.12	-90.45	24.77
1	0	15	34.46	30.89	13.04
2	0	15	93.94	68.14	15.74

h	k	l	F_c^2	F_o^2	σF_o^2
3	0	15	0.97	-24.87	33.59
4	0	15	8.28	-4.21	37
-4	1	15	3.74	39.31	14.74
-3	1	15	78.82	61.77	14.24
-2	1	15	232.43	232.34	14.24
-1	1	15	898.41	939.8	35.8
0	1	15	1225.46	1404.79	43.02
1	1	15	3.66	-109.3	28.78
2	1	15	82.1	84.13	15.94
3	1	15	18.14	-7.12	34.29
4	1	15	3.02	18.25	36.3
-4	2	15	36.27	46.73	14.94
-3	2	15	49.7	58.56	13.74
-2	2	15	0.01	1.8	12.53
-1	2	15	309.67	359.19	21.06
0	2	15	148.05	152.72	12.53
1	2	15	83.72	88.55	13.74
2	2	15	51.75	-2.61	32.59
3	2	15	170.71	157.84	18.65
4	2	15	0.07	25.67	18.45
-4	3	15	0.04	-3.51	28.68
-3	3	15	1.37	-15.14	26.77
-2	3	15	62.01	81.22	13.14
-1	3	15	1.32	21.36	23.97
0	3	15	37.89	45.02	12.23
1	3	15	0.85	12.13	13.94
2	3	15	203.41	163.15	17.35
3	3	15	25.8	27.58	34.6
4	3	15	1.49	1.7	37
-4	4	15	7.47	-12.53	30.79
-3	4	15	0.24	-56.86	28.78
-2	4	15	36.74	38.21	13.24
-1	4	15	9.67	-8.42	25.87
0	4	15	7.16	-22.46	26.77
1	4	15	153.72	172.28	15.64
2	4	15	2.34	-47.73	32.89
3	4	15	40.7	1.4	36.1
4	4	15	0.03	-9.73	38.31
-3	5	15	2.21	-14.44	27.88
-2	5	15	39.16	51.34	13.54
-1	5	15	1.76	3.31	26.87
0	5	15	8.96	-26.67	27.98
1	5	15	4.4	24.27	30.48
2	5	15	0	-31.49	33.69
3	5	15	2.74	-57.36	37.2
4	5	15	7.98	4.71	21.76
-3	6	15	2.62	-20.36	28.88
-2	6	15	32.29	17.75	26.87
-1	6	15	5.18	12.63	27.48
0	6	15	14.94	-2.81	28.18
1	6	15	6.4	-22.66	30.89
2	6	15	8.98	-2.01	33.39
3	6	15	0	-31.99	38.71
-3	7	15	25.77	18.45	31.79
-2	7	15	13.31	15.04	28.28
-1	7	15	15.71	-9.43	28.18
0	7	15	72.12	24.37	30.28
1	7	15	160.08	143.4	17.15
2	7	15	81.79	74	16.25
3	7	15	19.51	28.88	19.96
-2	8	15	16.22	-25.67	29.68
-1	8	15	29.13	39.71	14.84
0	8	15	25.7	-4.31	30.88
1	8	15	12.01	46.73	16.35
2	8	15	0.01	26.07	34.9
-2	9	15	15.05	-62.37	32.69
-1	9	15	11.22	-1.6	29.78
0	9	15	2.56	35.1	15.54
1	9	15	0.08	-14.14	33.19
2	9	15	1.81	-9.02	35.9
0	10	15	3.86	19.96	32.19
0	-8	16	2.09	21.26	32.59
-1	-7	16	2.32	3.41	29.88
0	-7	16	0.03	-89.49	29.78
1	-7	16	10.32	-11.93	30.68
-2	-6	16	7.66	-19.35	27.88
-1	-6	16	2.26	-13.74	29.18
0	-6	16	4.4	12.94	14.24
1	-6	16	2.27	20.16	14.74
2	-6	16	0.13	-20.96	30.99
-3	-5	16	51.46	-18.75	31.79
-2	-5	16	4.74	-2.31	27.88
-1	-5	16	22.9	-6.92	27.78
0	-5	16	11.75	-3.31	27.18
1	-5	16	7.02	26.07	27.58
2	-5	16	0.45	23.77	15.34
3	-5	16	2.26	-40.01	35
-3	-4	16	2.46	-59.67	29.88
-2	-4	16	21.36	3.51	13.94
-1	-4	16	95.63	89.75	13.74
0	-4	16	874.37	969.98	41.31
1	-4	16	1106.68	1121.7	44.72
2	-4	16	9.69	30.48	15.24
3	-4	16	56.28	62.47	17.35
-3	-3	16	39.17	47.63	14.54
-2	-3	16	3.45	-35.6	25.57
-1	-3	16	8.9	17.55	25.87
0	-3	16	45.9	-5.92	26.47
1	-3	16	110.72	116.02	14.44
2	-3	16	29.2	26.37	29.68
3	-3	16	1.4	-26.97	17.05
-4	-2	16	0	6.42	30.18
-3	-2	16	0	-31.69	28.68
-2	-2	16	6.73	-2.41	25.37
-1	-2	16	35.46	19.85	24.87
0	-2	16	0.01	9.93	25.47
1	-2	16	1.29	-46.73	27.98
2	-2	16	8.5	29.48	30.58
3	-2	16	64.43	31.69	17.75
4	-2	16	1.29	18.15	36
-4	-1	16	0.53	-7.12	15.14
-3	-1	16	0.27	-50.34	27.28
-2	-1	16	2.2	-51.14	25.57
-1	-1	16	107.97	117.83	12.84
0	-1	16	8.37	4.21	24.77
1	-1	16	8.87	-13.64	27.38
2	-1	16	43.25	55.85	15.34
3	-1	16	7.63	-2.11	33.29
4	-1	16	0.28	29.88	35.1
-4	0	16	0.89	2.21	15.14
-3	0	16	79.27	79.12	14.44
-2	0	16	1.54	-38.41	26.07
-1	0	16	7.88	17.85	24.57
0	0	16	38.14	-13.64	25.17
1	0	16	20.25	28.17	27.16
2	0	16	26.64	-9.33	31.59
3	0	16	4.84	-4.11	33.59
4	0	16	11.48	-23.26	37
-4	1	16	38.54	46.33	15.54
-3	1	16	32	26.77	13.94
-2	1	16	4.91	-24.27	25.47
-1	1	16	358.26	357.29	19.35
0	1	16	312.81	208.48	15.64
1	1	16	73.68	46.83	13.94
2	1	16	44.13	43.12	16.04
3	1	16	7.9	-8.12	33.89
4	1	16	31.94	-35.9	37.9
-4	2	16	1.24	17.45	30.18
-3	2	16	53.02	-9.63	27.78
-2	2	16	21.1	6.72	26.47
-1	2	16	84.77	67.49	12.74
0	2	16	277.74	302.44	17.55
1	2	16	48.63	45.33	14.04
2	2	16	759.43	767.22	40.31
3	2	16	118.72	125.55	18.45
4	2	16	2.49	40.01	18.75
-4	3	16	4.26	29.38	29.38
-3	3	16	7.17	21.96	26.57
-2	3	16	12.25	34.9	13.04
-1	3	16	232.75	225.22	14.34
0	3	16	4.52	-1.8	26.07
1	3	16	325.39	309.66	16.85
2	3	16	553.17	520.54	30.58
3	3	16	9.91	-2.11	35.5
4	3	16	5.36	28.88	37.9
-4	4	16	1.37	16.55	30.79
-3	4	16	24.18	-0.7	28.08
-2	4	16	0.01	0.6	27.18
-1	4	16	0.08	11.03	25.67
0	4	16	129.49	129.86	14.34
1	4	16	3.09	-6.52	15.04
2	4	16	26.82	36.5	16.85
3	4	16	0.94	-0.7	36.3
4	4	16	0.01	-38.81	38.71
-3	5	16	5.35	-3.11	28.28
-2	5	16	61.01	68.39	14.14
-1	5	16	1.78	-31.29	27.38
0	5	16	0.05	-22.08	28.08
1	5	16	74.41	63.68	15.74
2	5	16	15.07	24.37	33.89
3	5	16	0.04	2.31	37.6
-3	6	16	13.94	-29.18	29.68
-2	6	16	46.12	44.22	14.64
-1	6	16	33.41	10.03	27.48
0	6	16	0.06	13.64	26.58
1	6	16	55.51	40.61	15.94
2	6	16	0.04	-100.08	35.9
3	6	16	15.43	-9.02	38.61
-3	7	16	3.19	12.63	29.88
-2	7	16	2.53	-31.69	28.88
-1	7	16	1.7	10.63	14.34
0	7	16	82.2	65.48	15.54
1	7	16	65.33	95.97	16.65
2	7	16	5.91	-8.32	35.6
3	7	16	9.78	8.82	39.01
-2	8	16	28.09	59.46	15.44
-1	8	16	27.86	9.23	30.28
0	8	16	17.87	22.36	15.64
1	8	16	18.98	35.8	16.85
2	8	16	14.14	-53.45	37.2
-1	9	16	0.31	25.67	31.19
0	9	16	32.5	25.67	31.49
1	9	16	4.3	28.37	33.39
2	9	16	3.64	0.9	38.41
0	10	16	0.41	3.71	34.9
-1	-7	17	0.3	-21.28	29.58
0	-7	17	5.24	27.38	14.84
1	-7	17	4.85	-32.69	30.18
-2	-6	17	9.17	7.82	30.58
-1	-6	17	1.43	-45.43	28.18
0	-6	17	0.24	-25.47	28.98
1	-6	17	37.45	15.84	30.18
2	-6	17	1.03	9.53	31.39
-3	-5	17	44.85	64.58	16.14
-2	-5	17	3.93	-34.29	28.88
-1	-5	17	3.65	18.75	27.18
0	-5	17	9.07	-10.33	27.18
1	-5	17	68.5	79.42	14.94
2	-5	17	11.85	-5.62	30.99
3	-5	17	0.46	-39.81	34.9
-3	-4	17	15.32	-31.89	30.99
-2	-4	17	66.53	76.71	14.44
-1	-4	17	5.74	13.04	26.57
0	-4	17	44.57	42.92	14.34
1	-4	17	30.88	-10.43	29.68
2	-4	17	21.77	24.77	30.88
3	-4	17	25.26	55.75	16.85
-3	-3	17	20.8	21.76	28.18
-2	-3	17	23.63	21.06	27.38
-1	-3	17	1317.67	1338.6	47.13
0	-3	17	643.2	708.46	36.9
1	-3	17	34.08	32.39	14.34
2	-3	17	2.64	14.14	30.28
3	-3	17	10.87	-16.04	32.69
-3	-2	17	18.84	17.65	14.34
-2	-2	17	3.17	30.89	13.04
-1	-2	17	63.39	55.65	13.34
0	-2	17	168.56	166.76	14.14
1	-2	17	50.26	44.32	14.24
2	-2	17	87.89	72.2	15.94
3	-2	17	80.94	34.9	35
-4	-1	17	4.76	18.35	31.09
-3	-1	17	1.52	-38.41	27.28
-2	-1	17	6.99	10.93	25.07
-1	-1	17	1.54	-13.04	25.17
0	-1	17	53.93	65.78	12.94
1	-1	17	162.47	165.86	14.84
2	-1	17	0.75	0.6	30.08
3	-1	17	18.92	5.82	32.79
4	-1	17	0.43	-24.37	38.01
-4	0	17	19.72	7.22	29.88
-3	0	17	0.67	7.92	27.07
-2	0	17	26.72	37.7	12.63
-1	0	17	3.36	9.53	24.77
0	0	17	36.91	1.91	26.27
1	0	17	2.19	-9.43	27.68
2	0	17	13.28	31.69	15.34
3	0	17	16.71	-43.92	33.79
4	0	17	2.65	18.65	36
-4	1	17	45.05	28.58	30.68
-3	1	17	0.29	17.85	27.28
-2	1	17	12.46	-55.65	26.67
-1	1	17	112.78	125.25	13.54
0	1	17	56.52	-9.23	27.38
1	1	17	11.24	-99.98	29.28
2	1	17	107.34	106.7	16.35
3	1	17	18.51	-10.43	35.5
4	1	17	9	20.16	37.3
-4	2	17	10.73	-52.14	30.89
-3	2	17	8.75	24.47	26.37
-2	2	17	2.31	-15.74	25.97
-1	2	17	15.76	-4.01	24.67
0	2	17	208.73	198.85	14.44
1	2	17	2.07	-9.43	28.68
2	2	17	2.3	20.76	32.29
3	2	17	1.66	-27.58	35.2
4	2	17	4.47	17.55	37.4
-4	3	17	0.06	-14.64	31.19
-3	3	17	1.67	16.65	14.14
-2	3	17	183.98	173.18	14.54
-1	3	17	32.09	50.34	12.94
0	3	17	175.46	160.04	14.44
1	3	17	224.67	213.09	16.45
2	3	17	100.08	90.45	17.15
3	3	17	1.45	12.33	34.6
4	3	17	10.41	31.99	19.55
-3	4	17	2.59	14.54	28.38
-2	4	17	8.88	0.3	13.74
-1	4	17	90.56	77.72	13.74
0	4	17	0.91	13.94	13.74
1	4	17	54.68	52.04	15.34
2	4	17	13.12	19.25	16.85
3	4	17	1.08	24.77	36.3
4	4	17	2.8	34.19	40.11
-3	5	17	3.6	-74.31	28.88
-2	5	17	0.1	23.77	26.27
-1	5	17	3.06	1.8	26.87
0	5	17	0.05	13.94	14.04
1	5	17	30.05	13.64	15.74
2	5	17	128.15	94.66	17.85
3	5	17	1.61	-52.14	37.6
-3	6	17	10.2	-42.92	30.08
-2	6	17	6.08	9.43	28.48
-1	6	17	46.16	46.53	14.34
0	6	17	14.07	-24.77	26.88
1	6	17	0.15	-73.8	32.59
2	6	17	4.6	-8.62	34.9
3	6	17	2.6	-78.32	38.61
-3	7	17	36.12	-6.42	33.19
-2	7	17	151.5	137.28	16.14

h	k	l	F_c^2	F_o^2	σF_o^2
-1	7	17	0.03	25.07	28.68
0	7	17	34.92	22.56	30.28
1	7	17	0.45	10.53	31.69
2	7	17	21.95	21.86	35.3
3	7	17	0.09	-43.42	42.02
-2	8	17	62.52	67.09	15.94
-1	8	17	21.99	14.24	29.08
0	8	17	114.84	114.22	16.45
1	8	17	137.39	129.86	17.85
2	8	17	5.07	-18.85	36.6
-1	9	17	16.13	28.38	15.84
0	9	17	9.83	-3.31	32.59
1	9	17	3.05	6.12	33.39
-1	-7	18	0.73	-22.06	29.58
0	-7	18	11.47	1.8	31.39
1	-7	18	15.96	22.46	16.55
-2	-6	18	14.75	10.83	30.48
-1	-6	18	1.27	5.01	14.24
0	-6	18	1.77	0.8	14.54
1	-6	18	17.43	14.94	28.48
2	-6	18	3.38	-34.4	32.29
-2	-5	18	0.4	-15.74	26.47
-1	-5	18	91.18	136.98	14.84
0	-5	18	0.77	-45.02	28.28
1	-5	18	7.44	-1.5	29.28
2	-5	18	1.72	26.47	30.89
-3	-4	18	0.26	16.95	28.28
-2	-4	18	26.02	29.08	14.24
-1	-4	18	1.51	9.63	25.77
0	-4	18	4.14	24.97	26.17
1	-4	18	27.22	25.27	27.88
2	-4	18	3.34	18.85	15.44
3	-4	18	3.37	11.53	33.09
-3	-3	18	2.36	-13.44	28.38
-2	-3	18	80.98	94.06	14.14
-1	-3	18	15.67	-37.8	27.78
0	-3	18	663.64	627.74	32.99
1	-3	18	1.3	-16.95	27.38
2	-3	18	13.7	17.65	29.08
3	-3	18	0.22	-9.13	34.29
-3	-2	18	0.78	1.6	27.18
-2	-2	18	0.14	-6.42	13.34
-1	-2	18	187.74	201.86	14.64
0	-2	18	11.14	-31.79	27.07
1	-2	18	4.73	26.57	13.74
2	-2	18	67.67	66.99	16.04
3	-2	18	1.32	-26.87	33.69
-3	-1	18	3.8	-12.33	27.68
-2	-1	18	30.38	-14.64	25.97
-1	-1	18	11.34	21.66	26.57
0	-1	18	20.23	22.06	13.14
1	-1	18	14.64	17.55	27.98
2	-1	18	18.21	-36.5	31.09
3	-1	18	2.26	-18.95	33.89
-3	0	18	0.43	17.95	26.67
-2	0	18	2.59	9.23	25.67
-1	0	18	1.23	-4.31	24.77
0	0	18	1.9	-81.12	27.78
1	0	18	10.82	15.74	14.04
2	0	18	4.99	-52.45	31.09
3	0	18	72.5	91.75	17.85
4	0	18	3.34	-5.52	38.81
-4	1	18	8.67	-15.84	31.79
-3	1	18	0.06	25.17	25.67
-2	1	18	4.43	14.04	24.87
-1	1	18	61.68	48.94	12.84
0	1	18	22.46	11.93	26.27
1	1	18	6.31	-163.25	31.19
2	1	18	4.44	-34.9	30.99
3	1	18	25.05	7.32	34.6
4	1	18	6.09	3.71	36.9
-3	2	18	12.05	9.73	14.04
-2	2	18	368.52	398.2	23.67
-1	2	18	239.98	298.12	15.24
0	2	18	0.66	-15.54	13.34
1	2	18	24.23	4.81	29.88
2	2	18	6.92	18.65	15.64
3	2	18	49.03	16.14	34.7
4	2	18	6.24	9.02	39.71
-3	3	18	20.76	35.5	14.64
-2	3	18	0.24	21.96	13.34
-1	3	18	201.88	189.52	14.64
0	3	18	161.24	154.23	14.44
1	3	18	1049.44	1094.43	44.32
2	3	18	1055.66	1070.96	47.83
3	3	18	13.17	2.91	37
4	3	18	10.72	11.33	21.06
-3	4	18	1.88	8.32	27.38
-2	4	18	46.88	39.31	13.74
-1	4	18	1.06	-15.04	28.67
0	4	18	147.73	156.13	14.84
1	4	18	5.39	25.17	30.28
2	4	18	18.66	28.68	32.99
3	4	18	26.04	32.69	36.7
-3	5	18	0.67	44.32	14.64
-2	5	18	0.81	-7.02	28.08
-1	5	18	6.04	-3.11	26.37
0	5	18	79.98	96.77	14.44
1	5	18	13.25	14.14	30.79
2	5	18	0.59	-14.54	32.99
3	5	18	0.02	24.47	36.9
-3	6	18	0	-22.96	30.38
-2	6	18	3.2	-33.09	28.38
-1	6	18	3.86	-18.15	27.58
0	6	18	45.48	3.21	29.08
1	6	18	16.63	-34.09	32.19
2	6	18	0.09	19.25	17.65
3	6	18	12.53	19.05	39.11
-2	7	18	23.87	17.95	30.38
-1	7	18	24.89	-5.21	29.68
0	7	18	20.28	-21.26	28.98
1	7	18	0.11	-7.32	32.79
2	7	18	2.11	-36.2	35.8
-2	8	18	0.56	10.63	29.78
-1	8	18	20.57	4.11	31.19
0	8	18	14.37	9.43	31.29
1	8	18	1.09	6.32	16.75
2	8	18	17.05	0.9	37.5
-1	9	18	4.08	-25.07	32.49
0	9	18	14.32	-14.74	33.79
1	9	18	10.1	20.56	33.89
-1	-6	19	9.07	15.54	28.78
0	-6	19	2.2	-36.9	31.09
1	-6	19	0.93	22.06	14.84
-2	-5	19	3.63	-21.56	26.28
-1	-5	19	21.65	10.93	28.88
0	-5	19	0.56	11.43	14.24
1	-5	19	0.24	9.43	28.48
2	-5	19	0.01	-5.21	31.59
-3	-4	19	7.45	-37.9	31.59
-2	-4	19	0.89	19.15	26.87
-1	-4	19	0	20.96	26.47
0	-4	19	0.08	15.54	13.94
1	-4	19	60.21	62.47	15.14
2	-4	19	4.3	12.84	15.74
3	-4	19	1.73	-59.67	36
-3	-3	19	27.09	30.48	15.14
-2	-3	19	8.51	-42.32	28.88
-1	-3	19	676.11	675.77	35.8
0	-3	19	276.43	274.16	16.75
1	-3	19	7.78	11.73	14.34
2	-3	19	114.71	126.85	16.55
3	-3	19	10.1	8.62	34.09
-3	-2	19	2.04	14.34	14.34
-2	-2	19	27.28	22.66	13.74
-1	-2	19	81.3	83.63	13.54
0	-2	19	22.55	48.84	13.64
1	-2	19	22.66	14.24	27.68
2	-2	19	51.19	41.82	15.94
3	-2	19	106.33	115.12	17.65
-3	-1	19	5.62	-32.89	29.18
-2	-1	19	15.4	-10.03	26.37
-1	-1	19	64.49	73.9	13.44
0	-1	19	2.31	6.22	26.47
1	-1	19	58.98	52.34	14.54
2	-1	19	1.89	-7.92	30.08
3	-1	19	0.07	22.46	17.25
-3	0	19	2.93	14.84	27.38
-2	0	19	17.14	0.6	25.67
-1	0	19	5.05	5.41	13.04
0	0	19	47.7	48.13	13.34
1	0	19	63.39	41.21	14.74
2	0	19	46.42	42.32	16.24
3	0	19	6.68	20.76	34.5
-3	1	19	0.03	-39.41	27.58
-2	1	19	11.54	13.24	13.24
-1	1	19	0	23.97	25.17
0	1	19	22.12	-14.34	26.87
1	1	19	90.36	83.33	15.24
2	1	19	108.99	123.24	16.75
3	1	19	0.79	-50.14	35
-3	2	19	5.49	-7.72	27.98
-2	2	19	74.58	70.39	14.14
-1	2	19	17.93	23.06	13.14
0	2	19	4.29	3.71	26.47
1	2	19	75.94	89.55	14.94
2	2	19	6.17	-39.41	32.19
3	2	19	25.5	-16.75	35.6
-3	3	19	20.8	-5.62	27.98
-2	3	19	93.09	108.9	14.24
-1	3	19	228.78	271.75	16.55
0	3	19	9.75	20.36	13.74
1	3	19	401.45	392.39	21.36
2	3	19	2.47	26.67	32.39
3	3	19	28.37	15.64	18.45
-3	4	19	10.19	3.21	28.48
-2	4	19	0.08	-15.84	27.68
-1	4	19	73.08	76.11	13.84
0	4	19	174.38	183.01	15.44
1	4	19	621.07	655.92	36.5
2	4	19	41.3	26.47	33.79
3	4	19	5.95	13.74	38.01
-3	5	19	0.05	0	28.88
-2	5	19	8.31	9.43	28.38
-1	5	19	26.78	22.76	27.68
0	5	19	151.56	137.78	15.34
1	5	19	3.5	-3.81	31.39
2	5	19	12.06	-3.51	34.29
3	5	19	2.84	-42.92	38.81
-3	6	19	2.7	16.35	28.88
-2	6	19	1.46	9.33	28.58
-1	6	19	15.61	28.08	28.78
0	6	19	1.18	-6.72	29.88
1	6	19	15.05	13.24	31.79
2	6	19	2.69	19.15	35.4
3	6	19	10.55	32.49	19.85
-2	7	19	4.99	-11.83	29.48
-1	7	19	5.57	11.43	28.28
0	7	19	0.02	8.82	30.68
1	7	19	7.67	-33.29	33.79
2	7	19	6.7	-22.46	36.2
-2	8	19	1.32	-3.61	30.79
-1	8	19	57.53	72.9	15.94
0	8	19	14.74	-7.32	31.89
1	8	19	82.52	81.77	17.75
2	8	19	7.51	-30.68	37.6
-1	9	19	7.82	8.32	31.79
0	9	19	2.56	-25.87	32.59
1	9	19	4.2	37.8	18.55
-1	-6	20	0.35	0	29.08
0	-6	20	0	12.23	29.38
1	-6	20	2.33	31.19	15.64
-2	-5	20	0.51	-101.58	30.08
-1	-5	20	0.32	-3.81	14.54
0	-5	20	4.7	20.96	15.04
1	-5	20	2.52	8.22	29.68
2	-5	20	7.84	17.05	31.49
-2	-4	20	18.52	26.67	28.58
-1	-4	20	17.62	4.61	27.58
0	-4	20	46.56	47.23	14.54
1	-4	20	0.39	11.73	14.84
2	-4	20	3.57	-11.53	31.19
-3	-3	20	2.4	13.64	29.98
-2	-3	20	0.16	21.46	14.14
-1	-3	20	165.48	173.78	15.84
0	-3	20	7.25	-6.12	27.56
1	-3	20	6.97	24.47	28.66
2	-3	20	0.25	27.78	15.94
3	-3	20	0.35	28.68	34.19
-3	-2	20	5.24	-24.97	28.78
-2	-2	20	207.22	232.34	16.14
-1	-2	20	63.78	68.19	14.94
0	-2	20	119.73	105.59	14.84
1	-2	20	6.95	-19.85	14.74
2	-2	20	86.61	95.06	16.45
3	-2	20	12.13	-29.88	35.2
-3	-1	20	1.1	22.46	28.18
-2	-1	20	0.24	-18.25	26.87
-1	-1	20	1.72	-39.91	27.18
0	-1	20	29.71	22.76	13.74
1	-1	20	182.21	179.1	15.44
2	-1	20	109.45	90.25	16.75
3	-1	20	33.21	62.27	17.85
-3	0	20	0.14	-8.92	27.28
-2	0	20	0	4.81	25.97
-1	0	20	25.63	16.55	13.54
0	0	20	0.21	-48.13	28.08
1	0	20	10.38	-50.74	28.98
2	0	20	1.88	-14.84	30.68
3	0	20	22.73	41.11	18.05
-3	1	20	18.95	39.31	14.24
-2	1	20	0.06	4.01	25.37
-1	1	20	7.1	1.8	27.28
0	1	20	0.33	-45.02	27.88
1	1	20	0.61	-144.1	32.29
2	1	20	67.04	78.02	16.55
3	1	20	0.99	-55.45	36.4
-3	2	20	5.31	8.12	27.88
-2	2	20	1.89	20.96	25.57
-1	2	20	3.72	3.51	26.77
0	2	20	5.82	-9.02	27.38
1	2	20	21.29	21.46	15.34
2	2	20	0.02	12.74	31.49
3	2	20	0.06	11.83	34.6
-3	3	20	25.6	50.64	14.34
-2	3	20	28.35	15.34	14.24
-1	3	20	5.23	-47.63	27.18
0	3	20	109.08	110.91	14.54
1	3	20	8.18	-2.41	30.36
2	3	20	125.14	91.35	17.45
3	3	20	25.82	-50.04	38.51
-3	4	20	18.75	1.7	28.88
-2	4	20	38.8	65.08	14.34
-1	4	20	64.19	64.48	14.14
0	4	20	86.4	88.65	14.94
1	4	20	542.69	491.06	29.78
2	4	20	6.99	25.47	32.99
3	4	20	3.58	-66.68	37.8
-3	5	20	6	-7.12	30.89
-2	5	20	5.04	-3.01	28.36
-1	5	20	37.43	33.09	14.34
0	5	20	35.19	-26.57	30.38
1	5	20	60.7	49.44	16.35
2	5	20	5.12	-23.16	34.19
3	5	20	6.02	27.18	19.35
-2	6	20	1.69	-22.66	28.98
-1	6	20	14.08	14.84	14.74
0	6	20	11.11	12.53	29.58
1	6	20	7.54	0.7	31.99
2	6	20	0.56	-4.81	35.7

h	k	l	F_c^2	F_o^2	σF_o^2
3	6	20	2.99	24.97	21.06
-2	7	20	3.04	7.02	29.08
-1	7	20	4.86	-18.15	30.08
0	7	20	0.06	-58.66	31.59
1	7	20	1.27	-27.38	33.19
2	7	20	14.14	-3.41	36.7
-1	8	20	8.5	-18.15	31.39
0	8	20	0.19	-11.63	31.39
1	8	20	20.03	42.72	17.65
0	9	20	36.65	1.8	34.7
0	-6	21	13.6	-8.22	31.39
-1	-5	21	13.22	24.97	29.48
0	-5	21	59.82	79.42	15.34
1	-5	21	0.1	-33.49	31.39
-2	-4	21	3.2	-39.11	28.88
-1	-4	21	4.43	-10.33	28.48
0	-4	21	11.14	11.43	28.08
1	-4	21	0	-3.91	29.68
2	-4	21	0.09	31.09	31.89
-2	-3	21	14.2	7.32	27.78
-1	-3	21	8.87	8.12	27.88
0	-3	21	0.01	-5.72	27.78
1	-3	21	0.7	9.53	28.98
2	-3	21	3.14	4.91	31.39
-3	-2	21	0.71	-34.09	29.48
-2	-2	21	324.58	330.41	21.06
-1	-2	21	411.84	392.69	22.16
0	-2	21	20.85	-19.25	27.16
1	-2	21	9.24	-35.8	29.78
2	-2	21	6.69	-29.78	32.39
3	-2	21	2.79	38.91	17.65
-3	-1	21	2.12	-7.82	28.68
-2	-1	21	37.06	17.75	28.78
-1	-1	21	20.08	-34.29	27.98
0	-1	21	23.43	28.78	13.84
1	-1	21	11.4	20.96	30.08
2	-1	21	325.32	296.02	18.95
3	-1	21	7.09	-60.77	35.9
-3	0	21	0.44	21.96	28.08
-2	0	21	1.91	-35.1	27.58
-1	0	21	0.02	-74.51	28.18
0	0	21	22.24	6.72	27.88
1	0	21	19.81	-23.46	30.18
2	0	21	3.65	12.03	31.39
3	0	21	34.24	5.01	35.9
-3	1	21	2.01	-22.66	29.48
-2	1	21	0.02	13.54	25.57
-1	1	21	0	-38.21	27.28
0	1	21	6.18	15.04	27.78
1	1	21	21.09	19.35	15.44
2	1	21	0.63	19.55	30.99
3	1	21	0.05	-23.97	35.2
-3	2	21	10.91	26.07	28.68
-2	2	21	39.31	7.12	27.38
-1	2	21	2.27	-5.11	26.87
0	2	21	93.29	90.65	14.34
1	2	21	1.33	25.67	29.78
2	2	21	17.84	9.83	33.29
3	2	21	12.9	-18.15	36.4
-3	3	21	0.65	-19.65	29.28
-2	3	21	5.49	20.26	26.47
-1	3	21	55.24	57.46	14.14
0	3	21	5.46	14.24	27.68
1	3	21	6.04	0	30.48
2	3	21	125.65	114.72	17.95
3	3	21	1.64	-1.5	18.55
-3	4	21	38.3	-0.9	30.38
-2	4	21	80.27	94.36	14.94
-1	4	21	0.46	-7.42	27.38
0	4	21	852.84	942.81	42.92
1	4	21	363.96	386.77	22.46
2	4	21	7.43	30.99	32.29
3	4	21	35.99	-12.03	37.3
-3	5	21	0	-44.02	31.29
-2	5	21	17.29	14.24	28.08
-1	5	21	11.04	6.42	28.68
0	5	21	69.12	77.41	15.64
1	5	21	22.55	-5.01	31.49
2	5	21	6.21	-8.92	18.05
3	5	21	12.39	-3.51	37.9
-2	6	21	7.68	15.14	28.58
-1	6	21	2.49	-13.74	29.18
0	6	21	0.35	-1.4	29.18
1	6	21	34.27	-0.7	32.79
2	6	21	10.29	20.46	18.45
-2	7	21	0	-22.46	31.09
-1	7	21	3.55	24.67	28.98
0	7	21	0.37	3.91	31.29
1	7	21	0.71	-8.92	32.59
2	7	21	11.36	-37.1	36.3
-1	8	21	0.2	0.9	30.08
0	8	21	8.57	-7.82	32.39
1	8	21	7.81	9.73	34.09
-1	-5	22	7.03	-35.1	29.88
0	-5	22	4.05	28.78	30.08
1	-5	22	2.55	46.53	15.74
-2	-4	22	9.3	10.83	28.28
-1	-4	22	10.39	33.39	14.74
0	-4	22	0.03	-7.22	28.28
1	-4	22	0.29	15.74	30.48
2	-4	22	0.09	-18.05	33.59
-2	-3	22	12.22	0	14.94
-1	-3	22	1.65	35	13.84
0	-3	22	10.3	11.53	14.64
1	-3	22	4.37	17.75	29.38
2	-3	22	0	8.52	32.19
-2	-2	22	2.52	-25.87	29.88
-1	-2	22	1.92	-5.11	27.58
0	-2	22	0.93	12.63	27.98
1	-2	22	7.62	26.17	28.58
2	-2	22	3.76	-3.21	32.09
-3	-1	22	49.54	29.88	15.54
-2	-1	22	195.37	225.02	16.55
-1	-1	22	96.93	85.34	14.44
0	-1	22	2.04	-32.09	27.58
1	-1	22	281.54	250.99	17.15
2	-1	22	42.59	1.5	34.09
3	-1	22	22.11	8.92	35.5
-3	0	22	40.39	48.94	15.14
-2	0	22	0.01	-18.05	28.08
-1	0	22	13.34	-26.27	27.38
0	0	22	34.17	-18.75	28.38
1	0	22	124.12	96.77	16.04
2	0	22	17.37	6.02	31.99
3	0	22	8.59	2.61	35.8
-3	1	22	1.16	12.74	14.54
-2	1	22	11.84	21.86	13.84
-1	1	22	0.42	-31.19	27.18
0	1	22	0.16	-22.86	28.08
1	1	22	0.08	-69.89	30.48
2	1	22	0.09	8.82	32.39
3	1	22	0.05	0.8	36.4
-3	2	22	6.53	-22.66	28.08
-2	2	22	0.62	15.04	13.84
-1	2	22	1.31	3.31	26.27
0	2	22	16.66	-8.92	28.08
1	2	22	1.04	-15.84	29.78
2	2	22	6.62	16.95	32.69
3	2	22	4.93	-0.8	36.5
-3	3	22	27.27	-21.26	29.88
-2	3	22	14.6	13.64	28.18
-1	3	22	0.54	17.65	27.07
0	3	22	43.6	59.56	14.84
1	3	22	9.8	-7.42	30.08
2	3	22	8.38	19.45	33.79
3	3	22	6.27	16.55	36.2
-3	4	22	3.56	-41.92	32.79
-2	4	22	3.93	-7.82	28.38
-1	4	22	90.78	112.21	15.04
0	4	22	5.73	-56.76	30.18
1	4	22	342.29	332.72	19.25
2	4	22	42.77	1.5	35.4
3	4	22	19.48	36.2	19.75
-2	5	22	7.3	-38.1	29.08
-1	5	22	17.43	13.54	14.94
0	5	22	39.19	29.28	31.69
1	5	22	50.17	28.68	32.89
2	5	22	2.12	-63.07	35.3
-2	6	22	1.71	7.32	14.94
-1	6	22	0.42	-1.6	29.08
0	6	22	5.65	18.05	15.34
1	6	22	4.79	-35.3	32.89
2	6	22	11.29	-37.7	36.9
-1	7	22	1.15	18.65	15.24
0	7	22	3.59	0.8	31.99
1	7	22	0.5	-33.79	33.59
2	7	22	0	-59.36	39.41
-1	8	22	0.34	25.07	16.65
0	8	22	2.06	6.32	33.29
1	8	22	1.01	7.32	35.1
0	-5	23	0.13	-2.71	30.79
-1	-4	23	42.2	5.31	30.38
0	-4	23	0.79	18.65	28.58
1	-4	23	6.18	18.25	31.39
-2	-3	23	6.9	14.34	15.14
-1	-3	23	7.03	5.11	14.54
0	-3	23	0.12	4.71	27.98
1	-3	23	1.58	29.18	30.18
2	-3	23	0.48	3.51	32.59
-2	-2	23	65.5	66.08	15.34
-1	-2	23	14.23	3.81	27.98
0	-2	23	21.37	9.83	28.78
1	-2	23	11.49	13.34	15.14
2	-2	23	27.56	12.53	32.39
-2	-1	23	12.15	-108.1	33.19
-1	-1	23	3.42	-64.68	28.78
0	-1	23	10.51	29.58	14.34
1	-1	23	13.43	-41.62	30.18
2	-1	23	0.1	-1.6	32.99
-3	0	23	5.15	4.51	30.28
-2	0	23	23.82	26.07	14.24
-1	0	23	6.11	-53.35	28.38
0	0	23	21.85	-171.78	32.09
1	0	23	49.59	-51.64	32.19
2	0	23	3.36	-5.52	32.89
3	0	23	5.51	28.08	36.3
-3	1	23	3.06	-4.51	29.68
-2	1	23	8.87	30.08	13.84
-1	1	23	3.82	29.68	13.64
0	1	23	2.32	-32.99	28.48
1	1	23	0.01	-1.4	29.78
2	1	23	0.09	-3.41	16.75
3	1	23	13.56	0	36.3
-3	2	23	0.38	2.71	31.79
-2	2	23	0.56	27.38	27.98
-1	2	23	1.09	-10.53	26.47
0	2	23	1.6	6.52	14.34
1	2	23	17.07	-16.75	30.68
2	2	23	0.95	6.92	16.95
3	2	23	1.94	-130.46	38.61
-2	3	23	2.28	2.41	28.18
-1	3	23	0.98	2.21	14.14
0	3	23	1.85	-27.48	28.78
1	3	23	0.1	-9.93	30.89
2	3	23	0	-27.48	34.19
3	3	23	6.74	-29.88	38.31
-2	4	23	48.57	74.11	14.74
-1	4	23	1.55	1.5	27.88
0	4	23	47.67	64.18	15.14
1	4	23	89.95	116.52	16.75
2	4	23	0.34	-38.71	33.89
-2	5	23	0.95	8.52	29.78
-1	5	23	214.5	232.04	17.25
0	5	23	486.4	446.44	24.27
1	5	23	21.84	-6.92	32.59
2	5	23	0.9	26.17	35.1
-2	6	23	0.06	2.71	30.28
-1	6	23	13.05	-53.45	30.99
0	6	23	3.9	27.07	30.99
1	6	23	0.27	14.24	16.55
2	6	23	1.06	22.16	35.7
-1	7	23	6.25	12.33	31.29
0	7	23	10.07	8.52	31.49
1	7	23	10.96	-60.37	34.4
-1	-4	24	11.67	17.35	30.89
0	-4	24	0.05	18.25	15.14
1	-4	24	4.74	-4.51	32.59
-1	-3	24	0.04	7.72	27.28
0	-3	24	19.2	30.89	15.04
1	-3	24	2.13	-13.64	30.79
-2	-2	24	20.91	-4.41	29.28
-1	-2	24	10.96	-21.06	28.58
0	-2	24	3.22	-2.21	14.94
1	-2	24	27.75	3.21	30.48
2	-2	24	0.67	30.79	31.79
-2	-1	24	142.64	175.39	16.45
-1	-1	24	33.35	24.77	29.08
0	-1	24	7.76	-61.37	28.78
1	-1	24	1.05	-63.98	30.68
2	-1	24	26.58	28.48	16.75
-2	0	24	0.35	24.87	27.68
-1	0	24	1.49	-7.52	28.48
0	0	24	161.35	151.12	15.84
1	0	24	167.21	149.71	16.55
2	0	24	6.86	0.8	32.09
-2	1	24	23.94	52.34	14.34
-1	1	24	1.14	-15.54	26.17
0	1	24	5.4	-37	29.38
1	1	24	31.94	23.57	31.19
2	1	24	31.13	30.99	16.95
-2	2	24	3.22	-26.97	29.18
-1	2	24	0.04	3.71	28.48
0	2	24	4.48	11.43	27.98
1	2	24	4.48	-32.39	30.79
2	2	24	0.66	14.54	32.89
-2	3	24	0.42	14.94	29.38
-1	3	24	21.31	0.7	28.48
0	3	24	3.09	26.07	28.78
1	3	24	22.38	29.48	15.64
2	3	24	0.03	-4.91	33.99
-2	4	24	1.09	9.43	30.18
-1	4	24	4.18	-53.55	29.18
0	4	24	0.29	1.5	30.28
1	4	24	18.65	19.25	31.99
2	4	24	0.69	27.88	35.2
-2	5	24	8.76	0.9	15.14
-1	5	24	15.68	4.01	29.18
0	5	24	35.32	7.82	32.09
1	5	24	3.94	-19.35	33.09
2	5	24	5.61	2.61	36.3
-1	6	24	92.46	141.59	16.45
0	6	24	123.35	160.74	17.25
1	6	24	1.32	8.52	32.29
-1	7	24	3.64	-2.71	33.39
0	7	24	0.71	30.18	31.69
1	7	24	3.91	28.08	17.85
-1	-3	25	6.08	29.58	14.94
0	-3	25	0.51	15.64	28.88
1	-3	25	3.94	32.19	15.74
-1	-2	25	7.35	15.94	14.64
0	-2	25	13.04	-59.36	30.18
1	-2	25	3.4	17.05	31.09
2	-2	25	10.07	-6.72	17.95
-2	-1	25	98.53	-60.77	33.99
-1	-1	25	0.25	-49.84	29.18
0	-1	25	8.88	27.58	28.78
1	-1	25	19.95	24.97	15.74
2	-1	25	13.72	-3.51	32.89
-2	0	25	6.86	18.35	28.18
-1	0	25	0.81	-21.46	28.98

h	k	l	F_c^2	F_o^2	σF_o^2
0	0	25	3.04	-97.27	32.09
1	0	25	3.15	3.91	30.58
2	0	25	55.44	-60.27	34.8
-2	1	25	2.69	-7.02	15.04
-1	1	25	23.75	-0.8	28.58
0	1	25	17.41	-24.87	30.38
1	1	25	11.17	-25.67	16.14
2	1	25	4.03	-9.33	32.19
-2	2	25	4.55	19.75	27.68
-1	2	25	0.28	25.77	14.24
0	2	25	3.18	12.74	28.58
1	2	25	0	-16.24	31.99
2	2	25	1.23	-31.39	35.2
-2	3	25	0.13	-23.46	29.68
-1	3	25	0.26	-4.71	27.98
0	3	25	1.83	6.12	30.28
1	3	25	7.04	-7.12	32.19
2	3	25	0.42	-28.28	34.9
-2	4	25	1.07	19.35	15.04
-1	4	25	11.3	28.48	14.84
0	4	25	0.97	19.25	15.14
1	4	25	0.11	13.74	32.79
2	4	25	17.37	-15.84	34.5
-1	5	25	74.18	69.29	16.04
0	5	25	126.2	95.46	17.25
1	5	25	0.12	19.55	16.35
2	5	25	17.63	-6.42	37
-1	6	25	19.01	-8.12	31.69
0	6	25	3.48	-7.72	16.55
1	6	25	7.79	15.94	34.5
0	-3	26	1.06	-28.38	32.39
-1	-2	26	1.33	-3.51	29.18
0	-2	26	0.3	7.72	15.14
1	-2	26	0.01	30.38	30.48
-1	-1	28	8.53	-0.8	29.68
0	-1	26	4.12	19.55	15.04
1	-1	26	7.22	15.84	15.84
-2	0	26	46.3	20.96	31.39
-1	0	26	7.27	-6.72	30.28
0	0	26	7.86	-42.82	31.49
1	0	26	15.53	6.72	31.09
2	0	26	9.73	1.2	17.55
-2	1	26	0.44	10.83	28.48
-1	1	26	8.14	-8.22	30.18
0	1	26	48.23	-28.58	32.59
1	1	26	2.33	26.97	30.28
2	1	26	1.57	-25.77	34.6
-2	2	26	0.61	-80.02	30.79
-1	2	26	0.63	2.41	29.08
0	2	26	31.46	45.93	15.44
1	2	26	8.51	-13.84	31.59
2	2	26	0.05	4.41	34.5
-2	3	26	0.36	-42.82	31.29
-1	3	26	0.01	8.72	14.84
0	3	26	6.71	20.96	30.08
1	3	26	3.21	21.96	16.04
2	3	26	0.21	-56.56	35.4
-1	4	26	6.59	-28.98	29.78
0	4	26	0.67	-44.62	30.99
1	4	28	0.04	11.03	16.75
2	4	26	8.64	17.95	19.15
-1	5	28	2.89	14.14	30.99
0	5	26	3.29	-0.8	32.29
1	5	26	0.65	19.35	34.09
0	6	26	53.6	41.31	17.15
0	-2	27	0.03	-40.11	31.89
-1	-1	27	12.41	-24.37	30.79
0	-1	27	0.61	-24.57	30.18
1	-1	27	2.64	26.97	30.68
-1	0	27	0.15	-42.22	30.68
0	0	27	14.29	13.64	30.38
1	0	27	1.24	-11.33	32.19
-1	1	27	1.36	3.41	29.28
0	1	27	21.7	-52.75	31.99
1	1	27	8.13	-13.74	33.19
-1	2	27	0.6	8.82	14.84
0	2	27	0.11	-23.36	30.48
1	2	27	0.53	-18.05	32.39
-1	3	27	5.45	-12.23	31.09
0	3	27	10.1	6.82	15.64
1	3	27	12.31	7.02	32.69
-1	4	27	5.48	-8.92	31.69
0	4	27	3.43	16.45	31.09
1	4	27	0.82	13.34	33.29
0	5	27	0.86	8.12	30.79
1	5	27	0.69	-5.52	34.8
0	0	28	1.82	-39.41	31.09
1	0	28	0.07	13.74	33.19
-1	1	28	7.8	-8.42	31.69
0	1	28	18.81	-12.33	32.59
1	1	28	4.57	-6.42	33.09
-1	2	28	0.4	-12.74	30.68
0	2	28	0.76	19.35	31.19
1	2	28	2.01	-2.61	16.95
-1	3	28	5.82	33.79	16.14
0	3	28	10.31	17.75	31.49
1	3	28	0.25	-9.13	33.79
0	4	28	13.58	8.22	16.95

3.9 NAL3XL

h	k	l	F_c^2	F_o^2	σF_o^2
1	0	0	4002.75	4013.13	58.15
2	0	0	451.23	395.64	17.86
3	0	0	760.5	884.47	27.93
4	0	0	785.88	787.38	27.4
5	0	0	105.83	110.19	12.02
6	0	0	8.36	24.44	13.56
7	0	0	137.7	132.21	16.32
8	0	0	1704.66	1700.39	54.39
9	0	0	171.13	181.3	18.33
10	0	0	2.36	-56	32.23
1	1	0	514.44	495.4	9.17
2	1	0	205.48	212.42	8.42
3	1	0	1016.76	1013.83	21.44
4	1	0	112.66	116.43	7.41
5	1	0	93.5	85.77	8.52
6	1	0	79.29	68.99	9.95
7	1	0	569.34	560.14	20.7
8	1	0	260.36	245.59	12.96
9	1	0	7.29	-12.01	21.29
10	1	0	2.02	5.83	16.18
0	2	0	440.99	406.59	10.3
1	2	0	167.33	139.9	3.9
2	2	0	67.16	89.64	9.54
3	2	0	1458.32	1510.43	39.15
4	2	0	16.47	-2.89	18.47
5	2	0	0.65	-24.44	21.08
6	2	0	151.74	155.96	15.24
7	2	0	177.35	163.24	16.72
8	2	0	126.19	109.99	17.32
9	2	0	3.23	10.61	29.55
10	2	0	46.13	49.35	19.47
1	3	0	907.9	852.49	19.4
2	3	0	441.27	423.57	21.22
3	3	0	1179.65	1262.92	35.05
4	3	0	444.11	501.73	24.37
5	3	0	115.3	112.47	13.16
6	3	0	0.32	1.28	26.05
7	3	0	9.47	11.48	15.78
8	3	0	19.25	13.36	28.87
9	3	0	0.82	-25.72	30.35
10	3	0	1.96	-7.59	19.41
0	4	0	20691.13	19214.98	274.84
1	4	0	97.81	106.34	4.79
2	4	0	56.39	54.32	9.6
3	4	0	410.53	462.72	22.23
4	4	0	421.14	494.54	25.25
5	4	0	25.59	19.81	23.64
6	4	0	48.74	23.57	15.44
7	4	0	0	18.47	28.61
8	4	0	539.19	509.38	26.12
9	4	0	26.97	24.04	17.86
10	4	0	29.76	50.43	20.61
1	5	0	307.87	279.48	7.48
2	5	0	298.68	290.82	16.59
3	5	0	685.58	750.31	27.66
4	5	0	29.11	46.94	12.02
5	5	0	10.31	-8.06	14.1
6	5	0	117.36	146.85	16.05
7	5	0	210.93	228.3	18.4
8	5	0	228	246.7	19.34
9	5	0	39.59	37.2	18.4
0	6	0	15.65	11.98	7.65
1	6	0	4.78	-3.4	7.6
2	6	0	20.27	4.23	17.86
3	6	0	525.54	543.36	25.65
4	6	0	282.81	289.47	15.31
5	6	0	3.27	-0.87	24.98
6	6	0	24.28	31.69	15.85
7	6	0	29.09	34.85	16.59
8	6	0	186.87	190.9	19.27
9	6	0	24.1	7.45	31.49
1	7	0	108.23	102.74	5.23
2	7	0	15.53	33.51	10.74
3	7	0	1280.86	1321.2	40.36
4	7	0	113.28	119.86	14.24
5	7	0	36.66	63.86	15.04
6	7	0	2.46	26.19	27.93
7	7	0	91.14	92.19	17.39
8	7	0	43.11	52.64	18.13
9	7	0	33.81	26.32	34.45
0	8	0	70.99	60.76	7.64
1	8	0	228.09	235.15	6.47
2	8	0	27.16	15.31	12.02
3	8	0	188.07	244.49	14.71
4	8	0	405.27	400.27	20.48
5	8	0	149.43	160.28	16.05
6	8	0	2.4	-58.42	28.34
7	8	0	1.09	24.78	29.41
8	8	0	28.74	-35.86	32.7
1	9	0	1.89	10.31	7.27
2	9	0	0.06	21.69	22.43
3	9	0	31.75	42.5	13.77
4	9	0	78.23	73.46	14.84
5	9	0	111.93	128.99	16.38
6	9	0	11.01	8.06	16.32
7	9	0	5.18	8.12	17.19
8	9	0	0.04	28	31.63
0	10	0	192.31	192.69	13.23
1	10	0	0.17	-3.48	11.26
2	10	0	8.17	15.44	23.3
3	10	0	70.66	7.45	25.72
4	10	0	2.18	9.67	25.99
5	10	0	2.17	20.68	25.78
6	10	0	16.35	20.41	16.72
7	10	0	0.34	-9.4	30.28
8	10	0	19.94	15.04	19.67
1	11	0	38.78	47.54	6.7
2	11	0	0.35	-6.78	24.71
3	11	0	15.33	-7.12	25.78
4	11	0	2.87	5.3	26.59
5	11	0	2.01	9.4	15.78
8	11	0	5.76	-15.44	26.81
7	11	0	46.34	65.07	18.67
0	12	0	71.68	81.96	10.11
1	12	0	58.91	58.52	13.85
2	12	0	0.61	-30.75	24.51
3	12	0	48.82	61.91	15.04
4	12	0	50.69	43.91	15.91
5	12	0	15.19	0	28.81
6	12	0	61.94	81.32	18.26
1	13	0	29.35	30.69	8.92
2	13	0	6.67	-14.84	25.65
3	13	0	4.65	-33.51	27.46
4	13	0	1.58	3.56	26.39
5	13	0	2.82	-63.86	30.42
0	14	0	0.03	-1.52	21.05
1	14	0	27	16.61	11.77
2	14	0	0.34	-21.22	26.19
3	14	0	9.49	18.4	26.66
4	14	0	9.32	7.72	29.14
1	15	0	12.24	-16.61	15.88
2	15	0	0	15.58	27.53
-10	1	1	0.57	-2.64	22.17
-9	1	1	1.44	11.06	20.55
-8	1	1	161.25	134.95	12.01
-7	1	1	240.43	245.22	12.01
-6	1	1	54.06	58.91	9.85
-5	1	1	0.9	2.39	13.79
-4	1	1	3383.86	3864.36	60.13
-3	1	1	689.39	701.42	17.75
-2	1	1	1717.08	1684.82	50.23
-1	1	1	2534.7	2460.64	62.77
0	1	1	4300.66	3760.8	55.7
1	1	1	35.32	29.17	4.84
2	1	1	1947.43	1999.38	32.78
3	1	1	136.26	135.99	7.79
4	1	1	164.09	189.72	8.14
5	1	1	418.12	403.92	28.54
6	1	1	236.55	239.73	12.69
7	1	1	445.09	463.14	16.13
8	1	1	143.41	123.55	12.69
9	1	1	26.95	20.04	15.38
10	1	1	2.29	-22.7	26.59
-10	2	1	4.35	0	32.16
-9	2	1	30.47	69.36	16.85
-8	2	1	50.73	54.79	16.59
-7	2	1	1.92	-3.29	26.52
-6	2	1	0.09	0.4	24.64
-5	2	1	119.39	101.12	12.42
-4	2	1	140.58	143.63	10.88
-3	2	1	15.24	-23.03	18
-2	2	1	3212.54	3215.85	69.97
-1	2	1	3875.39	3720.7	91.16
0	2	1	361.22	288.18	7.25
1	2	1	1624.98	1530.1	37.26
2	2	1	509.14	524.96	22.23
3	2	1	3.33	-6.38	17.32
4	2	1	14.75	26.79	10.34
5	2	1	4.58	-2.35	12.49
6	2	1	56.17	46.67	14.71
7	2	1	3857.69	3710.59	90.31
8	2	1	189.41	216.69	18.2
9	2	1	2.39	22.63	30.75
10	2	1	50.5	3.96	34.31
-10	3	1	7.16	28.34	31.83
-9	3	1	3.72	3.49	17.19
-8	3	1	27.27	3.42	29.48
-7	3	1	163.09	181.37	16.45
-6	3	1	16.05	-0.4	25.18
-5	3	1	97.24	80.51	12.76
-4	3	1	952.66	1021.66	32.5
-3	3	1	641.81	689.34	25.45
-2	3	1	18.74	9.27	17.32
-1	3	1	19234.42	17909.18	229
0	3	1	5208.42	4884.73	50.99
1	3	1	3050.08	2978.92	34.76
2	3	1	26.33	33.1	9.74
3	3	1	1737.46	1661.31	42.37
4	3	1	4.22	-7.72	19.14
5	3	1	19.81	15.98	23.17
6	3	1	7.36	10.88	26.05
7	3	1	702.45	733.73	37.07
8	3	1	23.2	50.5	16.99
9	3	1	42.26	37.94	18.13
10	3	1	61.19	58.89	20.14
-10	4	1	8.64	22.83	19.61
-9	4	1	139.17	106.83	18.4
-8	4	1	447.87	415.51	22.7
-7	4	1	0.79	-2.48	28
-6	4	1	38.9	44.65	14.77
-5	4	1	0.11	-54.66	23.64
-4	4	1	2492.08	2770.88	65.8
-3	4	1	420.09	444.92	22.29
-2	4	1	90.95	78.21	9.8
-1	4	1	7699.7	7228.43	74.93
0	4	1	7566.12	7243.61	74.99
1	4	1	114.8	106.76	4.77
2	4	1	229.21	209.77	11.68
3	4	1	48.77	53.05	10.21
4	4	1	2325.47	2421.02	59.56
5	4	1	4.74	21.62	13.7
6	4	1	56.75	50.5	15.78
7	4	1	50.69	64.93	16.92
8	4	1	17.96	16.12	29.41
9	4	1	0	6.18	17.93
-9	5	1	149.6	142.62	19.27
-8	5	1	558.35	555.45	29.34
-7	5	1	45.37	29.08	29.34
-6	5	1	4	-36.73	27.86
-5	5	1	50.67	56.34	13.97
-4	5	1	292.39	304.78	15.44
-3	5	1	2.83	7.86	18.2
-2	5	1	180.34	163.44	10.41
-1	5	1	0.13	-24.14	7.86
0	5	1	77.8	86.08	4.61
1	5	1	161.58	153.94	4.9
2	5	1	84.94	78.56	9.67
3	5	1	238.76	256.37	13.16
4	5	1	1208.55	1219.27	38.74
5	5	1	3.16	-19.2	25.58
6	5	1	9.43	11.95	27.73
7	5	1	13.46	-3.89	29.34
8	5	1	5.23	7.85	30.69
9	5	1	2.86	2.89	31.22
-9	6	1	0	8.53	18.4
-8	6	1	2.9	-7.05	31.02
-7	6	1	96.69	101.19	17.26
-6	6	1	21.29	38.21	15.58
-5	6	1	36.51	46.53	14.57
-4	6	1	23.49	41.16	12.89
-3	6	1	172.63	166.59	12.42
-2	6	1	113.04	102.13	10.34
-1	6	1	1033.47	957.76	14.76
0	6	1	55.28	43.8	10.01
1	6	1	8.32	2.57	6.46
2	6	1	37.37	14.03	18.53
3	6	1	541.92	560.62	26.46
4	6	1	184.16	228.37	14.64
5	6	1	41.92	71.58	14.84
6	6	1	122.62	98.37	16.92
7	6	1	71.64	42.3	17.12
8	6	1	3.88	8.66	30.35
9	6	1	9.04	25.92	33.64
-9	7	1	7.99	32.97	19.74
-8	7	1	1.57	27.53	30.35
-7	7	1	41.27	-14.71	29.28
-6	7	1	17.27	11.75	16.25
-5	7	1	54.05	69.9	15.11
-4	7	1	0.71	11.62	23.7
-3	7	1	4.08	18.05	20.95
-2	7	1	55.3	10.41	19.94
-1	7	1	533.18	499.7	11.76
0	7	1	46.14	50.23	5.39
1	7	1	36.81	32.15	9.48
2	7	1	443.28	438.41	23.23
3	7	1	215.71	232	14.03
4	7	1	4.23	-5.77	13.83
5	7	1	0.02	3.76	26.46
6	7	1	2.84	15.11	27.53
7	7	1	41.71	41.43	16.99
8	7	1	40.27	18.2	32.37
9	7	1	3.4	-31.09	20.14
-9	8	1	50.97	76.82	20.41
-8	8	1	195.68	241.26	19.67
-7	8	1	10.8	8.92	29.14
-6	8	1	0	-20.55	28.07
-5	8	1	174.62	172.84	16.18
-4	8	1	123.96	110.53	14.91
-3	8	1	0.91	10.01	22.83

h	k	l	F_c^2	F_o^2	σF_o^2
-2	8	1	58.43	63.92	12.09
-1	8	1	447.49	447.25	11.83
0	8	1	325.22	331.37	8.59
1	8	1	31.92	33.26	8.75
2	8	1	86.71	110.73	12.56
3	8	1	237.54	274.1	15.38
4	8	1	258.68	256.57	16.32
5	8	1	16.21	6.71	26.59
6	8	1	52.62	47.94	16.52
7	8	1	15.6	34.98	17.26
8	8	1	3.24	0	30.69
-8	9	1	26.48	29.95	18.4
-7	9	1	144.32	127.92	18.47
-6	9	1	2.91	-37.07	28.54
-5	9	1	65.77	56.61	15.78
-4	9	1	91.56	82.19	15.11
-3	9	1	1.45	-35.32	24.04
-2	9	1	72.4	90.45	13.09
-1	9	1	27.32	32.94	6.53
0	9	1	104.43	110.55	6.28
1	9	1	146.49	162.2	8.56
2	9	1	13.03	-20.88	23.17
3	9	1	59.68	65.6	14.1
4	9	1	137.25	134.56	15.85
5	9	1	0.08	3.29	26.52
6	9	1	0.08	-7.39	27.6
7	9	1	8.3	-30.55	30.62
8	9	1	0.17	-4.63	32.1
-8	10	1	0.39	-21.49	33.91
-7	10	1	20.54	31.96	17.59
-6	10	1	5.87	17.39	29.01
-5	10	1	4.34	-33.98	27.46
-4	10	1	10.29	-3.22	25.72
-3	10	1	17.06	28.13	14.1
-2	10	1	14.37	-59.63	24.44
-1	10	1	21.35	43.84	14.51
0	10	1	3.5	-11.54	11.23
1	10	1	94.62	113.92	6.72
2	10	1	63.12	40.83	13.7
3	10	1	90.35	98.84	14.91
4	10	1	30.24	-1.68	26.05
5	10	1	37	1.21	27.8
6	10	1	25.92	-18.67	29.75
7	10	1	37.45	-8.12	31.83
-7	11	1	0.13	-35.25	32.1
-6	11	1	0.14	-3.49	29.34
-5	11	1	15.47	22.29	27.33
-4	11	1	114.75	135.77	16.25
-3	11	1	46.19	49.96	14.57
-2	11	1	5.77	-39.82	25.11
-1	11	1	0.16	13.12	9.53
0	11	1	5.32	14.33	9.34
1	11	1	9.81	-1.08	12
2	11	1	51.97	52.44	14.17
3	11	1	123	121.81	14.91
4	11	1	1.05	-24.78	26.52
5	11	1	0.04	-48.55	28.4
6	11	1	10.78	13.63	29.08
7	11	1	3.16	-4.77	31.16
-6	12	1	46.02	50.43	17.66
-5	12	1	110.58	96.69	17.32
-4	12	1	16	34.04	15.38
-3	12	1	16.82	27.4	14.57
-2	12	1	31.5	5.24	24.84
-1	12	1	20.01	17.79	9.75
0	12	1	0.02	-6.72	11.83
1	12	1	54.19	61.08	10.02
2	12	1	37.84	18.87	14.5
3	12	1	15.84	-34.65	25.78
4	12	1	7.67	-4.63	27.26
5	12	1	6.68	-39.89	29.14
6	12	1	11.71	-30.22	31.96
-5	13	1	17.11	8.26	30.08
-4	13	1	0.48	-2.15	27.93
-3	13	1	44.23	55.4	15.58
-2	13	1	5.88	25.11	25.38
-1	13	1	25.34	30.4	13.49
0	13	1	8.37	-11.97	12.38
1	13	1	84.57	94.57	7.56
2	13	1	5.33	11.68	25.45
3	13	1	2.64	-21.76	26.05
4	13	1	0.92	0.74	26.59
5	13	1	0.31	-0.81	30.15
-4	14	1	2.33	-14.71	29.61
-3	14	1	1.19	26.46	26.93
-2	14	1	6.34	-23.43	26.32
-1	14	1	0.11	5.84	17.05
0	14	1	22.35	36.09	13.29
1	14	1	60.3	81.65	8.94
2	14	1	0.31	-8.59	26.39
3	14	1	5.45	4.97	15.65
4	14	1	11.01	-63.66	30.35
-2	15	1	27.99	32.16	17.12
-1	15	1	8.97	-20.65	16.38
0	15	1	3.02	-4.36	13.69
1	15	1	1.46	-24.43	24.2
2	15	1	1.91	-4.63	16.72
-10	0	2	21.92	19	17.79
-9	0	2	69.56	19.88	30.42
-8	0	2	63.95	48.68	16.65
-7	0	2	29.69	22.7	15.18
-6	0	2	53.45	61.04	13.77
-5	0	2	1536.78	1969.05	50.83
-4	0	2	4502.7	5124.33	109.99
-3	0	2	39.73	47	9.6
-2	0	2	450.09	410.54	19.67
-1	0	2	1570.38	1500.2	25.16
0	0	2	3173.89	3124.12	47.09
1	0	2	184.72	175.55	6.91
2	0	2	4191.45	4456.14	95.08
3	0	2	408.49	502	22.49
4	0	2	617.44	665.44	27.33
5	0	2	164.21	174.45	13.7
6	0	2	105.73	106.9	15.04
7	0	2	0.99	-90.99	28.27
8	0	2	449.59	428.47	24.24
9	0	2	64.52	87.09	17.46
-10	1	2	2.76	-23.41	22.1
-9	1	2	40.17	53.88	12.23
-8	1	2	8.31	-9.86	19.81
-7	1	2	49.22	64.55	10.78
-6	1	2	99.36	122.4	10.04
-5	1	2	468.83	594.54	23.03
-4	1	2	27.68	39.38	6.98
-3	1	2	31.47	23.42	6.72
-2	1	2	267.68	254.66	9.64
-1	1	2	4.75	3.25	4.83
0	1	2	627.33	574.47	12.62
1	1	2	504.87	472.87	9.8
2	1	2	424.4	431.7	14.65
3	1	2	5354.25	5747.18	86.29
4	1	2	231.41	249.16	9.33
5	1	2	56.03	77.96	9.11
6	1	2	507.34	521.79	33.44
7	1	2	345.95	364.69	14.12
8	1	2	0	-28.62	20.3
9	1	2	8.55	13.48	21.06
-10	2	2	0.6	-0.74	30.89
-9	2	2	1.44	-9.06	29.34
-8	2	2	0.13	-31.36	28.13
-7	2	2	18.01	36.6	15.44
-6	2	2	24.44	43.44	13.83
-5	2	2	78.82	73.12	12.09
-4	2	2	83.31	92.4	10.54
-3	2	2	573.62	551.62	23.03
-2	2	2	6.83	27.87	9.4
-1	2	2	1182.35	1088.7	14.63
0	2	2	111.35	106.59	4.36
1	2	2	52.96	43.63	5.12
2	2	2	8.57	-12.02	16.85
h			F_c^2	F_o^2	σF_o^2
3	2	2	839.73	899.65	29.21
4	2	2	167.98	181.3	12.56
5	2	2	49.39	16.25	23.97
6	2	2	623.38	637.7	33.91
7	2	2	432.7	449.76	22.36
8	2	2	12.73	12.96	29.14
9	2	2	0.25	1.95	17.39
-10	3	2	22.5	40.42	19
-9	3	2	325.57	290.48	20.01
-8	3	2	6.06	-4.57	28.13
-7	3	2	1.45	25.18	15.31
-6	3	2	122.86	150.55	14.91
-5	3	2	92.72	110.59	13.09
-4	3	2	49.34	32.1	10.81
-3	3	2	91.07	96.02	9.87
-2	3	2	682.1	641.93	23.97
-1	3	2	11672.57	11358.05	115.96
0	3	2	712.8	694.47	11.82
1	3	2	0.06	8.98	6.47
2	3	2	777.07	725.8	25.72
3	3	2	757.19	788.25	27.87
4	3	2	16.7	23.7	11.68
5	3	2	100.37	98.44	14.1
6	3	2	67.53	64.06	15.51
7	3	2	533.89	472.79	26.79
8	3	2	1.76	-30.28	29.75
9	3	2	32.5	65	17.79
-10	4	2	0	-8.53	33.17
-9	4	2	0.35	-18.33	30.22
-8	4	2	20.73	-11.82	29.08
-7	4	2	1.05	15.78	28
-6	4	2	29.88	24.58	14.91
-5	4	2	208.18	234.55	14.97
-4	4	2	277.53	282.69	14.97
-3	4	2	210.08	223.2	13.97
-2	4	2	79.63	48.75	9.6
-1	4	2	2221.48	2173.81	25.42
0	4	2	10.74	-10.45	7.86
1	4	2	277.06	271.42	7.2
2	4	2	188.07	196	10.74
3	4	2	49.41	44.99	10.88
4	4	2	20.52	16.99	12.22
5	4	2	11.84	3.29	25.05
6	4	2	10.42	11.08	27.4
7	4	2	24.23	-16.32	29.75
8	4	2	59.03	28.27	17.59
9	4	2	16.42	41.23	17.79
-10	5	2	3.66	11.21	32.97
-9	5	2	51.45	38.61	17.86
-8	5	2	204.83	180.63	18.2
-7	5	2	1.53	-20.21	28.4
-6	5	2	0.26	10.54	27.19
-5	5	2	82.4	91.59	14.24
-4	5	2	59.04	58.02	12.36
-3	5	2	11.18	10.88	18.6
-2	5	2	7.03	-0.54	16.85
-1	5	2	759.66	708.28	12.43
0	5	2	537.85	539.64	10.99
1	5	2	13.48	-3.49	8.73
2	5	2	70.04	43.58	9.94
3	5	2	575.88	623.67	27.13
4	5	2	91.9	137.05	13.7
5	5	2	3.06	-15.24	25.58
6	5	2	594.42	599.16	32.1
7	5	2	46.29	33.24	17.06
8	5	2	31.17	37.94	17.53
9	5	2	14.09	16.12	32.63
-9	6	2	24.39	3.63	32.37
-8	6	2	8.2	-49.22	30.62
-7	6	2	4.15	-67.62	29.48
-6	6	2	42.67	47.94	15.78
-5	6	2	1.99	-3.36	25.99
-4	6	2	125.77	103.54	13.63
-3	6	2	32.37	42.77	11.42
-2	6	2	793.88	787.58	28.47
-1	6	2	1453.83	1444.03	19.47
0	6	2	2.25	-0.02	6.47
1	6	2	43.36	39.02	4.92
2	6	2	1.08	6.04	18.13
3	6	2	222.26	244.62	13.63
4	6	2	8.71	24.98	13.63
5	6	2	55.26	16.72	26.66
6	6	2	584.12	538.33	27.06
7	6	2	268.95	265.97	18.87
8	6	2	0.07	-24.37	31.22
9	6	2	15.88	22.96	34.25
-9	7	2	239.87	260.6	21.76
-8	7	2	9.76	-38.27	31.09
-7	7	2	0	24.24	28.13
-6	7	2	1.47	-5.24	28.07
-5	7	2	2.23	25.85	26.05
-4	7	2	12.15	25.78	13.56
-3	7	2	71.54	61.98	12.56
-2	7	2	872.55	810.95	30.49
-1	7	2	4396.13	4354.58	48.29
0	7	2	750.03	776.28	14.1
1	7	2	22.97	29.17	6.08
2	7	2	33.39	32.84	11.55
3	7	2	10.37	-14.17	23.03
4	7	2	18.79	-7.92	24.64
5	7	2	6.61	-39.01	27.4
6	7	2	29.06	25.52	28.2
7	7	2	90.71	122.21	17.53
8	7	2	56.07	48.82	18.33
-9	8	2	222.64	228.57	22.43
-8	8	2	2.26	7.79	30.75
-7	8	2	179.53	197.08	18.6
-6	8	2	13.22	32.23	15.91
-5	8	2	70.77	57.88	15.58
-4	8	2	126.45	112.81	14.77
-3	8	2	46.14	13.97	24.17
-2	8	2	446.02	465	24.91
-1	8	2	645.63	692.96	14.59
0	8	2	3.58	-0.95	10.05
1	8	2	14.57	10.87	7.03
2	8	2	103.03	114.62	13.16
3	8	2	76.66	83.25	13.7
4	8	2	23.8	51.77	14.3
5	8	2	14.76	-32.3	27.8
6	8	2	11.19	-10.27	29.21
7	8	2	1.07	28.52	29.28
8	8	2	2.07	-38.21	31.83
-8	9	2	175.6	217.29	19.81
-7	9	2	50.93	20.82	17.93
-6	9	2	15.3	-18.06	27.73
-5	9	2	2.09	-21.22	26.86
-4	9	2	10.34	29.81	14.71
-3	9	2	61.56	82.32	14.03
-2	9	2	24.01	13.56	13.23
-1	9	2	0.4	-6.57	10.85
0	9	2	139.84	161.61	7.42
1	9	2	14.64	9.42	6.77
2	9	2	30.38	15.65	24.17
3	9	2	9.24	17.32	24.37
4	9	2	4.95	4.77	15.11
5	9	2	32.03	15.11	27.33
6	9	2	33.77	52.58	16.65
7	9	2	0.26	-23.77	17.46
-8	10	2	0.17	22.29	33.1
-7	10	2	0.85	-66.01	32.03
-6	10	2	0.06	-5.84	28.13
-5	10	2	5.82	22.7	15.38
-4	10	2	5.26	5.98	26.05
-3	10	2	9.55	6.45	14.5
-2	10	2	10.4	-28.87	25.05
-1	10	2	137.34	146.97	7.57
0	10	2	239.71	267.32	7.64
1	10	2	159.86	151.77	7.04
2	10	2	278.68	278.73	16.18

h	k	l	F_c^2	F_o^2	σF_o^2
3	10	2	2.38	-41.9	25.38
4	10	2	3.48	34.11	14.5
5	10	2	37.71	20.75	28.34
6	10	2	1.01	9	28.34
7	10	2	15.19	-20.75	31.83
-7	11	2	0.02	18.4	31.83
-6	11	2	20.85	2.75	29.34
-5	11	2	30.39	12.83	28.4
-4	11	2	1.38	-41.77	26.86
-3	11	2	8.01	-16.79	25.52
-2	11	2	12.25	-38.01	24.71
-1	11	2	84.35	88.23	7.28
0	11	2	172.11	192.22	7.83
1	11	2	36.35	44.26	9.36
2	11	2	155.13	144.37	15.11
3	11	2	42.55	24.11	14.97
4	11	2	0.03	3.76	26.52
5	11	2	12.13	17.66	28.61
6	11	2	0.07	-3.69	30.42
-6	12	2	64.9	98.98	18.47
-5	12	2	7.21	18.2	29.08
-4	12	2	56.24	22.23	27.93
-3	12	2	25.3	45.53	15.24
-2	12	2	0.07	10.14	24.91
-1	12	2	8.74	-14.17	12.13
0	12	2	1.3	-2.97	11.87
1	12	2	1.26	-8.55	10
2	12	2	87.85	73.19	15.04
3	12	2	3.06	20.21	14.91
4	12	2	14.51	54.59	15.51
5	12	2	16.77	30.42	16.72
6	12	2	0.02	12.76	32.1
-5	13	2	13.11	-31.18	30.08
-4	13	2	60.92	44.38	16.45
-3	13	2	273.06	309.69	18.94
-2	13	2	7.27	4.57	25.45
-1	13	2	11.9	0.94	13.27
0	13	2	0.72	4.96	10.09
1	13	2	1.89	-9.32	12.29
2	13	2	7.43	10.74	25.25
3	13	2	8.37	2.28	15.58
4	13	2	7.57	-11.15	28.47
5	13	2	22.29	4.77	30.89
-4	14	2	20.94	25.85	17.46
-3	14	2	140.42	155.58	17.32
-2	14	2	2.04	-18.73	27.73
-1	14	2	0.02	0.2	14.76
0	14	2	8.25	12.95	10.53
1	14	2	8.28	4.73	15.33
2	14	2	44.73	46.6	15.58
3	14	2	2.15	13.03	28
-2	15	2	4.97	22.16	28.47
-1	15	2	4.48	-5.92	16.03
0	15	2	1.2	-0.24	12.19
1	15	2	22.9	4.34	16.08
-10	1	3	39.46	19.8	22.48
-9	1	3	49.94	-2.12	21.46
-8	1	3	26.61	8	14.37
-7	1	3	23.59	11.34	13.13
-6	1	3	0.63	-22.22	16.8
-5	1	3	525.76	595.64	19.47
-4	1	3	39.15	22.79	6.93
-3	1	3	100.98	92.27	19.74
-2	1	3	1977.58	1846.46	31.57
-1	1	3	274.55	262.67	9.37
0	1	3	90.17	79.4	4.81
1	1	3	540.08	507.98	24.88
2	1	3	112.61	89.96	6.69
3	1	3	119.19	109.9	7.48
4	1	3	64.35	59.78	8.33
5	1	3	188.56	192.7	10.49
6	1	3	111.42	101.04	15.58
7	1	3	12.63	9.32	19.46
8	1	3	32.22	30.87	11.99
9	1	3	0.58	-21.12	21.62
-10	2	3	0	-0.74	31.76
-9	2	3	36.14	-2.62	30.55
-8	2	3	181.19	176.93	17.19
-7	2	3	7.69	-27.4	26.79
-6	2	3	23.03	38.61	13.77
-5	2	3	990.22	1162.26	37
-4	2	3	3.4	-30.96	19.2
-3	2	3	88.26	80.85	9.74
-2	2	3	595.24	548.06	22.36
-1	2	3	582.49	523.65	20.14
0	2	3	583.23	548.99	10.9
1	2	3	1.24	-20.23	7.86
2	2	3	1639.95	1737.39	43.58
3	2	3	3015.29	3422.46	77.69
4	2	3	163.54	185.26	13.03
5	2	3	22.14	12.89	24.51
6	2	3	136.13	127.04	15.78
7	2	3	37.58	31.69	16.18
8	2	3	0.13	-19.07	29.68
9	2	3	137.36	176.26	18.73
-10	3	3	0.73	11.55	32.43
-9	3	3	0	8.06	17.19
-8	3	3	6.84	-5.84	27.87
-7	3	3	2.41	23.64	25.92
-6	3	3	11.75	-21.55	26.46
-5	3	3	695.91	745.34	31.76
-4	3	3	0.9	-15.58	19.41
-3	3	3	35.61	25.92	9.67
-2	3	3	148.88	136.51	9.8
-1	3	3	13.46	-10.38	6.26
0	3	3	0.01	-13.52	7.62
1	3	3	18.74	-4.9	6.46
2	3	3	5.02	24.11	9.27
3	3	3	382.27	375.76	19.67
4	3	3	54.87	62.04	12.76
5	3	3	128.03	119.93	14.91
6	3	3	95.46	83.53	15.85
7	3	3	2.91	-12.22	27.93
8	3	3	0.11	8.73	30.42
9	3	3	1.77	7.65	31.56
-10	4	3	24.84	-19.67	34.18
-9	4	3	0.62	7.59	29.55
-8	4	3	1.44	1.21	27.46
-7	4	3	115.88	92.66	16.92
-6	4	3	91.6	69.23	15.24
-5	4	3	762.53	774.95	32.77
-4	4	3	147.92	137.32	12.49
-3	4	3	135.47	111.13	11.21
-2	4	3	94.17	98.84	9.74
-1	4	3	81.96	80.68	4.56
0	4	3	243.74	241.09	8.01
1	4	3	20.32	19.17	5.54
2	4	3	708.35	714.19	27.13
3	4	3	1.19	16.99	19.81
4	4	3	178.75	205.81	14.44
5	4	3	2.67	18.87	25.25
6	4	3	1.2	21.89	15.91
7	4	3	50.31	0	29.28
8	4	3	0.25	22.02	29.68
9	4	3	3.21	-33.04	33.1
-9	5	3	4.66	0	29.88
-8	5	3	252.32	238.51	18.4
-7	5	3	16.02	2.69	27.19
-6	5	3	55.07	16.59	26.79
-5	5	3	1.82	8.26	24.11
-4	5	3	90.27	89.98	12.83
-3	5	3	780.05	745.95	29.01
-2	5	3	1009.74	909.79	30.28
-1	5	3	129.27	154.54	5.06
0	5	3	1095.28	1016.89	15.48
1	5	3	416.03	389.03	10.2
2	5	3	1.37	-29.01	18.67
3	5	3	1.03	9	20.55
4	5	3	85.35	64.06	13.97
5	5	3	96.43	135.57	15.38
6	5	3	1281.34	1287.63	46.28
7	5	3	0.92	-76.48	29.08
8	5	3	0.73	24.84	30.08
-9	6	3	0.64	5.17	31.96
-8	6	3	172.92	137.38	18.26
-7	6	3	26.68	15.44	28.67
-6	6	3	18.38	21.69	15.31
-5	6	3	263.54	269.8	16.65
-4	6	3	62.21	81.72	13.43
-3	6	3	1.14	5.64	20.01
-2	6	3	1298.9	1366.73	39.55
-1	6	3	15.23	14.17	6.2
0	6	3	741.91	761.78	13.75
1	6	3	44.8	32.39	5.19
2	6	3	24.38	38.41	11.28
3	6	3	86.12	84.81	13.3
4	6	3	50.73	53.72	14.17
5	6	3	123.9	129.06	15.85
6	6	3	717.91	718.01	36.46
7	6	3	1.69	-54.52	29.95
8	6	3	0.8	-29.48	31.36
-9	7	3	21.34	17.59	19.81
-8	7	3	9.74	12.29	30.89
-7	7	3	0.59	-9.06	28.81
-6	7	3	4.93	14.3	15.98
-5	7	3	7.62	-3.83	26.52
-4	7	3	0.09	-21.69	24.58
-3	7	3	4.59	1.21	22.16
-2	7	3	1380.46	1227.06	39.35
-1	7	3	1878.52	1989.9	25.85
0	7	3	272.47	292.22	7.54
1	7	3	53.36	47.04	8.37
2	7	3	159.57	150.48	13.09
3	7	3	123.28	129.13	13.9
4	7	3	7.93	41.09	14.24
5	7	3	9.35	-10.21	26.52
6	7	3	285.36	284.57	18.8
7	7	3	77.93	62.58	17.86
8	7	3	13.95	-35.32	33.44
-8	8	3	0.93	-22.96	31.9
-7	8	3	6.19	11.55	28.87
-6	8	3	9.56	-30.42	28.81
-5	8	3	210.95	215.28	17.19
-4	8	3	0.34	20.88	14.1
-3	8	3	11.35	22.96	23.84
-2	8	3	71.87	105.89	12.89
-1	8	3	26.3	17.22	8.57
0	8	3	3.83	9.62	10.21
1	8	3	73.45	78.8	8.04
2	8	3	18.99	39.35	12.83
3	8	3	6.71	5.3	13.7
4	8	3	9.06	9.8	25.58
5	8	3	35.43	37.8	15.31
6	8	3	15.04	8.73	16.65
7	8	3	29.1	22.02	17.46
8	8	3	0	17.59	19.41
-8	9	3	0.24	-29.61	32.84
-7	9	3	21.78	30.08	30.55
-6	9	3	1.49	-6.18	27.26
-5	9	3	151.85	165.25	16.32
-4	9	3	273.66	272.49	17.26
-3	9	3	43.41	19.14	25.99
-2	9	3	209.82	194.33	14.84
-1	9	3	45.88	43.2	6.4
0	9	3	22.04	20.04	9.78
1	9	3	28.49	30.08	7.03
2	9	3	21.27	15.31	24.04
3	9	3	45.72	62.92	14.5
4	9	3	33.36	51.5	15.04
5	9	3	45.24	28.94	15.91
6	9	3	201.32	224.21	18.53
7	9	3	30.23	18.6	18.47
-7	10	3	6.39	18.2	30.35
-6	10	3	1.65	20.55	27.93
-5	10	3	19.08	12.15	27.46
-4	10	3	349.96	346.75	18.67
-3	10	3	0.68	11.08	25.25
-2	10	3	1148.23	1092.63	40.83
-1	10	3	9.13	8.22	11.5
0	10	3	256.85	278.86	9.55
1	10	3	0.31	-9.84	14
2	10	3	6.14	1.07	23.9
3	10	3	0.12	-12.89	24.37
4	10	3	47.8	-1.86	27.19
5	10	3	26.3	21.22	28.87
6	10	3	201.45	171.63	18.8
-7	11	3	5.75	-20.28	31.76
-6	11	3	4.9	-27.13	30.55
-5	11	3	6.26	26.32	28.27
-4	11	3	222.98	228.17	17.73
-3	11	3	177.5	203.73	16.18
-2	11	3	353.88	324.46	17.66
-1	11	3	115.88	123.19	8.61
0	11	3	6.89	-21.19	9.85
1	11	3	0	-5.22	11.84
2	11	3	5.29	-2.69	14.24
3	11	3	2.75	-35.59	24.98
4	11	3	146.68	142.09	17.19
5	11	3	0.03	-30.02	28.81
6	11	3	8.9	-14.77	31.02
-6	12	3	3.84	5.37	30.49
-5	12	3	0.38	20.75	28
-4	12	3	6.2	-10.07	27.53
-3	12	3	47.97	62.25	15.38
-2	12	3	70.87	81.85	15.11
-1	12	3	32.92	28.29	8.21
0	12	3	7.85	-3.17	8.51
1	12	3	0.42	-5.86	10.08
2	12	3	1.78	-14.71	25.18
3	12	3	3.95	18.13	25.92
4	12	3	35.67	-15.78	28.54
5	12	3	0.26	20.82	28.87
-5	13	3	2.37	-39.62	30.55
-4	13	3	103.91	106.43	17.19
-3	13	3	79.25	75.88	16.18
-2	13	3	41.24	46.06	15.31
-1	13	3	1.71	-5.62	12.58
0	13	3	8.42	1.9	14.64
1	13	3	16.47	-0.92	12.86
2	13	3	1.08	-35.66	27.06
3	13	3	4.35	-13.16	27.66
4	13	3	0	18.6	28.67
-4	14	3	121.83	114.82	18.73
-3	14	3	47.83	25.92	29.88
-2	14	3	40.46	39.28	15.65
-1	14	3	0.45	-11.25	15.34
0	14	3	0	9.68	13.41
1	14	3	68.13	82.1	9.28
2	14	3	51.67	44.92	16.72
3	14	3	0.5	-0.27	17.32
-1	15	3	0.19	-13.17	16.38
0	15	3	0.29	7.75	11.38
-10	0	4	84.36	79.84	18.47
-9	0	4	42.89	36.33	16.99
-8	0	4	44.54	19.94	16.32
-7	0	4	0.73	-19.61	26.19
-6	0	4	132.1	151.15	14.71
-5	0	4	100.73	102.4	12.69
-4	0	4	191.63	174.38	12.09
-3	0	4	0.04	-13.3	16.79
-2	0	4	144.62	138.93	9.74
-1	0	4	2859.15	2880.08	45.95
0	0	4	16.85	-11.65	10.8
1	0	4	472.57	482.17	15.09
2	0	4	226.57	261.41	13.77
3	0	4	110.62	111	11.62
4	0	4	1.47	8.12	12.36
5	0	4	55.13	81.57	14.37
6	0	4	4.5	-61.04	26.86
7	0	4	0.25	25.52	15.38

h	k	l	F_c^2	F_o^2	σF_o^2
8	0	4	1.01	12.09	16.59
9	0	4	6.31	-2.22	18.8
-10	1	4	3.95	-7.67	22.46
-9	1	4	107.37	82.65	21.35
-8	1	4	46.85	57.17	11.11
-7	1	4	6.5	13.08	20.35
-6	1	4	3.11	4.61	17.18
-5	1	4	5.02	22.74	10.59
-4	1	4	353.51	370.4	14.19
-3	1	4	16.62	6.72	8.05
-2	1	4	140.47	141.9	6.91
-1	1	4	233.03	211.89	5.59
0	1	4	52.15	45.15	4.39
1	1	4	20.43	18.25	5.15
2	1	4	1668.93	1887.04	33.76
3	1	4	111.92	94.84	8.12
4	1	4	0.02	9.87	15.52
5	1	4	160.01	161.95	10.63
6	1	4	27.07	15.41	18.77
7	1	4	0.62	-11.88	19.55
8	1	4	0.05	15.27	14.43
9	1	4	2.09	3.93	16.14
-10	2	4	1.69	-31.76	31.63
-9	2	4	14.26	-4.03	29.68
-8	2	4	10.64	34.85	15.71
-7	2	4	25.29	28.2	15.51
-6	2	4	113.51	118.52	15.04
-5	2	4	30.47	53.05	12.96
-4	2	4	15.04	15.65	11.15
-3	2	4	115.6	119.05	10.68
-2	2	4	7.64	-4.97	16.12
-1	2	4	387.44	372.5	15.44
0	2	4	246.44	237.92	6.68
1	2	4	3.07	-10.54	8.07
2	2	4	796.13	832.3	29.28
3	2	4	24.11	18.53	11.48
4	2	4	6.34	13.63	23.43
h			F_c^2	F_o^2	σF_o^2
5	2	4	18.77	20.35	14.44
6	2	4	1.71	-19.88	26.66
7	2	4	5.99	21.02	28.13
8	2	4	9.85	-26.93	28.87
-10	3	4	3	-7.12	19.14
-9	3	4	82.41	86.76	17.79
-8	3	4	5.34	20.14	16.05
-7	3	4	6.72	-17.86	27.73
-6	3	4	123.21	105.49	15.58
-5	3	4	18.76	4.77	23.57
-4	3	4	9.66	9.74	20.82
-3	3	4	0	5.51	17.46
-2	3	4	534.03	521.2	23.37
-1	3	4	3465.14	3739.28	64.96
0	3	4	25.17	27.73	6.1
1	3	4	68.52	74.63	4.93
2	3	4	1116.72	1164.88	35.32
3	3	4	45.01	51.17	12.02
4	3	4	187.27	200.91	14.64
5	3	4	21.49	50.97	14.37
6	3	4	125.58	99.11	16.32
7	3	4	193.65	202.45	17.86
8	3	4	6.86	-12.29	29.68
-10	4	4	48.7	66.14	19.07
-9	4	4	27.91	20.01	17.53
-8	4	4	6.85	11.21	28.34
-7	4	4	22.3	14.1	27.93
-6	4	4	112.33	97.57	15.44
-5	4	4	3.71	-17.06	24.51
-4	4	4	0.06	-2.22	21.69
-3	4	4	24.19	11.48	19
-2	4	4	105.18	108.51	10.74
-1	4	4	1100.38	1174.95	20.92
0	4	4	207.88	212.57	6.07
1	4	4	49.21	49.42	5.57
2	4	4	761.35	837.74	30.42
3	4	4	0.91	5.77	21.62
4	4	4	53.77	40.49	13.83
5	4	4	0.44	-4.97	25.65
6	4	4	1.97	-7.32	15.65
7	4	4	1.94	14.91	28.47
8	4	4	0.75	24.31	29.41
-9	5	4	13.03	19.87	17.53
-8	5	4	15.91	24.44	28.81
-7	5	4	21.37	31.02	15.71
-6	5	4	4.93	-36.46	26.86
-5	5	4	70.89	25.65	25.85
-4	5	4	55.89	63.66	13.16
-3	5	4	1.18	14.57	11.35
-2	5	4	61.62	54.19	10.88
-1	5	4	42.83	26.86	9.31
0	5	4	23.53	27.69	6.65
1	5	4	57.17	53.31	5.33
2	5	4	272.91	273.43	14.03
3	5	4	46.84	17.53	23.17
4	5	4	35.52	16.52	25.18
5	5	4	88	122.07	15.85
6	5	4	154.91	116.97	16.79
7	5	4	28.21	2.01	29.81
8	5	4	11.01	-6.11	31.63
-9	6	4	8.23	23.9	18.13
-8	6	4	6.39	-30.15	29.95
-7	6	4	59.29	69.97	16.45
-6	6	4	543.17	543.83	28.4
-5	6	4	823.67	807.45	35.72
-4	6	4	244.95	211.45	15.38
-3	6	4	87.52	120.26	12.69
-2	6	4	78.86	91.12	11.82
-1	6	4	15.54	8.02	7.78
0	6	4	213.26	245.31	10.94
1	6	4	43.66	37.15	6.23
2	6	4	1210.49	1213.63	38.61
3	6	4	32.8	6.98	23.64
4	6	4	22.07	39.62	14.3
5	6	4	29.32	12.02	27.53
6	6	4	10.06	-30.28	28.4
7	6	4	6.3	21.62	29.81
8	6	4	5.32	0.81	32.16
-9	7	4	0.01	-67.69	33.37
-8	7	4	15.99	-4.9	17.59
-7	7	4	3.36	-2.48	28.94
-6	7	4	61.65	-21.89	28.34
-5	7	4	57.06	24.78	26.12
-4	7	4	358.42	343.86	18.06
-3	7	4	32.52	38.74	13.3
-2	7	4	53.55	47.34	12.76
-1	7	4	652.39	693.03	14.89
0	7	4	1.66	0.6	9.04
1	7	4	84.56	79.97	6.26
2	7	4	76.13	57.41	13.3
3	7	4	19.85	23.23	13.7
4	7	4	0.01	-1.61	26.05
5	7	4	9.57	-10.48	26.66
6	7	4	23.41	16.25	28.94
7	7	4	100.83	82.26	18.47
-8	8	4	27.87	-12.56	31.96
-7	8	4	36.96	54.19	17.06
-6	8	4	0.61	0	27.4
-5	8	4	253.03	248.98	17.19
-4	8	4	210.13	185.33	16.05
-3	8	4	90.87	81.58	14.03
-2	8	4	27.64	21.35	12.83
-1	8	4	12.73	-12.12	8.77
0	8	4	24.45	26.59	14.64
1	8	4	23.69	23.85	10.11
2	8	4	72.37	82.39	13.83
3	8	4	186.79	231.12	15.98
4	8	4	3.43	0	14.77
5	8	4	427.81	414.24	20.75
6	8	4	2.78	-7.52	29.28
7	8	4	57.45	25.99	32.3
-8	9	4	3.41	2.35	31.96
-7	9	4	71.15	70.77	17.53
-6	9	4	35.13	35.45	16.38
-5	9	4	9.57	15.85	26.46
-4	9	4	407.95	361.86	20.01
-3	9	4	0.44	6.65	14.44
-2	9	4	71.4	42.77	14.03
-1	9	4	9.66	14.91	9.39
0	9	4	0.04	-16.66	14.92
1	9	4	6.66	11.75	8.12
2	9	4	0.16	-39.42	25.11
3	9	4	8.04	-17.19	24.78
4	9	4	0	-9.67	25.65
5	9	4	495.61	529.26	27.33
6	9	4	227.92	207.35	19.2
-7	10	4	1.23	-23.23	31.69
-6	10	4	20.8	2.08	28.74
-5	10	4	164.4	165.59	17.12
-4	10	4	416.49	392.21	21.69
-3	10	4	307.14	288.4	18.53
-2	10	4	326.5	301.56	17.32
-1	10	4	4.5	10.67	9.55
0	10	4	13.23	6.03	9.7
1	10	4	63.59	59.39	7.09
2	10	4	0.04	12.49	24.11
3	10	4	14.61	8.46	25.05
4	10	4	85.17	103.07	15.98
5	10	4	203.18	192.98	18.2
6	10	4	79.23	83.26	18.33
-7	11	4	0.16	19.2	31.43
-6	11	4	32.03	-4.43	30.08
-5	11	4	60.61	54.32	16.59
-4	11	4	251.66	205.67	17.79
-3	11	4	40.1	37.87	15.18
-2	11	4	219.16	194.8	18.38
-1	11	4	19.18	17.07	9.97
0	11	4	17.42	7.73	11.21
1	11	4	1.51	-14.12	12.23
2	11	4	5.3	-19.88	25.25
3	11	4	347.24	353.2	19.14
4	11	4	173.12	174.99	17.12
5	11	4	2.14	-6.04	30.22
-6	12	4	10.96	-3.96	31.76
-5	12	4	5.59	32.57	16.65
-4	12	4	32.73	26.32	16.45
-3	12	4	11.34	24.51	15.31
-2	12	4	0.35	-20.01	25.99
-1	12	4	0.27	-3.52	12.26
0	12	4	2.16	-15.52	12.49
1	12	4	0.53	-0.37	10.14
2	12	4	7.93	-56.74	26.52
3	12	4	116.65	116.3	16.92
4	12	4	29	-4.57	30.28
-5	13	4	0.04	23.84	17.73
-4	13	4	13.94	15.98	29.01
-3	13	4	66.57	76.15	15.91
-2	13	4	44.26	39.15	15.65
-1	13	4	19.42	2.81	10.57
0	13	4	0.46	9.41	9.05
1	13	4	0.95	2.7	13.14
2	13	4	0.05	6.65	26.46
3	13	4	29.44	23.1	29.21
-3	14	4	100.81	82.32	18.06
-2	14	4	87.48	78.29	16.99
-1	14	4	3.48	2.05	12.39
0	14	4	8.23	13.7	8.76
1	14	4	13.49	7.41	12.53
2	14	4	0.42	-14.44	28.87
-10	1	5	35.68	29.44	16.24
-9	1	5	3.08	-14.82	24.11
-8	1	5	70.56	82.02	11.18
-7	1	5	33.58	18.94	20.48
-6	1	5	104.93	124.26	10.52
-5	1	5	30.52	-2.71	19.94
-4	1	5	10.12	16.44	14.6
-3	1	5	14.14	12.29	9.24
-2	1	5	1570.36	1572.18	29.89
-1	1	5	36.54	40.34	5.36
0	1	5	0.37	-12.02	13.22
1	1	5	48.62	41.69	10.14
2	1	5	115.32	120.33	8.36
3	1	5	51.81	42	8.81
4	1	5	4.72	20.91	18.53
5	1	5	47.4	49.33	10.54
6	1	5	289.6	249.41	14.71
7	1	5	0.04	-42.08	19.87
8	1	5	4.91	-1.01	21.53
-10	2	5	25.99	12.83	31.36
-9	2	5	182.6	161.09	18.33
-8	2	5	59.39	46.67	16.38
-7	2	5	9.5	4.9	26.39
-6	2	5	86.97	93.47	14.91
-5	2	5	158.73	176.8	14.64
-4	2	5	43.49	-1.88	22.49
-3	2	5	228.13	213.46	12.83
-2	2	5	15.16	-11.75	17.79
-1	2	5	560.82	619.34	14.22
0	2	5	169.7	150.59	5.44
1	2	5	46.74	39.27	5.2
2	2	5	64.44	55.4	11.75
3	2	5	144.16	162.7	13.63
4	2	5	22.97	24.37	13.77
5	2	5	20.22	7.25	26.25
6	2	5	108.35	77.62	16.25
7	2	5	28.85	2.08	29.68
8	2	5	7.05	23.7	29.68
-9	3	5	1.86	20.14	29.48
-8	3	5	75.34	66.61	17.12
-7	3	5	0.49	6.38	15.65
-6	3	5	60.02	25.18	26.66
-5	3	5	499.62	532.55	28.2
-4	3	5	31.35	25.38	12.62
-3	3	5	354.37	373.68	19.67
-2	3	5	381.02	429.48	23.1
-1	3	5	466.14	512.92	11.98
0	3	5	51.6	56.98	5.2
1	3	5	152.18	141.1	5.87
2	3	5	0.63	19.61	11.55
3	3	5	15.55	31.76	13.03
4	3	5	10.92	15.18	24.11
5	3	5	13.61	-7.99	26.52
6	3	5	68.61	6.71	28.4
7	3	5	9.77	19.27	29.08
8	3	5	0	27.26	31.29
-9	4	5	2.13	-8.8	30.62
-8	4	5	0.45	17.59	28.67
-7	4	5	5.02	8.06	26.99
-6	4	5	12.04	25.25	15.31
-5	4	5	846.2	828.93	35.99
-4	4	5	30.1	37.13	12.96
-3	4	5	0.4	-10.21	21.62
-2	4	5	5.82	-7.05	11.01
-1	4	5	61.05	56.02	6.8
0	4	5	188.6	184.31	5.98
1	4	5	146.5	141.88	6.09
2	4	5	136.08	138.73	13.23
3	4	5	247.33	274.64	15.38
4	4	5	136.67	150.34	14.97
5	4	5	0.06	-27.06	26.19
6	4	5	74.33	65.54	16.25
7	4	5	40.89	36.93	16.99
8	4	5	0.75	27.8	30.28
-9	5	5	3.35	-81.79	32.57
-8	5	5	4.6	7.45	16.99
-7	5	5	1.1	5.37	27.6
-6	5	5	33.02	29.41	15.44
-5	5	5	28.24	8.66	25.65
-4	5	5	132.91	164.71	14.3
-3	5	5	43.71	-7.18	22.56
-2	5	5	0.33	-23.23	20.75
-1	5	5	85.29	97.29	6.73

h	k	l	F_c^2	F_o^2	σF_o^2
0	5	5	192.55	195.59	8.57
1	5	5	269.92	268.69	10.91
2	5	5	32.76	48.01	12.83
3	5	5	96	102.6	14.1
4	5	5	48.41	23.7	27.06
5	5	5	25.12	-5.77	26.12
6	5	5	269.87	265.77	18.87
7	5	5	6.28	-32.03	29.75
-9	6	5	23.94	-14.1	33.51
-8	6	5	23.42	11.21	28.94
-7	6	5	19.06	20.08	28.54
-6	6	5	0.39	-3.36	15.18
-5	6	5	449.92	435.92	23.84
-4	6	5	272.84	254.09	15.91
-3	6	5	131.34	149.74	13.97
-2	6	5	34.64	13.63	21.62
-1	6	5	6.93	-11.8	10.44
0	6	5	222.01	245.73	7.14
1	6	5	36	37.07	6.19
2	6	5	175	177.4	14.44
3	6	5	37.91	32.63	14.17
4	6	5	3.01	15.24	25.11
5	6	5	1.12	1.21	25.78
6	6	5	4.22	25.58	28.13
7	6	5	16.54	25.38	17.19
-8	7	5	8.17	-16.85	30.42
-7	7	5	0.03	0.67	29.01
-6	7	5	37.26	19.67	27.33
-5	7	5	701.11	709.69	36.06
-4	7	5	129.97	141.48	15.24
-3	7	5	19.13	21.49	23.97
-2	7	5	3.33	17.46	22.56
-1	7	5	53.25	70.47	6.4
0	7	5	106.38	108.07	6.56
1	7	5	45.56	55.55	10.27
2	7	5	131.81	125.7	14.44
3	7	5	873.53	898.37	37.27
4	7	5	73.02	80.58	15.11
5	7	5	20.93	31.78	15.51
6	7	5	29.09	23.7	16.99
7	7	5	9.79	-8.93	18.13
-8	8	5	0.02	-29.14	31.29
-7	8	5	1.78	13.9	28.27
-6	8	5	0.22	25.31	27.8
-5	8	5	293.96	250.39	17.93
-4	8	5	8.79	10.95	14.71
-3	8	5	15.57	-0.54	24.17
-2	8	5	38.97	50.7	13.7
-1	8	5	20.67	12.15	9.39
0	8	5	14.85	21.61	7.94
1	8	5	163.72	149.54	7.08
2	8	5	378.42	351.18	18
3	8	5	455.63	479.84	25.65
4	8	5	0.09	-17.12	26.19
5	8	5	33.26	9.4	28.2
6	8	5	0.74	-21.55	29.55
-7	9	5	50.58	36.13	17.59
-6	9	5	95.66	103	16.92
-5	9	5	17.32	3.69	26.79
-4	9	5	2.9	12.76	25.72
-3	9	5	8.95	1.14	24.44
-2	9	5	13.69	-4.23	13.63
-1	9	5	24.6	17.72	9.91
0	9	5	3.1	18.1	9.52
1	9	5	196.02	198.87	10.5
2	9	5	10.57	10.81	23.84
3	9	5	352.06	327.28	20.08
4	9	5	23.67	36.66	15.58
5	9	5	100.46	115.56	16.99
6	9	5	2.07	26.59	29.81
-7	10	5	0.35	7.05	30.75
-6	10	5	35.99	17.53	17.06
-5	10	5	27.97	10.07	26.72
-4	10	5	12.65	22.83	15.24
-3	10	5	41.61	27.93	14.91
-2	10	5	6.46	-17.39	24.84
-1	10	5	15.27	1.52	10.11
0	10	5	0.7	-4.35	11.85
1	10	5	8.53	1.26	12.05
2	10	5	104.94	112.2	15.31
3	10	5	0.89	24.17	25.38
4	10	5	0.52	-11.28	26.86
5	10	5	1.16	1.54	29.81
-6	11	5	2.58	13.09	17.73
-5	11	5	52.1	23.77	28.34
-4	11	5	0	-16.99	27.53
-3	11	5	0.34	-13.63	26.66
-2	11	5	2.12	-33.44	26.66
-1	11	5	3.11	6.45	10
0	11	5	10.53	20.86	8.61
1	11	5	21.05	8.22	10.28
2	11	5	10.98	1.34	25.58
3	11	5	169.84	183.85	17.39
4	11	5	2.54	-51.17	28.74
-5	12	5	2.82	-43.44	29.41
-4	12	5	2.51	-16.25	27.46
-3	12	5	48.94	47.27	15.65
-2	12	5	0.11	-0.94	14.91
-1	12	5	26.87	-2.6	12.94
0	12	5	19.68	16.54	9.01
1	12	5	0.96	-1.91	12.64
2	12	5	22.64	-5.1	26.59
3	12	5	76.36	64.93	17.06
-4	13	5	29.5	23.1	30.35
-3	13	5	85.3	49.62	17.46
-2	13	5	0.21	-4.5	26.39
-1	13	5	39.13	38.86	10.01
0	13	5	10.75	12.8	10.69
1	13	5	16.73	4.83	11.2
2	13	5	0.3	21.96	27.4
-9	0	6	13.79	13.97	28.2
-8	0	6	4.56	7.18	27.93
-7	0	6	14.25	-53.32	26.68
-6	0	8	815.05	917.58	38.74
-5	0	6	339.2	315.46	18.06
-4	0	8	92.09	93.4	13.36
-3	0	6	288.61	319.62	17.79
-2	0	6	1950.81	2140.47	54.99
-1	0	6	199.7	193.66	8.85
0	0	6	4.87	-0.25	9.61
1	0	6	138.38	121.04	10.54
2	0	6	304.18	323.65	17.26
3	0	6	37.41	-22.18	24.04
4	0	6	5.98	14.97	24.51
5	0	6	172.62	129.26	15.98
6	0	6	299.48	299.14	18.33
7	0	8	3.27	14.64	28.2
-9	1	6	0.34	6.27	33.54
-8	1	6	46.78	26.31	11.49
-7	1	6	158.79	159.78	11.58
-6	1	6	2.31	7.97	18.11
-5	1	6	1.24	-23.08	17.09
-4	1	6	12.88	31.2	10.99
-3	1	6	0.83	-16.52	14.83
-2	1	6	326.5	353.83	13.39
-1	1	6	281.63	279.72	7.19
0	1	8	4.11	10.92	7.89
1	1	6	93.09	85.9	5.45
2	1	6	262.1	281.02	10.6
3	1	6	5.67	8.18	11.5
4	1	6	9.22	1.43	12.46
5	1	6	178.79	174.39	11.47
6	1	6	9.71	-17.02	19.06
7	1	6	4.87	-48.46	20.58
-9	2	6	15.42	41.43	17.19
-8	2	6	37.16	31.83	16.72
-7	2	6	0.92	-14.17	26.93
-6	2	6	17.21	5.84	26.72
-5	2	6	353.91	330.84	18.47
-4	2	6	56.25	48.28	13.03
-3	2	6	5.62	15.85	11.95
-2	2	6	6.25	-2.28	11.62
-1	2	6	122.3	133.27	6.05
0	2	6	8.31	2.79	6.98
1	2	6	1.51	-5.59	8.96
2	2	6	191	206.68	14.1
3	2	6	10.74	-6.18	23.97
4	2	6	6.5	1.61	24.37
5	2	6	0.06	2.42	25.58
6	2	6	0.81	0	27.46
7	2	6	0.86	-3.69	28.13
-9	3	6	13.63	24.96	17.53
-8	3	6	0.01	2.08	28.13
-7	3	6	195.86	190.36	17.39
-6	3	6	354.7	329.16	18.26
-5	3	6	320.23	325	17.46
-4	3	6	29.17	2.62	23.5
-3	3	6	124.87	121.81	13.23
-2	3	6	39.64	45.93	12.09
-1	3	6	7.36	12.9	6.99
0	3	6	22.46	23.54	6.4
1	3	6	91.74	94.06	8.29
2	3	6	93.21	106.77	13.5
3	3	6	129.04	159.68	14.57
4	3	6	0.11	4.3	24.58
5	3	6	55.84	64.46	15.38
6	3	6	0.89	4.03	15.85
7	3	6	8.71	11.35	29.81
-9	4	6	1.03	-19.34	31.22
-8	4	6	1.88	5.51	28.34
-7	4	6	21.44	26.66	26.99
-6	4	6	411.14	426.05	23.03
-5	4	6	303.37	316.4	18.53
-4	4	6	0.47	14.37	23.3
-3	4	6	92.04	118.25	13.56
-2	4	6	167.98	175.73	13.56
-1	4	6	212.63	237.11	10.1
0	4	6	1.95	9.61	7.27
1	4	6	38.41	34.36	7.82
2	4	6	1083.44	1089.48	38.86
3	4	6	84.94	65.94	14.17
4	4	6	6.94	-2.75	25.58
5	4	6	16.98	16.12	26.32
6	4	6	10.1	-35.19	28.13
7	4	6	3.16	12.36	30.22
-9	5	6	0.04	27.87	31.56
-8	5	6	19.75	69.43	16.79
-7	5	6	10.57	-3.63	28
-6	5	6	92.77	92.06	15.78
h	k	l	F_c^2	F_o^2	σF_o^2
-5	5	6	15.95	27.66	14.77
-4	5	6	90.46	69.3	14.37
-3	5	6	124.45	148.4	13.77
-2	5	6	221.32	228.24	14.71
-1	5	6	0.78	-2.17	10.67
0	5	6	20.42	28.66	7.8
1	5	6	53.06	54.37	6.51
2	5	6	782.77	838.61	34.85
3	5	8	42.86	1.07	28.12
4	5	6	53.04	46.53	14.97
5	5	6	0.01	-6.45	27.6
6	5	6	2.5	11.42	28.13
7	5	6	0.43	26.99	30.55
-8	6	6	0.86	16.32	16.85
-7	6	6	21.52	-24.78	29.81
-6	6	6	11.57	-30.42	27.26
-5	6	8	195.74	202.32	16.32
-4	6	6	38.15	23.77	14.64
-3	6	8	13.64	36.8	13.36
-2	6	6	1.41	-12.62	22.98
-1	6	6	6.02	22.38	7.66
0	6	6	38.53	51.62	13.08
1	6	6	7.42	14.42	11.22
2	6	6	507.86	564.92	30.96
3	6	8	0.01	-5.57	14.17
h			F_c^2	F_o^2	σF_o^2
4	6	8	8.63	18.2	14.84
5	8	6	26.08	-19.34	27.87
6	6	6	8.32	11.82	28.67
-8	7	6	26.86	48.55	18
-7	7	6	5.91	-9.8	29.48
-6	7	6	27.23	21.15	28.34
-5	7	8	93.03	79.97	15.58
-4	7	6	10.18	-54.99	25.58
-3	7	6	0.73	-6.24	24.11
-2	7	6	14.3	47.68	13.3
-1	7	6	1.02	6.23	10.78
0	7	6	0.34	-3.22	10.22
1	7	8	9.62	13.79	13.12
2	7	6	64.54	84.67	14.37
3	7	6	57.37	48.01	14.77
4	7	6	4.17	-14.71	25.99
5	7	6	9.44	15.18	16.05
6	7	6	1.57	-0.81	30.02
-7	8	6	33.54	21.42	30.89
-6	8	6	5.88	-26.46	28.4
-5	8	6	2.23	-49.56	27.4
-4	8	6	18.01	-49.35	26.52
-3	8	6	3.84	-8.39	24.37
-2	8	6	18.19	14.1	24.11
-1	8	6	107.71	97.61	7.19
0	8	6	0.27	-6.16	13.66
1	8	6	144.64	142.62	7.56
2	8	6	291.41	302.1	17.19
3	8	6	58.29	51.3	14.77
4	8	6	0.77	-4.3	15.04
5	8	6	4.37	-21.55	16.59
-7	9	6	4.65	-17.86	31.09
-6	9	6	3.52	-18.67	28.61
-5	9	6	19.44	41.9	15.71
-4	9	6	17.8	34.85	15.11
-3	9	6	2.55	-4.23	24.04
-2	9	6	15.6	6.45	24.51
-1	9	6	152.45	159.31	7.59
0	9	6	8.06	2.93	12.05
1	9	6	33.5	44.28	11.65
2	9	6	98.65	77.49	15.24
3	9	6	16.11	2.62	25.85
4	9	6	10.38	-6.45	27.13
5	9	6	10.69	24.71	17.06
-6	10	6	3.5	23.7	29.28
-5	10	6	11.75	37.87	15.98
-4	10	6	21.93	22.56	15.58
-3	10	6	12.26	-1.95	25.65
-2	10	6	37.84	29.41	14.97
-1	10	6	0.11	-9.1	6.63
0	10	6	22.03	12.67	12.27
1	10	6	87.44	95.59	7.6
2	10	6	1.58	-0.67	25.45
3	10	6	6.86	22.09	26.12
4	10	6	21.66	28.81	16.99
-5	11	6	2.22	13.77	28.54
-4	11	6	0.14	-32.7	27.93
-3	11	6	2.87	-30.02	27.19
-2	11	6	0.99	0.67	25.92
-1	11	6	42.3	44.33	9.51
0	11	6	53.1	62.75	7.49
1	11	6	48.92	44.7	10.23
2	11	6	0.24	10.95	25.92
3	11	6	4.17	4.57	27.8
-4	12	6	13.66	-25.78	29.61
-3	12	6	4.32	0.74	27.6
-2	12	6	3.45	25.05	25.99
-1	12	6	72.28	24.54	17.4
0	12	6	0.06	1.91	10.8
1	12	6	29.26	15.27	15.18
2	12	6	16.36	-55.46	29.28
-2	13	6	0.63	14.37	27.19
-1	13	6	35.51	37.63	9.19
0	13	6	7.9	-3.77	16.03
-9	1	7	24.93	13.05	15.63

h	k	l	F_c^2	F_o^2	σF_o^2
-8	1	7	3.5	2.03	19.76
-7	1	7	293.27	324.37	13.36
-6	1	7	1349.28	1403.31	40.09
-5	1	7	11.06	14.55	10.04
-4	1	7	86.45	95.24	9.83
-3	1	7	127.67	120.02	9.52
-2	1	7	27.5	23.12	8.92
-1	1	7	17.14	7.51	7.63
0	1	7	196.51	207.01	8
1	1	7	514.53	508.49	12.02
2	1	7	645.28	719.87	23.5
3	1	7	45.42	52.56	9.99
4	1	7	11.87	41.34	36.33
5	1	7	0.7	-20.39	18.34
6	1	7	20.71	-20.13	19.65
-9	2	7	21.15	12.69	31.83
-8	2	7	6.08	19.94	29.14
-7	2	7	0.37	10.27	27.06
-6	2	7	0.85	2.89	25.52
-5	2	7	371.59	373.88	21.15
-4	2	7	41.53	59.83	13.7
-3	2	7	0.94	-14.44	22.23
-2	2	7	20.28	14.84	22.16
-1	2	7	190.37	204.83	8.91
0	2	7	126.83	130.53	6.77
1	2	7	690.51	694.15	24.52
2	2	7	202.42	216.69	15.11
3	2	7	65.75	49.62	14.77
4	2	7	71.25	76.35	14.64
5	2	7	92.91	107.17	16.25
6	2	7	6.74	-31.56	28.81
-9	3	7	11.42	29.75	31.56
-8	3	7	8.18	24.64	16.65
-7	3	7	32.29	-27.46	28.54
-6	3	7	455.3	463.12	23.84
-5	3	7	0.82	-2.69	25.11
-4	3	7	4.03	-8.8	14.17
-3	3	7	154.89	171.03	14.17
-2	3	7	6.24	-9.27	22.49
-1	3	7	45.32	34.16	9.74
0	3	7	0.04	5.35	11.12
1	3	7	13.57	25.48	7.25
2	3	7	121.46	99.18	14.91
3	3	7	3.14	-15.71	25.11
4	3	7	106.19	73.06	15.91
5	3	7	176.14	174.99	16.72
6	3	7	1.55	-41.83	28.4
-8	4	7	24.47	28.13	28.94
-7	4	7	75.91	68.56	16.92
-6	4	7	13.4	16.59	26.66
-5	4	7	3.44	-38.34	26.05
-4	4	7	0.81	-3.16	24.31
-3	4	7	283.08	298	16.05
-2	4	7	80.84	88.89	13.7
-1	4	7	8.81	1.67	11.18
0	4	7	0.37	-15.26	11.36
1	4	7	164.9	148.88	7.22
2	4	7	535.92	546.85	29.75
3	4	7	1.36	-4.43	14.17
4	4	7	5.62	1.28	25.78
5	4	7	73.42	85.94	15.91
6	4	7	6.48	-22.16	29.28
-8	5	7	0.02	-48.82	31.22
-7	5	7	14.42	-41.63	28.54
-6	5	7	75.03	59.69	15.91
-5	5	7	26.7	14.64	26.12
-4	5	7	4.73	-2.69	24.58
-3	5	7	0.47	-3.63	23.64
-2	5	7	387.76	339.43	18.2
-1	5	7	42.95	44.16	8.36
0	5	7	2.98	11.25	9.49
1	5	7	195.09	190.82	7.67
2	5	7	235.87	240.26	16.32
3	5	7	13.82	-15.04	24.78
4	5	7	0.05	-13.03	26.12
5	5	7	32.53	-14.3	29.08
6	5	7	13.55	6.31	30.49
-8	6	7	34.92	50.56	18.47
-7	6	7	9.99	-7.92	27.26
-6	6	7	2.53	-11.95	26.99
-5	6	7	0.46	-7.32	25.92
-4	6	7	22.98	-11.55	25.25
-3	6	7	28.63	42.3	14.03
-2	6	7	14.94	19.2	23.7
-1	6	7	2.91	20.86	9.57
0	6	7	126.6	125.66	7.2
1	6	7	16.91	9.1	9.65
2	6	7	13.8	42.57	13.7
3	6	7	0.52	-25.05	25.58
4	6	7	9.93	14.24	26.19
5	6	7	5.97	-14.84	26.99
-7	7	7	16.77	28.81	16.72
-6	7	7	0.93	1.41	27.26
-5	7	7	0.48	5.84	26.32
-4	7	7	10.39	19.07	14.5
-3	7	7	110.55	91.52	14.64
-2	7	7	1.57	22.49	13.56
-1	7	7	15.8	13.38	9.65
0	7	7	0.03	-9.39	11.7
1	7	7	0.16	7.6	11.84
2	7	7	12.68	16.92	14.44
3	7	7	1.66	12.49	25.72
4	7	7	9.07	-13.5	27.46
5	7	7	3.6	-5.44	29.61
-7	8	7	13.72	-7.12	30.82
-6	8	7	1.99	-29.95	28.2
-5	8	7	2.89	24.37	15.58
-4	8	7	4.49	2.55	25.72
-3	8	7	57.18	87.63	14.84
-2	8	7	21.95	-47.07	25.05
-1	8	7	55.48	41.94	7.09
0	8	7	41.13	57.55	7.04
1	8	7	46.07	45.7	11.55
2	8	7	20.15	35.19	14.57
3	8	7	34.07	34.98	15.58
4	8	7	20.5	-27.6	27.93
-6	9	7	0.77	8.26	17.12
-5	9	7	1.01	-34.04	28.13
-4	9	7	31.39	32.77	15.51
-3	9	7	3.19	16.52	14.5
-2	9	7	120.08	121.4	15.24
-1	9	7	9.44	13.61	10.16
0	9	7	9.12	5.88	12.33
1	9	7	1.75	4.94	12.17
2	9	7	3	10.01	14.5
3	9	7	3.49	6.65	25.99
4	9	7	1.43	1.61	29.48
-5	10	7	0.15	-24.64	28.81
-4	10	7	0.91	-8.8	27.87
-3	10	7	2.43	-29.01	26.19
-2	10	7	8.37	-25.58	26.39
-1	10	7	2.86	-1.05	10.46
0	10	7	5.43	12.47	12.82
1	10	7	0.64	-6.41	10.4
2	10	7	0.47	-11.08	28.19
3	10	7	0.53	5.51	27.87
-4	11	7	3.32	-10.21	28.87
-3	11	7	43.53	47.94	16.92
-2	11	7	18.39	5.98	26.59
-1	11	7	2.9	3.87	12.04
0	11	7	45.9	54.23	7.73
1	11	7	5.01	-2.03	13.72
2	11	7	4.7	-32.5	28.61
-2	12	7	24.1	-11.28	16.99
-1	12	7	8.36	-2.36	11.54
0	12	7	26.42	8.21	14.31
-8	0	8	0.01	15.04	16.85
-7	0	8	165.61	152.96	17.46
-6	0	8	222.64	202.18	17.32
-5	0	8	24.3	26.39	14.24
-4	0	8	17.97	20.55	13.97
-3	0	8	0.32	2.62	23.3
-2	0	8	51.99	72.99	13.7
-1	0	8	10.32	9	21.55
0	0	8	0.83	12.83	16.57
1	0	8	641.15	631.96	23.62
2	0	8	522.09	527.58	28.47
3	0	8	16.79	12.36	24.31
4	0	8	1.85	-5.37	26.19
5	0	8	11.57	-2.22	16.12
-8	1	8	53.57	65.72	13.93
-7	1	8	18.26	12.18	39.48
-6	1	8	33.96	42.3	22.49
-5	1	8	7.04	-9.83	17.49
-4	1	8	2.55	11.26	18.9
-3	1	8	1.9	3.97	16.59
-2	1	8	69.57	78.67	9.8
-1	1	8	0.37	-2.89	10.42
0	1	8	136.29	125.72	7.19
1	1	8	1433.31	1447.66	35.04
2	1	8	7.05	4.08	16.83
3	1	8	10.6	3.86	13.77
4	1	8	28.87	24.71	10.74
5	1	8	10.18	12.52	19.43
-8	2	8	13.78	20.82	30.22
-7	2	8	44.98	35.92	16.32
-6	2	8	0.78	14.71	15.18
-5	2	8	84.29	72.32	14.84
-4	2	8	41.92	40.02	14.24
-3	2	8	90.82	58.82	14.3
-2	2	8	22.66	4.77	24.04
-1	2	8	97.48	92.44	7.13
0	2	8	72.86	78.11	7.03
1	2	8	9.75	5.84	11.99
2	2	8	17.2	16.99	23.7
3	2	8	16.42	9.47	24.84
4	2	8	54.85	60.9	15.51
5	2	8	5.2	27.6	27.86
-8	3	8	0.24	20.35	29.41
-7	3	8	248.78	283.97	19.14
-6	3	8	29.51	-5.3	27.13
-5	3	8	4.1	11.86	25.65
-4	3	8	5.6	22.49	24.37
-3	3	8	0.5	-29.28	24.71
-2	3	8	73.43	93.74	13.97
-1	3	8	24.72	28.18	7.38
0	3	8	70.26	68.11	6.97
1	3	8	823.55	829.92	23.63
2	3	8	0	-22.16	24.24
3	3	8	0.03	2.55	25.18
4	3	8	13.81	-31.22	26.32
5	3	8	27.89	39.62	16.59
-8	4	8	17.93	-37.67	31.36
-7	4	8	93.91	117.58	16.99
-6	4	8	67.36	73.06	16.18
-5	4	8	28.25	42.03	14.97
-4	4	8	2.47	-11.89	24.98
-3	4	8	28.41	10.27	24.17
-2	4	8	25.85	19.47	23.7
-1	4	8	34.77	13.85	9.86
0	4	8	36.54	28.82	8.53
1	4	8	139.21	136.05	10.66
2	4	8	15.07	9.27	24.64
3	4	8	15.02	19.07	25.45
4	4	8	3.1	-23.5	27.8
5	4	8	0.8	10.07	29.21
-7	5	8	38.82	21.96	29.34
-6	5	8	108.06	89.91	16.85
-5	5	8	11.95	24.84	25.85
-4	5	8	11.44	11.15	25.52
-3	5	8	28.96	23.7	24.51
-2	5	8	225.83	159.81	15.65
-1	5	8	0.35	-33.73	11.89
0	5	8	5.19	-1.82	11.91
1	5	8	61.23	53.16	16.75
2	5	8	30.29	-9.8	25.92
3	5	8	7.28	18.6	14.84
4	5	8	20.81	34.25	15.85
5	5	8	1.76	2.75	17.39
-7	6	8	17.37	-3.89	30.08
-6	6	8	1.03	2.22	28.13
-5	6	8	26.78	8.11	27.8
-4	6	8	6.95	19.34	24.91
-3	6	8	40.47	14.91	25.52
-2	6	8	84.78	85.61	14.64
-1	6	8	15.71	7.32	12.05
0	6	8	13.35	8.53	9.92
1	6	8	18.5	19.74	13.73
2	6	8	0.54	-10.01	25.65
3	6	8	0	27.6	14.57
4	6	8	150.53	90.18	18.13
-6	7	8	10.04	4.7	17.39
-5	7	8	1.44	-8.53	27.13
-4	7	8	6.29	14.91	25.85
-3	7	8	27.36	49.09	14.64
-2	7	8	37.26	74.67	13.9
-1	7	8	7.53	1.18	12.25
0	7	8	5.08	18.98	8.52
1	7	8	10.35	-5.2	17.07
2	7	8	4.3	-31.36	25.45
3	7	8	24.11	38.61	15.71
4	7	8	20.87	6.38	29.21
-6	8	8	2.08	-33.31	31.02
-5	8	8	0.02	21.62	26.86
-4	8	8	50.57	50.09	15.65
-3	8	8	118.56	133.02	15.78
-2	8	8	49.83	56	14.84
-1	8	8	0.01	-2.73	13.06
0	8	8	0.11	-12.14	12.78
1	8	8	4.28	1.77	9.09
2	8	8	9.41	41.56	15.18
3	8	8	0.01	-36.39	28.4
-5	9	8	8.31	11.82	29.41
-4	9	8	0.85	-28.67	28.4
-3	9	8	4.24	-48.82	26.72
-2	9	8	30.38	16.45	15.18
-1	9	8	3.03	-10.02	14.32
0	9	8	15.74	13.68	9.13
1	9	8	30.29	42.16	8.45
2	9	8	6.53	-18.99	28.67
-4	10	8	5.15	-11.21	30.49
-3	10	8	1.81	-45.73	28.13
-2	10	8	4.64	17.93	15.91
-1	10	8	0.16	-8.88	13.6
0	10	8	0.47	-11.52	11.17
1	10	8	4.75	6.71	11.36
-7	1	9	5.55	-65.89	20.27
-6	1	9	6.01	12.26	11.06
-5	1	9	13.05	-10.95	16.51
-4	1	9	3.14	8.39	12.43
-3	1	9	36.19	49.76	18.5
-2	1	9	129.94	124.16	10.61
-1	1	9	83.75	91.53	7.35
0	1	9	61.2	54.35	7.94
1	1	9	0.77	7.03	11.06
2	1	9	29.73	34.23	24.91
3	1	9	5.15	-7.45	28.77
4	1	9	1.27	-1.71	24.07
-7	2	9	7.78	5.44	28.94
-6	2	9	41.14	41.3	16.18
-5	2	9	1.84	13.5	24.91
-4	2	9	12.79	26.79	14.3
-3	2	9	427.75	424.44	22.76
-2	2	9	28.46	26.99	13.97
-1	2	9	21.82	4.8	10.13
0	2	9	285.25	287.81	8.54
1	2	9	91.36	80.01	7.53
2	2	9	12.42	20.21	24.84
3	2	9	0.01	-21.55	26.25
4	2	9	10.85	-20.82	28.34

h	k	l	F_c^2	F_o^2	σF_o^2
-7	3	9	46.69	16.52	30.62
-6	3	9	2.11	-2.22	26.86
-5	3	9	1.66	21.42	26.19
-4	3	9	0.13	3.02	14.71
-3	3	9	32.08	42.24	14.44
-2	3	9	4.05	-1.88	24.84
-1	3	9	52.86	49	7.84
0	3	9	156.57	149.16	7.8
1	3	9	263.55	268.52	11.18
2	3	9	4.18	28.61	14.5
3	3	9	0.08	11.01	25.38
4	3	9	24.84	52.17	17.12
-6	4	9	1.57	-9	26.72
-5	4	9	21.55	38.61	15.18
-4	4	9	3.68	14.84	25.38
-3	4	9	13.33	24.04	25.72
-2	4	9	20.82	-38.27	24.98
-1	4	9	0.16	-11.39	15.45
0	4	9	22.32	29.41	7.96
1	4	9	38.89	56.89	8.14
2	4	9	68.47	57.48	15.44
3	4	9	7.65	1.54	26.93
4	4	9	23.06	25.25	17.06
-6	5	9	24.09	-20.82	30.08
-5	5	9	6.64	1.48	26.05
-4	5	9	2.16	-26.39	26.93
-3	5	9	38.62	26.66	14.5
-2	5	9	0.09	-19.81	24.91
-1	5	9	0.52	1.49	12.02
0	5	9	235.27	225.25	10.51
1	5	9	26.53	29.12	9.17
2	5	9	1.2	-18.13	25.58
3	5	9	0.04	-23.84	27.33
-6	6	9	37.55	66.81	17.32
-5	6	9	6.26	-41.43	28.13
-4	6	9	0.02	-5.77	26.99
-3	6	9	19.26	0.74	26.25
-2	6	9	0.19	-23.37	24.71
-1	6	9	11.01	9.8	10.23
0	6	9	101.81	109.31	7.85
1	6	9	10.53	9.6	9.24
2	6	9	10.37	25.58	25.92
3	6	9	5.93	23.9	28.2
-5	7	9	0.79	-3.89	29.21
-4	7	9	14.37	29.61	15.38
-3	7	9	3.48	-2.22	26.79
-2	7	9	1.79	-18	25.99
-1	7	9	1.47	16.2	12.7
0	7	9	62.48	66.42	7.64
1	7	9	60.59	58.33	16.22
2	7	9	0.1	-31.36	27.87
-4	8	9	0.91	-21.29	26.93
-3	8	9	1.07	-30.62	26.99
-2	8	9	0.04	-25.65	26.66
-1	8	9	5.8	1.25	9.52
0	8	9	0.05	8.61	14.46
1	8	9	5.16	-2.18	13.58
-2	9	9	0	15.18	27.46
-1	9	9	5.22	20.33	10.81
-6	0	10	0.09	-42.84	28.13
-5	0	10	47.61	19.54	27.8
-4	0	10	2.27	-40.29	25.72
-3	0	10	9.44	-37.8	25.78
-2	0	10	24.15	23.7	14.5
-1	0	10	2.29	-32.99	36.93
0	0	10	1.59	18.62	18.21
1	0	10	0.96	1.27	18.32
2	0	10	26.23	48.55	16.18
-6	1	10	8.45	9.55	19.89
-5	1	10	13.61	-1.33	22.23
-4	1	10	80.52	71.26	11.04
-3	1	10	57.43	56.32	31.36
-2	1	10	18.93	27.78	20.18
-1	1	10	0.65	18.98	7.85
0	1	10	3.74	-20.76	16.09
1	1	10	15.89	35.59	8.06
2	1	10	0.53	12.55	13.47
-6	2	10	1.74	-41.7	29.01
-5	2	10	0.36	7.59	16.25
-4	2	10	2.69	-10.21	26.93
-3	2	10	17.81	5.71	26.59
-2	2	10	8.29	-25.18	25.31
-1	2	10	11.99	-0.5	10.44
0	2	10	55.19	52.82	7.63
1	2	10	1.8	11.59	9.04
2	2	10	4.19	3.83	27.4
-5	3	10	0.17	0.81	28.4
-4	3	10	10.41	6.71	26.25
-3	3	10	13.19	-0.74	26.25
-2	3	10	7.52	14.24	15.04
-1	3	10	2.42	11.32	10.43
0	3	10	15.09	2.94	12.94
1	3	10	0.05	1.29	13.06
2	3	10	1.75	18.8	26.93
-5	4	10	4.94	-49.82	29.55
-4	4	10	0	-6.85	27.19
-3	4	10	6.07	1.48	25.72
-2	4	10	4.29	-9.47	26.66
-1	4	10	17.27	18.15	10.03
0	4	10	14.31	5.03	11.79
1	4	10	17.52	7.42	13.32
2	4	10	0.26	-8.8	28.4
-4	5	10	23.49	0	28
-3	5	10	16.5	26.59	28.13
-2	5	10	8.69	2.22	26.59
-1	5	10	19.37	27.77	8.36
0	5	10	36.59	20.7	11.37
1	5	10	2.5	0.04	12.93
-3	6	10	1.22	7.86	16.32
-2	6	10	6.3	26.32	15.85
-1	6	10	78.37	87.45	14.85
0	6	10	258.09	285.02	11.65
-3	1	11	4.9	-2.76	19.46
-2	1	11	2.63	-4.82	19.37
-1	1	11	0.04	-23.36	19.27
-2	2	11	4.27	20.75	26.86
-1	2	11	52.52	64.13	16.25