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# The Crystalline Structure of MM3, A Derivative of Dapsone

Tommie L. Heltcel

# The Edwin P. McCabe Honors Program

Senior Thesis

# "The Crystalline Structure of MM3, A Derivative of Dapsone"

## Tommie L. Heltcel

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THE CRYSTALLINE STRUCTURE OF MM3,

A DERIVATIVE OF DAPSONE

by

Tommie Lee Heltcel

Chemistry/Mathematics Major

Departments of Natural Sciences and Mathematics

Division of Arts and Sciences

Langston University

Langston, Oklahoma

# THE CRYSTALLINE STRUCTURE OF MM3, A DERIVATIVE OF DAPSONE

Thesis Approved:

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Thesis Committee Chairman

_____
Thesis Committee Co-Chairman

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Thesis Committee Member

_____
Director of the Honors Program

_____
Vice President for Academic Affairs

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# Table of Contents

# Chapter I

## Introduction

Dapsone is a drug which has recently been discovered as a potential treatment for the disease of leprosy. Many of the derivatives of dapsone have been sent to the United States by Dr. M. Muhundam and Professor M.S.R. Naidu of the Department of Chemistry, S.V. University, Tirupati, India, for structure analysis. One such derivative is (E)-3-[2-[(4-Chlorophenyl) sulphonyl] ethenyl]-4H-1-benzopyran-4-one, which will hereafter be referred to as MM3. MM3 was synthesized and the initial data for the structural analysis taken in the departments of Physics and Chemistry at S.V. University, Tirupati, India. The drug has been found to have a high antibacterial activity and hence may become a treatment for the cure of leprosy. However, to understand the full potential of the drug, the structural and conformational study needs to be performed.

The "structural formula and geometric details ... [are] of primary interest to the chemist and biochemist who are concerned with the relation of the structural features to chemical properties" (Glusker and Trueblood 5). These chemical properties may help the chemist and biochemist to determine what functional groups need to be added to the drug to make it more effective by increasing the activity of the drug.

The author of this work has determined the crystal structure of MM3 by X-ray diffraction analysis. X-ray crystallography has become standard in structure determination since 1913 when W.L.

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Bragg first used X-ray diffraction to determine the crystalline structure of sodium chloride, ordinary table salt. The X-ray diffraction technique had been first discovered just a year before by Max von Laue, a physicist interested in X-rays. Von Laue suggested that "Friedrich and Knipping try diffracting X rays by crystals in order to test the hypothesis that X rays are wavelike with wavelengths of the order of 1 ..." angstrom ($10**-10$ m) (Glusker and Trueblood 9). X-rays are used for structural study since the wavelength is comparable to the interatomic dimensions. He used surmises of Kepler (1611) and Hooke (1665) and logical conclusions by Bergman (1773) and Hauy (1782) "that crystals have an internal structure that is periodic (regularly repeating) in three dimensions ..." (Glusker and Trueblood 8). The experiment was surprisingly successful and led to the technique for determining crystal structure employed by Bragg. Von Laue guessed that X-rays have wavelengths near the dimensions of atomic bonds and nuclei in a crystal.

The determination of the structure of crystals has become increasingly popular to chemists and physicists because of the relationship between structure and activity of all kinds of crystallized materials. From simple sodium chloride to complex proteins and viruses, the crystal structure has greatly contributed in an essential way to the understanding of biochemistry and molecular biology (Glusker and Trueblood 9).

This study finds the exact bond angles and lengths between atoms in the molecule, the unit cell (basic regular repeating

block) in a crystal of MM3, and the symmetrical way in which the molecules are packed together in this cell.

# Chapter II
## Measuring the Unit Cell and Intensities of Reflections

The precession photograph of the crystal was taken.  A few
spots and their coordinates were identified and serve as input to
a computer program to calculate the unit cell.  The axes lengths
a, b, and c, and angles alpha, beta, and gamma, were then
determined for the primitive cell.  These axes and angles are
named according to the standard convention.
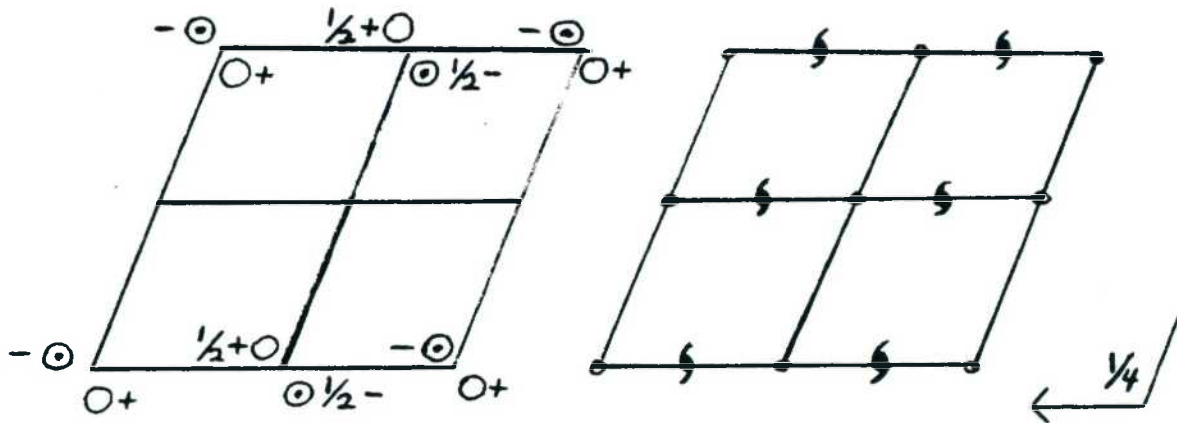


Figure 1

The data was collected on a Syntax Diffractometer at Oklahoma
State University, Stillwater, Oklahoma.

The x-rays are produced by rapidly accelerating electrons
hitting a molybdenum target.  When one of the electrons hits the
target, an electron attached to an atom is knocked off and
replaced by an electron from a higher orbital.  The second
electron loses a definite amount of potential energy, which is
omitted as radiation.  The replacing electrons come from orbitals

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of several different energy levels and produce several different wavelengths of radiation.  Therefore, the X-rays are filtered by a zirconium foil, leaving only K-alpha-1 and K-alpha-2 radiations (Glusker and Trueblood 5).  A parallel beam of the filtered X-rays is produced by a collimator and directed at the crystal.  The X-rays diffracted (deflected) by the crystal enter a movable counter.  The counter measures the peak height of each reflection and the left and right background of each.

## THE SPACE GROUP

The reflections' intensities and settings of the crystal were used to determine the space group.  The space group (defined in Appendix A) is the collection of symmetry operations which generates the entire infinite crystalline structure by acting on the basic "asymmetric unit."  In this case of the crystal structure of MM3, there is one molecule per asymmetric unit.

The translational subgroup of every space group is comprised of all the translations (see Fig. 1) which leave the infinite structure unchanged.  The space group may also contain an inversion center.  The space group is then called centrosymmetric. The space group of MM3 is of this kind.  (The X-ray reflection data usually show the presence of a center of symmetry even when the crystal does not.)  The space group may also contain rotation axes, mirror planes or glide planes.
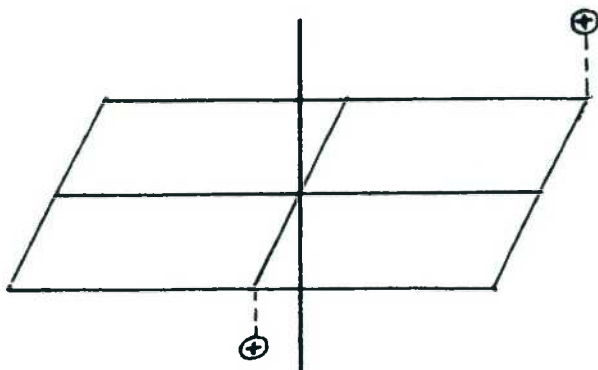
(Glide Plane)

Figure 2
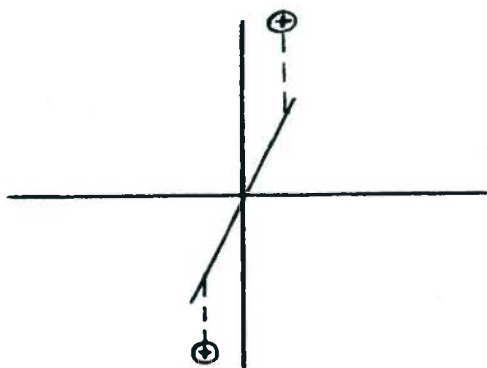


(2-Fold Screw Axes)

Figure 3

Only certain special combinations of these symmetry operations can be put together to become a space group. There are 230 possible groups for three-dimensional space. These are listed in the International Tables for X-ray Crystallography, Volume I.

Chapter III

Data Correction and Deriving the Structure Factor

The data for the experiment was processed at the Department of
Physics at the University of Central Oklahoma where this study was
done.  The processing was done using the SDP-Software developed by
Bert Frent Association.  The information was transferred from disk
to computer.  Then the computer read the peak intensities and left
and right backgrounds of each diffracted X-ray beam.  It averaged
the backgrounds and subtracted the averaged backgrounds from the
peak intensities to get the real value of each intensity.

Since the X-ray beam used was not polarized, a polarization
factor, depending on reflection angle, multiplies each intensity.
This polarization factor averages all of the possible polarized
light vectors in the unpolarized X-ray beam to correct from the
average intensity to the maximum value for each.

Another factor which must be introduced to the process is the
Lorenzo factor, which adjusts the data for the different rates at
which each of the intensities was recorded.

Next, the intensities were examined to see if a correction
for absorption of X-rays by the crystal should be applied.  This
correction is used when irregular crystal shape causes absorption
to differ for different reflections during the diffraction
process.  A graph of the absorption of the crystal (see next page)
showed very little absorption of X-rays, so there was no need to

correct the intensities.

The next step was to construct a Wilson plot. The Wilson plot is a graph that plots the natural log of the intensities versus (sin theta/lambda). Theoretically, the graph should be a straight line, so the curve is fitted by least squares to the best possible line. This line helps put the intensities on an absolute scale by finding the scale factor and temperature factors simultaneously (see page 10). The slope of the graph gives the temperature factor and the intercept gives the scale factor.

The graph shows that ln K = 1.6. The slope of the graph is

equal to $\dfrac{-1.6 + 0.3}{.3} = \dfrac{-1.3}{.3} = -4.3 = -2B$. So B = +2.1.

Then the squares root of the intensities are taken to get the structure factors for the crystal. In general the structure factors for a crystal allow the observer to choose one of several space groups for the crystal. There is a detailed listing of all of the structure factors observed (Fobs) and calculated (Fcal) for each intensity in Appendix E.

CRYSTAL DECAY

FOBS SQUARED

EXPOSURE (HRS)

WILSON PLOT

ln(F(obs)²/Σf²)

((SIN Θ)/l)²
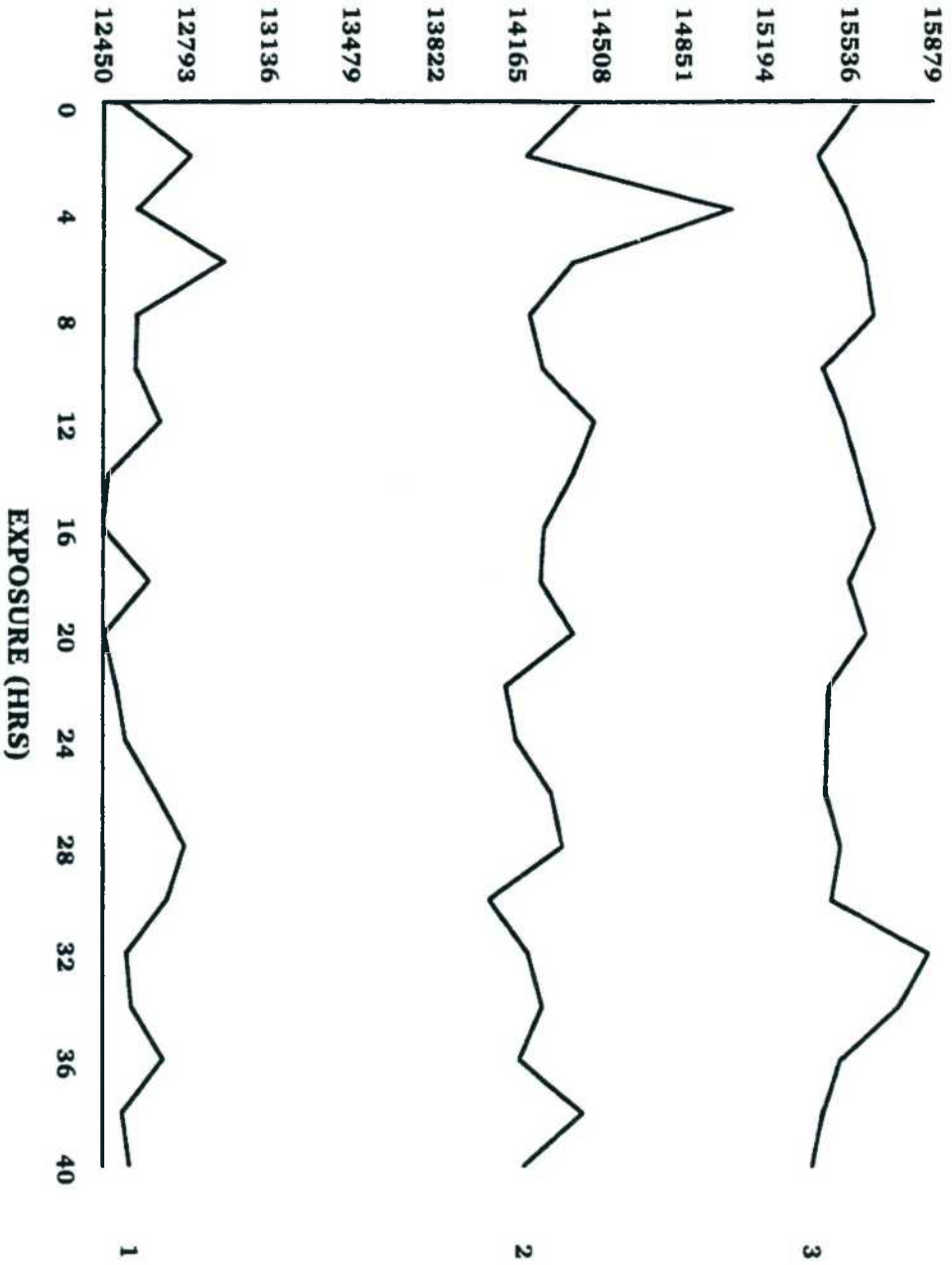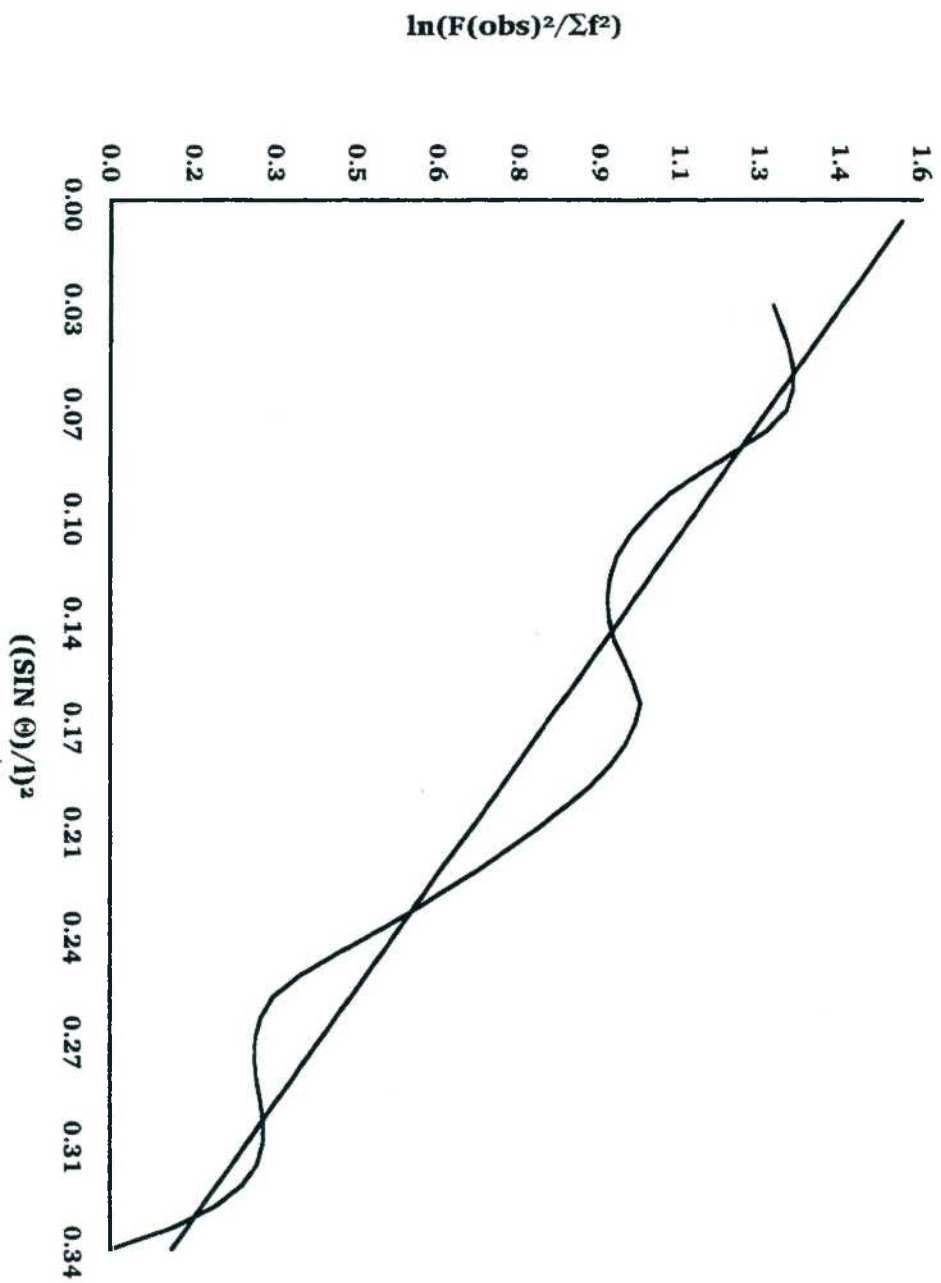
## Chapter IV

## Determination of the Space Group

The structure factors, $F(h,k,l)$, are indexed by trios of integers h, k, l. Their values are real numbers for centrosymmetric crystals like MM3. The elements of the space group outside the translation subgroup produce relations between structure factors with indices related by characteristic equations. The screw axes and glide plane cause certain sets of structure factors to have zero value. Thus, a screw axis parallel to the b axis (see Fig. 1) causes $F(0,k,0)$ with k odd to be absent. A glide plane with translation parallel to the a axis causes $F(h,0,l)$ with h odd to be absent.

The corrected intensities for MM3 were examined and it was found that both of the sets of reflections mentioned above were absent. It was therefore deduced that the space group P21/a was consistent with the observed systematic absences. The space group was therefore P21/a, a variant of #14 in the International Tables for X-ray Crystallography, Volume I.

The presence of both the screw and glide symmetries establishes the presence of a center of symmetry in the crystal. The three elements generate three additional atoms for each independent atom in the unit cell, making a total of a multiple of four molecules per unit cell. From the molecular weight, the calculated unit cell volume and the density of the crystal, the

calculated unit cell volume and the density of the crystal, the number of molecules in the unit cell is found to be four.

Chapter V

Solving the Phase Problem

The crystal structure of MM3 was determined by using direct
methods of phase determination in a Shelx Program.  The
crystallographer can only experimentally measure the absolute
values of the structure factors and not the phases.  In the case
of a centrosymmetric structure like MM3, this means that the sign
(+ or -) of the structure factors is initially unknown.  To
determine signs, relations between values of structure factors
derived from inequalities based on the theory of probability are
used.  There are many kinds of these relations, and a number of
computer programs employ these relations in different ways.  For
MM3, the ShelX option of SDP program was used.

The program uses normalized structure factors $E(h,k,l)$.  The
program first removes the temperature dependence from the
structure factors $F(h,k,l)$ using the Wilson plot.  It then divides
each corrected $F(h,k,l)$ by the square root of the sum of the
squares of the atomic scattering factors of all atoms in the unit
cell.  These resulting E values are the structure factors of the
crystal modified by substituting stationary point atoms for the
actual ones.

The program first assigns phases to three suitable E values
to choose one of the eight symmetry centers in the unit cell.  It
next ranks the modified E values from highest to lowest.  It

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assigns phases at random to a group of the largest values. Then it calculates new phases by using triplet and negative quartet relationships shifts between those E's with already assigned phases. It uses a "figure of merit," NQUAL, to estimate the correctness of the set of phases it has determined.

A calculated set of E values is then used in a Fourier summation to give an E map, a picture of the electron density in the unit cell. This picture also shows all the computed possible bonds between the peaks in the unit cell.

Bonds and atoms were dropped from the E map. Any bond between two atoms which differed in length from known values or which made an unusual angle with another bond was removed. Also the molecular structure discovered by Muhundam and Naidu was used to indicate spurious peaks in the E map, and these atoms were also removed. The molecular structure after refinement of coordinates is shown on the next page.
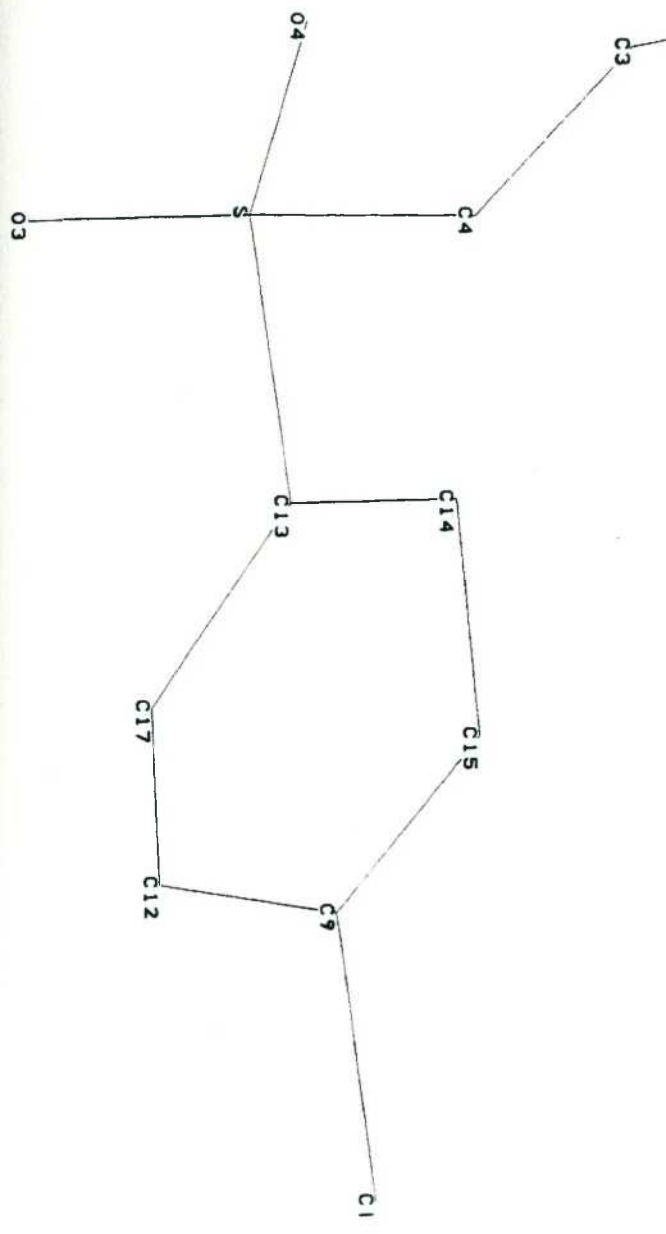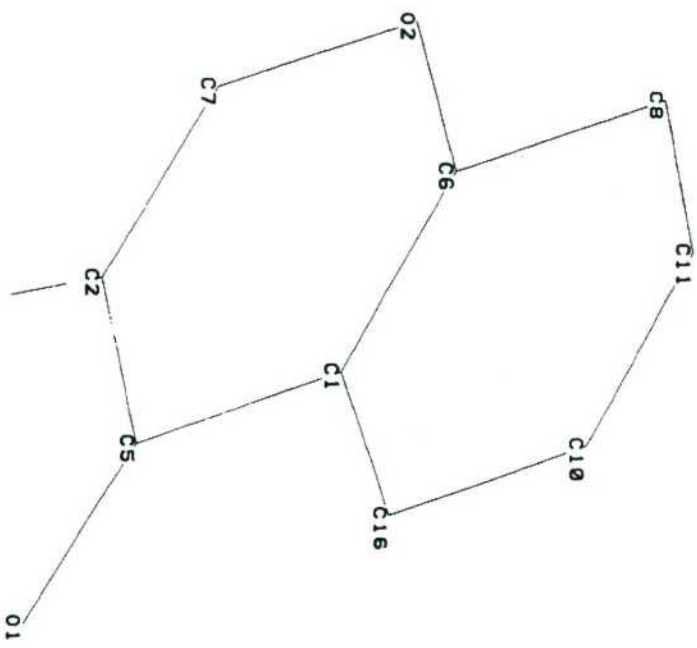
Chapter VI

Structure Refinement

Structure refinement for MM3 was done using the method of least squares using the full matrix. The best parameters for the assumed model are obtained by minimizing the weighted sum of the squares of the differences between the observed structure factors (Fobs) and the structure factors calculated from the parameters (Fcal).

If a reasonable trial structure close to the correct one can be found, then a linear approximation to the structure factor allows one to derive a linear equation using the shifts of the trial structure parameters as the variables for the structure factor. This can be done by using an expanded Taylor series about the trial parameters and only retaining the first derivative, making the assumption that higher order derivatives are negligibly small. Then Newton's method is used to find the parameter shifts. The method is iterated until all shifts are negligible. However, this can only succeed if the trial structure is very close to the correct one. If the structure is not of good quality, then the method will refine to a false minimum or not refine at all. Three cycles of full matrix least square refinement were executed using the Poisson weight scheme. Isotropic temperature factors were used in the structure factors expressions. Hydrogen atoms were omitted. The final parameters are listed in Appendix E. The

correctness of a structure is measured by the value of the reliability factor R1. This index is defined as the summation of the absolute value of the difference between the Fobs and Fcal divided by the summation of the Fobs values for all reflections.

The final R1 value of the trial structure of MM3 was 0.103. Generally, correct structures containing the same number of atoms in the asymmetric unit of MM3 have values ranging from 0.03 to 0.06. In order for the R1 value for this structure to be reduced, several more full matrix least squares needed to be performed after adding hydrogen atoms and changing the isotropic temperature factors to anisotropic ones.

The final results of this experiment showed that the trial structure of MM3 was nearly correct according to the final R value and the conformance of the bond angles and lengths to those expected for this structure. The hydrogen atoms have been omitted due to the lack of time.

Chapter VII

Discussion of Results

The structure of MM3 found in this experiment seems to be one of good quality because all of the bond lengths and angles are close to the accepted values found by other experiments. The mean value, variance, and standard deviation of the carbon to carbon bond lengths in the benzene rings of MM3 are listed in Table #1 on the next page. This table and the calculations below it show that the mean value of the bonds is 1.39 angstroms, the variance 0.00037 angstroms, and the standard deviation 0.019 angstroms. From these values the average bond length for this kind of bond in this experiment is 1.39 ± 0.019 angstroms, which is the known value for benzene rings from other experiments. The average bond angle in the benzene rings is also very close to expected value. The carbon to sulfur, carbon to oxygen, carbon to carbon, and sulfur to oxygen single bond distances in the molecule also closely agree with results obtained by others. From this data the structure for MM3 seems to agree with the expected structure quite well. However, more work needs to be performed on the structure before definite confirmation can be obtained.

The next steps to be done are as follows:

1.  Insert the hydrogen atoms at the locations which can be calculated from the known carbon to hydrogen bond distances and the expected bond angles.

2.  Replace the isotropic temperature factors for the heavy
    atoms by anisotropic factors which allow these atoms to
    move different amounts in different directions.

3.  Use several cycles of full matrix least squares
    refinement allowing the temperature factors to change,
    but keeping the hydrogen parameters fixed.  Repeat until
    shifts are negligible.

4.  Execute a difference Fourier summation to examine the
    difference between the calculated electron density and
    the observed (with calculated signs).

    If the resulting difference of the two densities is
    small, then the structure is demonstrated to be correct.

The bond lengths and angles will be recalculated and
estimated standard deviations (esd's) of these values will be
derived from the full matrix of refinement.  On the basis of these
esd's, the bond lengths and angles can be compared with values
from other structure determinations to ascertain whether the
structure of MM3 exhibits any deviation from normal behavior.

A packing diagram showing the way in which a molecule is
separated from its neighbors will be derived and discussed.

Table 1

Table for Average Carbon to Carbon Bond

Length in Benzene Rings Found in MM3

| From | To | Length (in Angstroms) | Length minus Mean X-U | Value Squared (X-U)**2 |
|------|------|------|------|------|
| C9 | C15 | 1.39 | 0.00 | 0.0000 |
| C9 | C12 | 1.39 | 0.00 | 0.0000 |
| C14 | C15 | 1.36 | -0.03 | 0.0009 |
| C12 | C17 | 1.39 | 0.00 | 0.0000 |
| C13 | C14 | 1.41 | 0.02 | 0.0004 |
| C13 | C17 | 1.41 | 0.02 | 0.0004 |
| C1 | C6 | 1.40 | 0.01 | 0.0001 |
| C6 | C8 | 1.37 | -0.02 | 0.0004 |
| C8 | C11 | 1.40 | 0.01 | 0.0001 |
| C11 | C10 | 1.43 | 0.04 | 0.0016 |
| C10 | C16 | 1.40 | 0.01 | 0.0001 |
| C16 | C1 | 1.37 | -0.02 | 0.0004 |
| | total | 16.72 | | total   0.0041 |

$$\text{Mean} = \frac{\text{Sum of all Lengths}}{\text{Number of Entries}} = \frac{16.72}{12} = 1.3933333$$

$$\text{Variance} = \frac{\text{Sum of all Lengths Squared}}{\text{Number of Entries minus one}} = \frac{0.0041}{11} = 0.0003727$$

Standard Deviation = Square Root of Variance = 0.0193061

Appendices

Appendix A

Glossary

Glossary

**Absent reflections**. Reflections too weak to be observed
by the method of measurement used. The fact that they are so
weak provides structural information to the crytallographer.
Systematically absent reflections are those which the space
group symmetry causes to be zero - for example, $F(0,k,0)$ with
$\underline{k}$ odd. Systematic absences are used in deriving the space
group.

**Accuracy**. Deviation of a result obtained by a
particular method from the value accepted as true.

**Asymmetric unit**. The smallest part of a crystal from
which the complete structure can be obtained from the space
group symmetry operations (including translations). The
asymmetric unit may consist of only part of a molecule or of
several molecules not related by symmetry.

**Atomic scattering factor**. X-rays set the electrons of
atoms into vibration, causing them to act as sources of
secondary radiation. The scattering power of a single atom
depends on its electronic structure and the angle of
scattering and is modified if the X-rays used are appreciably
absorbed by the atom. These effects are expressed in atomic
scattering factors, which represent the scattering power of
an atom measured relative to the scattering by a single
electron under similar conditions; the scattering power falls

off as the scattering angle increases. Atomic scattering is computed from theoretical wave functions for free atoms. Atomic scattering factors are modified by anomalous scattering and become complex.

**Automated diffractometer**. An instrument for automatically measuring and recording the intensities of diffracted beams. The orientations of the crystal and of the detector with respect to the source of radiation are computed from some unit cell data. The computer calculates these orientation angles and drives the gears that move the crystal orienter and detector to the desired angular settings.

**Crystal**. A solid having a regular repeating internal arrangement of atoms which is periodic in three dimensions.

**Crystal structure**. The arrangement of the atoms, molecules, or ions that are in a crystal.

**Diffraction pattern**. The experimentally measured values of intensities, diffracting angle (direction), and order of diffraction for each diffracted beam obtained when a crystal is placed in a narrow beam of X-rays or neutrons (usually monochromatic).

**Electron density**. The number of electrons per unit volume (usually per cubic angstrom).

**Electron density map**. A contoured representation of electron density at various points in a crystal structure. Electron density is expressed in electrons per cubic angstrom and is highest near atomic centers. The map is calculated using a Fourier synthesis, that is, a summation of waves

known amplitude, frequency, and phase.  For three-dimensional
maps it is customary to superimpose maps, representing two
dimensional sections, parallel to one another and at
different heights in the cell.

**Glide plane**. A glide plane is a symmetry element for
which each point is reflected across the plane and then
translated in a direction parallel to the plane.

**Monochromatic**. Consists of radiation of a single
wavelength or of a very small range of wavelengths.

**Normalized structure factor**. The ratio of the value of
the structure amplitude to the square root of the sum of the
squares of the atomic scattering factors of the atom in the
unit cell.

**Refinement**. A process of improving the parameters of an
approximate (trial) structure until the best fit of
calculated structure factor amplitudes to those observed is
obtained.  The process usually requires many successive
stages.

**Screw axis**. For a screw axis, the corresponding symmetry
operations is a rotation about the axis by some fraction
of 360 coupled with a translation parallel to the axis and
equal to a fraction of the unit-cell length.

**Space group**. A group of symmetry operations consistent
with an infinitely extended, regular repeating pattern.  The
space group can be derived by the addition of translational
symmetry to the 32 point groups appropriate for structures
arranged on lattices.  These include translations, glide

planes, and screw axes. Hence a space group may be considered as the group of operations that converts one molecule or asymmetric unit into an infinite extended pattern.

**Translation.** Refers to a motion in which all points of a body move the same distance in the same direction.

**Trial structure.** A possible structure for a crystal, which is tested by comparison of calculated and observed structure factors and by the results of an attempted refinement of the structure.

**Unit cell.** The basic building block of a crystal, repeated infinitely in three dimensions. It is characterized by three vectors - $\underline{a}$, $\underline{b}$, and $\underline{c}$ - that form the edges of a parallelepiped and the angles between them are alpha, gamma, and beta.

**X-rays.** Electromagnetic radiation produced by bombarding a target (usually a metal such as copper or molybdenum) with fast electrons. As a result, electrons from the innermost shells ($\underline{K}$ or $\underline{L}$) may be ejected from atoms in the target material. When an electron from an outer shell falls back into the vacant shell, energy is emitted in the form of X-rays.

Appendix B

Table of Bond Angles

## Table of Bond Angles in Degrees

| Atom 1 | Atom 2 | Atom 3 | Angle | Atom 1 | Atom 2 | Atom 3 | Angle |
|========|========|========|=======|========|========|========|=======|
| O3 | S | O4 | 117.9(6) | S | C4 | C3 | 118.7(9) |
| O3 | S | C4 | 107.7(5) | C1 | C5 | C2 | 115(1) |
| O3 | S | C13 | 108.2(6) | O2 | C6 | C1 | 120(1) |
| O4 | S | C4 | 110.1(6) | O2 | C6 | C8 | 117(1) |
| O4 | S | C13 | 108.6(6) | C1 | C6 | C8 | 124(1) |
| C4 | S | C13 | 103.5(6) | O2 | C7 | C2 | 125(1) |
| C6 | O2 | C7 | 120.2(9) | C6 | C8 | C11 | 118(1) |
| C5 | C1 | C6 | 121(1) | C1 | C9 | C12 | 118(1) |
| C3 | C2 | C5 | 125(1) | C8 | C11 | C10 | 120(1) |
| C3 | C2 | C7 | 116(1) | C9 | C12 | C17 | 118(1) |
| C5 | C2 | C7 | 119(1) | S | C13 | C14 | 120(1) |
| C2 | C3 | C4 | 126(1) | C13 | C14 | C15 | 120(1) |

Numbers in parentheses are estimated standard deviations in
the least significant digits.

Appendix C

Table of Bond Lengths

# Table of Bond Distances in Angstroms
-----------------------------------------

| Atom 1 | Atom 2 | Distance | | Atom 1 | Atom 2 | Distance |
|========|========|==========|---|========|========|==========|
| C1 | C9 | 1.74(1) | | C6 | O2 | 1.39(1) |
| S | O3 | 1.459(9) | | C6 | C1 | 1.40(2) |
| S | O4 | 1.44(1) | | C6 | C8 | 1.37(2) |
| S | C4 | 1.75(1) | | C7 | O2 | 1.33(1) |
| S | C13 | 1.76(1) | | C7 | C2 | 1.37(2) |
| O2 | C6 | 1.39(1) | | C8 | C6 | 1.37(2) |
| O2 | C7 | 1.33(1) | | C8 | C11 | 1.40(2) |
| O3 | S | 1.459(9) | | C9 | C1 | 1.74(1) |
| O4 | S | 1.44(1) | | C9 | C12 | 1.39(2) |
| C1 | C5 | 1.45(2) | | C10 | C11 | 1.43(2) |
| C1 | C6 | 1.40(2) | | C11 | C8 | 1.40(2) |
| C2 | C3 | 1.45(2) | | C11 | C10 | 1.43(2) |
| C2 | C5 | 1.47(2) | | C12 | C9 | 1.39(2) |
| C2 | C7 | 1.37(2) | | C12 | C17 | 1.39(2) |
| C3 | C2 | 1.45(2) | | C13 | S | 1.76(1) |
| C3 | C4 | 1.34(2) | | C13 | C14 | 1.41(2) |
| C4 | S | 1.75(1) | | C14 | C13 | 1.41(2) |
| C4 | C3 | 1.34(2) | | C14 | C15 | 1.36(2) |
| C5 | C1 | 1.45(2) | | C15 | C14 | 1.36(2) |
| C5 | C2 | 1.47(2) | | C17 | C12 | 1.39(2) |

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Numbers in parentheses are estimated standard deviations in
the least significant digits.

Appendix D

Table of Fobs and Fcal

Values of 10*Fobs and 10*Fcalc

| h | k | l | Fobs | Fcalc | Í(F) | h | k | l | Fobs | Fcalc | Í(F) |
|---|---|---|------|-------|------|---|---|---|------|-------|------|
| 1 | -7 | 0 | 125 | 123 | 5 | -13 | -6 | 2 | 109 | 140 | 6 |
| 5 | -7 | 0 | 92 | 103 | 6 | -5 | -6 | 2 | 168 | 171 | 4 |
| 6 | -7 | 0 | 70 | 44 | 8 | -3 | -6 | 2 | 275 | 318 | 3 |
| 8 | -7 | 0 | 114 | 142 | 6 | -2 | -6 | 2 | 151 | 83 | 4 |
| -8 | -7 | 1 | 90 | 81 | 7 | 3 | -6 | 2 | 247 | 205 | 3 |
| -6 | -7 | 1 | 126 | 156 | 5 | 4 | -6 | 2 | 94 | 93 | 6 |
| -2 | -7 | 1 | 77 | 60 | 8 | 5 | -6 | 2 | 141 | 117 | 4 |
| 4 | -7 | 1 | 198 | 184 | 4 | 7 | -6 | 2 | 97 | 65 | 6 |
| -8 | -7 | 2 | 104 | 147 | 6 | 10 | -6 | 2 | 101 | 87 | 6 |
| -5 | -7 | 2 | 81 | 136 |  | 13 | -6 | 2 | 153 | 155 | 5 |
| -2 | -7 | 2 | 93 | 89 | 6 | -12 | -6 | 3 | 75 | 116 | 7 |
| 0 | -7 | 2 | 130 | 182 | 5 | -9 | -6 | 3 | 161 | 122 | 4 |
| 3 | -7 | 2 | 90 | 105 | 7 | -8 | -6 | 3 | 125 | 132 | 5 |
| -3 | -7 | 3 | 167 | 211 | 4 | -6 | -6 | 3 | 407 | 447 | 3 |
| -1 | -7 | 3 | 68 | 51 | 8 | -5 | -6 | 3 | 182 | 144 | 4 |
| 3 | -7 | 3 | 124 | 137 | 5 | -4 | -6 | 3 | 180 | 189 | 4 |
| -5 | -7 | 4 | 187 | 250 | 4 | -3 | -6 | 3 | 91 | 86 | 6 |
| -2 | -7 | 4 | 70 | 67 | 8 | -2 | -6 | 3 | 200 | 183 | 4 |
| 2 | -7 | 4 | 134 | 109 | 5 | -1 | -6 | 3 | 224 | 206 | 4 |
| 7 | -7 | 4 | 119 | 117 | 6 | 2 | -6 | 3 | 480 | 481 | 3 |
| -7 | -7 | 5 | 81 | 120 | 7 | 3 | -6 | 3 | 221 | 171 | 4 |
| -6 | -7 | 5 | 106 | 127 | 6 | 6 | -6 | 3 | 135 | 174 | 4 |
| 4 | -7 | 5 | 99 | 69 | 7 | 11 | -6 | 3 | 243 | 285 | 4 |
| 5 | -7 | 5 | 123 | 154 | 6 | -9 | -6 | 4 | 72 | 87 | 8 |
| 0 | -7 | 6 | 92 | 109 | 7 | -8 | -6 | 4 | 153 | 210 | 4 |
| 3 | -7 | 6 | 183 | 212 | 5 | -2 | -6 | 4 | 193 | 188 | 4 |
| 0 | -6 | 0 | 417 | 439 | 3 | 0 | -6 | 4 | 348 | 341 | 3 |
| 1 | -6 | 0 | 181 | 120 | 4 | 1 | -6 | 4 | 311 | 321 | 3 |
| 2 | -6 | 0 | 103 | 138 | 6 | 2 | -6 | 4 | 120 | 67 | 5 |
| 8 | -6 | 0 | 81 | 71 | 6 | 6 | -6 | 4 | 87 | 72 | 6 |
| 9 | -6 | 0 | 104 | 150 | 5 | 9 | -6 | 4 | 221 | 268 | 4 |
| 11 | -6 | 0 | 78 | 77 | 7 | -12 | -6 | 5 | 95 | 114 | 6 |
| 12 | -6 | 0 | 113 | 136 | 5 | -10 | -6 | 5 | 142 | 143 | 5 |
| -13 | -6 | 1 | 76 | 87 | 7 | -9 | -6 | 5 | 201 | 219 | 4 |
| -12 | -6 | 1 | 81 | 103 | 7 | -8 | -6 | 5 | 129 | 152 | 5 |
| -11 | -6 | 1 | 142 | 159 | 5 | -6 | -6 | 5 | 170 | 157 | 4 |
| -10 | -6 | 1 | 145 | 128 | 4 | -5 | -6 | 5 | 177 | 161 | 4 |
| -5 | -6 | 1 | 129 | 81 | 5 | -2 | -6 | 5 | 320 | 342 | 3 |
| -2 | -6 | 1 | 582 | 617 | 3 | -1 | -6 | 5 | 342 | 284 | 3 |
| -1 | -6 | 1 | 225 | 114 | 4 | 0 | -6 | 5 | 194 | 214 | 4 |
| 1 | -6 | 1 | 173 | 119 | 4 | 2 | -6 | 5 | 119 | 148 | 5 |
| 2 | -6 | 1 | 70 | 48 | 7 | 4 | -6 | 5 | 90 | 65 | 7 |
| 3 | -6 | 1 | 199 | 179 | 4 | 6 | -6 | 5 | 113 | 160 | 6 |
| 4 | -6 | 1 | 103 | 110 | 5 | 7 | -6 | 5 | 365 | 399 | 3 |
| 6 | -6 | 1 | 263 | 259 | 3 | 8 | -6 | 5 | 116 | 106 | 6 |
| 7 | -6 | 1 | 233 | 215 | 4 | 10 | -6 | 5 | 131 | 145 | 5 |
| 9 | -6 | 1 | 102 | 80 | 6 | 11 | -6 | 5 | 108 | 97 | 6 |
| 10 | -6 | 1 | 109 | 103 | 5 | -10 | -6 | 6 | 69 | 46 | 7 |

| h | k | l | Fobs | Fcalc | Í(F) | h | k | l | Fobs | Fcalc | Í(F) |
|---|---|---|------|-------|------|---|---|---|------|-------|------|
| -7 | -6 | 6 | 125 | 124 | 5 | 1 | -5 | 1 | 95 | 80 | 5 |
| -6 | -6 | 6 | 146 | 179 | 5 | 2 | -5 | 1 | 691 | 688 | 3 |
| -5 | -6 | 6 | 146 | 173 | 5 | 3 | -5 | 1 | 243 | 170 | 3 |
| -4 | -6 | 6 | 148 | 124 | 5 | 4 | -5 | 1 | 105 | 33 | 5 |
| -2 | -6 | 6 | 179 | 194 | 4 | 6 | -5 | 1 | 277 | 322 | 3 |
| -1 | -6 | 6 | 155 | 162 | 4 | 7 | -5 | 1 | 336 | 324 | 3 |
| 4 | -6 | 6 | 239 | 281 | 4 | 8 | -5 | 1 | 126 | 158 | 4 |
| 7 | -6 | 6 | 110 | 91 | 6 | 10 | -5 | 1 | 155 | 145 | 4 |
| -10 | -6 | 7 | 98 | 101 | 6 | 11 | -5 | 1 | 238 | 265 | 3 |
| -8 | -6 | 7 | 167 | 202 | 4 | 12 | -5 | 1 | 109 | 119 | 5 |
| -6 | -6 | 7 | 187 | 219 | 4 | 14 | -5 | 1 | 70 | 42 | 7 |
| -5 | -6 | 7 | 186 | 152 | 4 | -13 | -5 | 2 | 103 | 72 | 5 |
| -4 | -6 | 7 | 100 | 140 | 6 | -11 | -5 | 2 | 135 | 119 | 4 |
| -3 | -6 | 7 | 123 | 151 | 5 | -8 | -5 | 2 | 210 | 235 | 3 |
| -1 | -6 | 7 | 115 | 121 | 5 | -7 | -5 | 2 | 80 | 27 | 6 |
| 0 | -6 | 7 | 88 | 62 | 7 | -6 | -5 | 2 | 147 | 163 | 4 |
| 1 | -6 | 7 | 177 | 175 | 4 | -5 | -5 | 2 | 97 | 102 | 5 |
| 3 | -6 | 7 | 338 | 326 | 3 | -2 | -5 | 2 | 202 | 170 | 3 |
| 4 | -6 | 7 | 144 | 168 | 5 | -1 | -5 | 2 | 144 | 142 | 4 |
| 5 | -6 | 7 | 114 | 153 | 5 | 0 | -5 | 2 | 373 | 361 | 3 |
| 7 | -6 | 7 | 191 | 216 | 4 | 1 | -5 | 2 | 322 | 289 | 3 |
| -7 | -6 | 8 | 131 | 144 | 5 | 2 | -5 | 2 | 255 | 244 | 3 |
| -1 | -6 | 8 | 123 | 158 | 5 | 3 | -5 | 2 | 69 | 69 | 7 |
| 0 | -6 | 8 | 113 | 84 | 6 | 4 | -5 | 2 | 168 | 138 | 4 |
| 1 | -6 | 8 | 149 | 203 | 5 | 6 | -5 | 2 | 213 | 210 | 3 |
| 2 | -6 | 8 | 270 | 245 | 4 | 7 | -5 | 2 | 125 | 107 | 4 |
| 7 | -6 | 8 | 153 | 147 | 5 | 8 | -5 | 2 | 232 | 199 | 3 |
| -7 | -6 | 9 | 82 | 86 | 7 | 9 | -5 | 2 | 146 | 195 | 4 |
| -1 | -6 | 9 | 219 | 205 | 4 | 11 | -5 | 2 | 142 | 159 | 4 |
| 0 | -6 | 9 | 244 | 295 | 4 | -15 | -5 | 3 | 160 | 186 | 4 |
| 3 | -6 | 9 | 118 | 93 | 6 | -13 | -5 | 3 | 146 | 131 | 4 |
| 5 | -6 | 9 | 99 | 141 | 7 | -12 | -5 | 3 | 125 | 129 | 5 |
| -3 | -6 | 10 | 148 | 118 | 5 | -10 | -5 | 3 | 346 | 362 | 3 |
| -1 | -6 | 10 | 116 | 118 | 6 | -9 | -5 | 3 | 143 | 190 | 4 |
| 0 | -6 | 10 | 83 | 78 | 8 | -8 | -5 | 3 | 267 | 280 | 3 |
| 3 | -5 | 0 | 217 | 252 | 3 | -7 | -5 | 3 | 243 | 277 | 3 |
| 9 | -5 | 0 | 154 | 132 | 4 | -6 | -5 | 3 | 84 | 13 | 6 |
| -13 | -5 | 1 | 117 | 108 | 5 | -2 | -5 | 3 | 672 | 680 | 3 |
| -12 | -5 | 1 | 125 | 136 | 5 | -1 | -5 | 3 | 398 | 338 | 3 |
| -11 | -5 | 1 | 243 | 255 | 3 | 0 | -5 | 3 | 67 | 18 | 7 |
| -10 | -5 | 1 | 263 | 300 | 3 | 2 | -5 | 3 | 455 | 450 | 3 |
| -9 | -5 | 1 | 174 | 96 | 4 | 3 | -5 | 3 | 347 | 389 | 3 |
| -8 | -5 | 1 | 136 | 111 | 4 | 4 | -5 | 3 | 188 | 238 | 4 |
| -6 | -5 | 1 | 236 | 280 | 3 | 5 | -5 | 3 | 289 | 225 | 3 |
| -5 | -5 | 1 | 213 | 187 | 3 | 7 | -5 | 3 | 199 | 228 | 4 |
| -4 | -5 | 1 | 322 | 271 | 3 | 8 | -5 | 3 | 117 | 140 | 5 |
| -3 | -5 | 1 | 147 | 149 | 4 | 10 | -5 | 3 | 255 | 245 | 3 |
| -1 | -5 | 1 | 284 | 139 | 3 | 12 | -5 | 3 | 101 | 68 | 5 |

Values of 10*Fobs and 10*Fcalc

| h | k | l | Fobs | Fcalc | Í(F) | h | k | l | Fobs | Fcalc | Í(F) |
|---|---|---|------|-------|------|---|---|---|------|-------|------|
| 13 | -5 | 3 | 111 | 92 | 5 | 4 | -5 | 6 | 133 | 90 | 4 |
| -12 | -5 | 4 | 141 | 151 | 4 | 5 | -5 | 6 | 138 | 120 | 4 |
| -7 | -5 | 4 | 73 | 61 | 6 | 6 | -5 | 6 | 131 | 109 | 4 |
| -6 | -5 | 4 | 130 | 128 | 4 | 7 | -5 | 6 | 126 | 114 | 5 |
| -3 | -5 | 4 | 130 | 185 | 4 | 9 | -5 | 6 | 83 | 86 | 6 |
| -1 | -5 | 4 | 106 | 91 | 5 | 10 | -5 | 6 | 99 | 96 | 6 |
| 0 | -5 | 4 | 121 | 131 | 5 | -12 | -5 | 7 | 123 | 143 | 5 |
| 1 | -5 | 4 | 174 | 133 | 4 | -11 | -5 | 7 | 115 | 124 | 5 |
| 2 | -5 | 4 | 298 | 260 | 3 | -10 | -5 | 7 | 102 | 105 | 5 |
| 3 | -5 | 4 | 345 | 305 | 3 | -9 | -5 | 7 | 259 | 274 | 3 |
| 4 | -5 | 4 | 90 | 154 | 6 | -7 | -5 | 7 | 178 | 204 | 4 |
| 5 | -5 | 4 | 83 | 105 | 6 | -6 | -5 | 7 | 162 | 151 | 4 |
| 6 | -5 | 4 | 140 | 210 | 4 | -4 | -5 | 7 | 191 | 205 | 4 |
| 7 | -5 | 4 | 184 | 258 | 4 | -1 | -5 | 7 | 398 | 377 | 3 |
| 9 | -5 | 4 | 123 | 77 | 4 | 0 | -5 | 7 | 344 | 383 | 3 |
| 10 | -5 | 4 | 99 | 80 | 5 | 1 | -5 | 7 | 268 | 333 | 3 |
| 12 | -5 | 4 | 146 | 134 | 4 | 2 | -5 | 7 | 214 | 199 | 4 |
| -15 | -5 | 5 | 168 | 163 | 4 | 3 | -5 | 7 | 95 | 82 | 6 |
| -13 | -5 | 5 | 70 | 115 | 8 | 4 | -5 | 7 | 65 | 35 | 8 |
| -12 | -5 | 5 | 271 | 313 | 3 | 6 | -5 | 7 | 262 | 283 | 3 |
| -10 | -5 | 5 | 82 | 60 | 7 | 7 | -5 | 7 | 139 | 154 | 5 |
| -9 | -5 | 5 | 204 | 147 | 4 | 8 | -5 | 7 | 68 | 87 | 8 |
| -8 | -5 | 5 | 243 | 267 | 3 | 11 | -5 | 7 | 229 | 254 | 4 |
| -7 | -5 | 5 | 286 | 313 | 3 | -7 | -5 | 8 | 170 | 114 | 4 |
| -6 | -5 | 5 | 170 | 185 | 4 | -6 | -5 | 8 | 112 | 95 | 5 |
| -5 | -5 | 5 | 186 | 196 | 3 | -4 | -5 | 8 | 92 | 95 | 5 |
| -4 | -5 | 5 | 246 | 186 | 3 | -2 | -5 | 8 | 84 | 136 | 6 |
| -3 | -5 | 5 | 307 | 365 | 3 | -1 | -5 | 8 | 103 | 65 | 5 |
| -2 | -5 | 5 | 359 | 408 | 3 | 0 | -5 | 8 | 139 | 157 | 5 |
| -1 | -5 | 5 | 223 | 214 | 3 | 4 | -5 | 8 | 106 | 149 | 6 |
| 0 | -5 | 5 | 249 | 204 | 3 | 5 | -5 | 8 | 148 | 111 | 4 |
| 2 | -5 | 5 | 234 | 238 | 3 | 11 | -5 | 8 | 85 | 53 | 7 |
| 3 | -5 | 5 | 579 | 562 | 3 | -11 | -5 | 9 | 119 | 119 | 5 |
| 4 | -5 | 5 | 99 | 93 | 6 | -8 | -5 | 9 | 204 | 229 | 4 |
| 5 | -5 | 5 | 274 | 307 | 3 | -5 | -5 | 9 | 67 | 57 | 7 |
| 6 | -5 | 5 | 279 | 315 | 3 | -4 | -5 | 9 | 134 | 177 | 5 |
| 8 | -5 | 5 | 157 | 143 | 4 | -3 | -5 | 9 | 277 | 320 | 3 |
| | | | | | | | | | | | |
| -13 | -5 | 6 | 83 | 112 | 7 | 4 | -5 | 9 | 218 | 236 | 4 |
| -10 | -5 | 6 | 96 | 74 | 5 | 6 | -5 | 9 | 115 | 139 | 5 |
| -7 | -5 | 6 | 145 | 118 | 4 | 7 | -5 | 9 | 143 | 145 | 5 |
| -6 | -5 | 6 | 173 | 182 | 4 | -6 | -5 | 10 | 160 | 160 | 4 |
| -5 | -5 | 6 | 72 | 57 | 6 | 1 | -5 | 10 | 121 | 200 | 5 |
| -3 | -5 | 6 | 222 | 160 | 3 | 2 | -5 | 10 | 191 | 151 | 4 |
| -2 | -5 | 6 | 284 | 222 | 3 | 3 | -5 | 10 | 100 | 157 | 6 |
| 0 | -5 | 6 | 128 | 107 | 5 | 6 | -5 | 10 | 98 | 73 | 6 |
| 1 | -5 | 6 | 435 | 482 | 3 | 7 | -5 | 10 | 88 | 49 | 7 |
| 2 | -5 | 6 | 105 | 26 | 5 | -7 | -5 | 11 | 124 | 166 | 5 |
| 3 | -5 | 6 | 117 | 177 | 5 | -3 | -5 | 11 | 97 | 95 | 6 |

Values of 10*Fobs and 10*Fcalc

| h | k | l | Fobs | Fcalc | Í(F) | h | k | l | Fobs | Fcalc | Í(F) |
|---|---|---|------|-------|------|---|---|---|------|-------|------|
| -1 | -5 | 11 | 145 | 168 | 5 | 0 | -4 | 2 | 138 | 134 | 3 |
| 0 | -5 | 11 | 226 | 273 | 4 | 1 | -4 | 2 | 164 | 147 | 3 |
| 1 | -4 | 0 | 219 | 157 | 2 | 3 | -4 | 2 | 211 | 142 | 3 |
| 2 | -4 | 0 | 283 | 258 | 2 | 4 | -4 | 2 | 101 | 165 | 4 |
| 3 | -4 | 0 | 237 | 195 | 2 | 5 | -4 | 2 | 79 | 51 | 5 |
| 4 | -4 | 0 | 136 | 124 | 3 | 6 | -4 | 2 | 155 | 129 | 3 |
| 5 | -4 | 0 | 140 | 120 | 3 | 8 | -4 | 2 | 115 | 76 | 4 |
| 6 | -4 | 0 | 203 | 207 | 3 | 11 | -4 | 2 | 448 | 463 | 3 |
| 8 | -4 | 0 | 77 | 39 | 5 | 12 | -4 | 2 | 138 | 152 | 4 |
| 9 | -4 | 0 | 125 | 83 | 4 | 13 | -4 | 2 | 154 | 144 | 4 |
| 10 | -4 | 0 | 84 | 72 | 5 | 14 | -4 | 2 | 92 | 112 | 5 |
| 13 | -4 | 0 | 221 | 180 | 3 | 15 | -4 | 2 | 114 | 101 | 5 |
| 14 | -4 | 0 | 79 | 129 | 6 | -17 | -4 | 3 | 177 | 150 | 4 |
| 16 | -4 | 0 | 155 | 173 | 4 | -16 | -4 | 3 | 240 | 234 | 4 |
| 17 | -4 | 0 | 131 | 124 | 5 | -15 | -4 | 3 | 71 | 64 | 7 |
| -17 | -4 | 1 | 167 | 178 | 4 | -14 | -4 | 3 | 71 | 49 | 7 |
| -15 | -4 | 1 | 216 | 183 | 4 | -12 | -4 | 3 | 147 | 190 | 4 |
| -14 | -4 | 1 | 106 | 83 | 5 | -11 | -4 | 3 | 572 | 565 | 3 |
| -12 | -4 | 1 | 447 | 419 | 3 | -10 | -4 | 3 | 71 | 108 | 6 |
| -10 | -4 | 1 | 106 | 94 | 4 | -9 | -4 | 3 | 264 | 194 | 3 |
| -9 | -4 | 1 | 133 | 69 | 4 | -8 | -4 | 3 | 109 | 56 | 4 |
| -8 | -4 | 1 | 328 | 321 | 3 | -7 | -4 | 3 | 362 | 355 | 3 |
| -7 | -4 | 1 | 505 | 477 | 2 | -6 | -4 | 3 | 172 | 195 | 3 |
| -6 | -4 | 1 | 327 | 361 | 2 | -5 | -4 | 3 | 87 | 102 | 4 |
| -5 | -4 | 1 | 123 | 159 | 3 | -4 | -4 | 3 | 207 | 195 | 3 |
| -4 | -4 | 1 | 379 | 245 | 2 | -3 | -4 | 3 | 94 | 52 | 4 |
| -3 | -4 | 1 | 295 | 293 | 2 | -2 | -4 | 3 | 365 | 354 | 2 |
| -2 | -4 | 1 | 320 | 381 | 2 | -1 | -4 | 3 | 395 | 333 | 2 |
| -1 | -4 | 1 | 177 | 201 | 3 | 0 | -4 | 3 | 85 | 43 | 5 |
| 0 | -4 | 1 | 178 | 90 | 3 | 1 | -4 | 3 | 414 | 344 | 2 |
| 2 | -4 | 1 | 403 | 328 | 2 | 2 | -4 | 3 | 174 | 172 | 3 |
| 3 | -4 | 1 | 557 | 505 | 2 | 3 | -4 | 3 | 182 | 186 | 3 |
| 4 | -4 | 1 | 87 | 137 | 4 | 4 | -4 | 3 | 393 | 326 | 2 |
| 5 | -4 | 1 | 216 | 172 | 3 | 5 | -4 | 3 | 461 | 433 | 2 |
| 8 | -4 | 1 | 361 | 317 | 3 | 6 | -4 | 3 | 499 | 512 | 2 |
| 10 | -4 | 1 | 366 | 330 | 3 | 7 | -4 | 3 | 463 | 473 | 3 |
| 11 | -4 | 1 | 441 | 405 | 3 | 9 | -4 | 3 | 163 | 112 | 3 |
| -14 | -4 | 2 | 99 | 99 | 5 | 13 | -4 | 3 | 142 | 139 | 4 |
| -13 | -4 | 2 | 133 | 119 | 4 | 14 | -4 | 3 | 65 | 104 | 7 |
| -12 | -4 | 2 | 236 | 245 | 3 | 16 | -4 | 3 | 145 | 134 | 5 |
| -11 | -4 | 2 | 154 | 173 | 4 | 17 | -4 | 3 | 92 | 86 | 6 |
| -10 | -4 | 2 | 316 | 274 | 3 | -14 | -4 | 4 | 130 | 151 | 5 |
| -9 | -4 | 2 | 144 | 123 | 4 | -12 | -4 | 4 | 115 | 68 | 5 |
| -8 | -4 | 2 | 228 | 218 | 3 | -8 | -4 | 4 | 95 | 58 | 4 |
| -7 | -4 | 2 | 165 | 131 | 3 | -4 | -4 | 4 | 56 | 49 | 6 |
| -6 | -4 | 2 | 180 | 174 | 3 | -3 | -4 | 4 | 115 | 102 | 4 |
| -2 | -4 | 2 | 200 | 141 | 3 | -2 | -4 | 4 | 70 | 22 | 5 |
| -1 | -4 | 2 | 141 | 115 | 3 | -1 | -4 | 4 | 154 | 91 | 3 |

Values of 10*Fobs and 10*Fcalc

| h | k | l | Fobs | Fcalc | Í(F) | h | k | l | Fobs | Fcalc | Í(F) |
|---|---|---|------|-------|------|---|---|---|------|-------|------|
| 0 | -4 | 4 | 128 | 151 | 4 | 12 | -4 | 6 | 232 | 192 | 4 |
| 1 | -4 | 4 | 126 | 67 | 4 | 13 | -4 | 6 | 131 | 198 | 5 |
| 4 | -4 | 4 | 97 | 132 | 5 | 14 | -4 | 6 | 129 | 125 | 5 |
| 7 | -4 | 4 | 69 | 66 | 6 | -15 | -4 | 7 | 136 | 120 | 5 |
| 8 | -4 | 4 | 66 | 15 | 6 | -13 | -4 | 7 | 107 | 119 | 5 |
| 13 | -4 | 4 | 127 | 105 | 4 | -11 | -4 | 7 | 100 | 80 | 5 |
| 15 | -4 | 4 | 133 | 132 | 5 | -10 | -4 | 7 | 189 | 165 | 4 |
| -16 | -4 | 5 | 254 | 274 | 4 | -8 | -4 | 7 | 351 | 372 | 3 |
| -15 | -4 | 5 | 146 | 152 | 4 | -7 | -4 | 7 | 222 | 234 | 3 |
| -14 | -4 | 5 | 79 | 55 | 6 | -6 | -4 | 7 | 138 | 138 | 4 |
| -13 | -4 | 5 | 108 | 64 | 5 | -4 | -4 | 7 | 152 | 182 | 4 |
| -12 | -4 | 5 | 106 | 101 | 5 | -3 | -4 | 7 | 447 | 492 | 3 |
| -11 | -4 | 5 | 317 | 302 | 3 | -2 | -4 | 7 | 436 | 464 | 3 |
| -9 | -4 | 5 | 148 | 170 | 4 | 0 | -4 | 7 | 254 | 214 | 3 |
| -8 | -4 | 5 | 257 | 226 | 3 | 2 | -4 | 7 | 153 | 174 | 4 |
| -7 | -4 | 5 | 96 | 124 | 5 | 3 | -4 | 7 | 167 | 190 | 4 |
| -6 | -4 | 5 | 194 | 185 | 3 | 5 | -4 | 7 | 304 | 300 | 3 |
| -4 | -4 | 5 | 167 | 192 | 3 | 7 | -4 | 7 | 76 | 100 | 6 |
| -3 | -4 | 5 | 560 | 501 | 2 | 8 | -4 | 7 | 74 | 95 | 6 |
| -1 | -4 | 5 | 282 | 278 | 3 | 9 | -4 | 7 | 130 | 130 | 4 |
| 1 | -4 | 5 | 617 | 648 | 2 | 10 | -4 | 7 | 191 | 157 | 4 |
| 2 | -4 | 5 | 646 | 650 | 2 | 13 | -4 | 7 | 89 | 119 | 7 |
| 3 | -4 | 5 | 350 | 392 | 3 | 14 | -4 | 7 | 268 | 297 | 4 |
| 4 | -4 | 5 | 235 | 152 | 3 | -13 | -4 | 8 | 77 | 77 | 6 |
| 5 | -4 | 5 | 108 | 124 | 5 | -11 | -4 | 8 | 91 | 80 | 6 |
| 6 | -4 | 5 | 182 | 176 | 3 | -10 | -4 | 8 | 125 | 97 | 5 |
| 7 | -4 | 5 | 168 | 170 | 3 | -9 | -4 | 8 | 74 | 25 | 6 |
| 8 | -4 | 5 | 196 | 194 | 3 | -8 | -4 | 8 | 156 | 148 | 4 |
| 9 | -4 | 5 | 135 | 130 | 4 | -7 | -4 | 8 | 194 | 206 | 4 |
| 11 | -4 | 5 | 99 | 96 | 5 | -6 | -4 | 8 | 157 | 175 | 4 |
| 12 | -4 | 5 | 315 | 312 | 3 | -4 | -4 | 8 | 93 | 148 | 5 |
| 13 | -4 | 5 | 169 | 156 | 4 | -3 | -4 | 8 | 145 | 183 | 4 |
| -12 | -4 | 6 | 92 | 67 | 5 | -1 | -4 | 8 | 120 | 110 | 4 |
| -11 | -4 | 6 | 195 | 230 | 4 | 1 | -4 | 8 | 143 | 73 | 4 |
| -10 | -4 | 6 | 220 | 216 | 3 | 2 | -4 | 8 | 94 | 17 | 5 |
| -9 | -4 | 6 | 96 | 73 | 5 | 3 | -4 | 8 | 114 | 72 | 5 |
| -8 | -4 | 6 | 80 | 27 | 5 | 4 | -4 | 8 | 93 | 54 | 5 |
| -3 | -4 | 6 | 67 | 66 | 6 | -13 | -4 | 9 | 104 | 126 | 5 |
| -2 | -4 | 6 | 237 | 277 | 3 | -12 | -4 | 9 | 146 | 154 | 4 |
| -1 | -4 | 6 | 196 | 228 | 3 | -11 | -4 | 9 | 182 | 214 | 4 |
| 0 | -4 | 6 | 80 | 90 | 6 | -10 | -4 | 9 | 114 | 103 | 5 |
| 1 | -4 | 6 | 115 | 145 | 4 | -8 | -4 | 9 | 122 | 154 | 5 |
| 3 | -4 | 6 | 85 | 34 | 5 | -7 | -4 | 9 | 298 | 332 | 3 |
| 5 | -4 | 6 | 231 | 186 | 3 | -6 | -4 | 9 | 103 | 95 | 5 |
| 8 | -4 | 6 | 111 | 63 | 4 | -4 | -4 | 9 | 128 | 116 | 4 |
| 9 | -4 | 6 | 142 | 97 | 4 | -3 | -4 | 9 | 110 | 85 | 5 |
| 10 | -4 | 6 | 104 | 55 | 5 | -2 | -4 | 9 | 153 | 187 | 4 |
| 11 | -4 | 6 | 144 | 206 | 4 | 0 | -4 | 9 | 178 | 188 | 4 |

Values of 10*Fobs and 10*Fcalc

| h | k | l | Fobs | Fcalc | Í(F) | h | k | l | Fobs | Fcalc | Í(F) |
|---|---|---|------|-------|------|---|---|---|------|-------|------|
| 1 | -4 | 9 | 199 | 251 | 3 | -12 | -3 | 1 | 382 | 366 | 3 |
| 5 | -4 | 9 | 221 | 194 | 4 | -11 | -3 | 1 | 694 | 644 | 3 |
| 6 | -4 | 9 | 120 | 116 | 4 | -10 | -3 | 1 | 181 | 149 | 3 |
| 10 | -4 | 9 | 233 | 261 | 4 | -9 | -3 | 1 | 179 | 160 | 3 |
| 11 | -4 | 9 | 181 | 183 | 4 | -6 | -3 | 1 | 535 | 448 | 2 |
| 12 | -4 | 9 | 104 | 88 | 6 | -5 | -3 | 1 | 502 | 378 | 2 |
| -12 | -4 | 10 | 130 | 125 | 5 | -4 | -3 | 1 | 394 | 281 | 2 |
| -10 | -4 | 10 | 139 | 145 | 5 | -3 | -3 | 1 | 927 | 757 | 3 |
| -9 | -4 | 10 | 144 | 18₄ | 4 | -2 | -3 | 1 | 288 | 190 | 2 |
| -4 | -4 | 10 | 117 | 73 | 5 | -1 | -3 | 1 | 477 | 400 | 2 |
| -3 | -4 | 10 | 116 | 53 | 4 | 1 | -3 | 1 | 547 | 483 | 2 |
| -2 | -4 | 10 | 82 | 39 | 6 | 2 | -3 | 1 | 406 | 319 | 2 |
| 1 | -4 | 10 | 8₂ | ₁46 | 6 | 3 | -3 | 1 | 460 | 428 | 2 |
| 4 | -4 | 10 | 118 | 131 | 5 | 4 | -3 | 1 | 285 | 211 | 2 |
| 5 | -4 | 10 | 89 | 84 | 6 | 5 | -3 | 1 | 370 | 344 | 2 |
| 7 | -4 | 10 | 80 | 62 | 6 | 6 | -3 | 1 | 493 | 440 | 2 |
| -10 | -4 | 11 | 114 | 119 | 5 | 7 | -3 | 1 | 229 | 242 | 2 |
| -9 | -4 | 11 | 149 | 161 | 5 | 8 | -3 | 1 | 136 | 140 | 3 |
| -8 | -4 | 11 | 192 | 199 | 4 | 9 | -3 | 1 | 145 | 126 | 3 |
| -6 | -4 | 11 | 79 | 131 | 6 | 10 | -3 | 1 | 243 | 261 | 3 |
| -4 | -4 | 11 | 168 | 195 | 4 | 11 | -3 | 1 | 387 | 375 | 3 |
| -3 | -4 | 11 | 145 | 190 | 4 | 12 | -3 | 1 | 534 | 505 | 3 |
| -2 | -4 | 11 | 90 | 82 | 5 | 13 | -3 | 1 | 109 | 108 | 5 |
| 1 | -4 | 11 | 182 | 189 | 4 | 14 | -3 | 1 | 205 | 168 | 3 |
| 5 | -4 | 11 | 71 | 77 | 7 | 15 | -3 | 1 | 134 | 145 | 4 |
| 6 | -4 | 11 | 243 | 291 | 4 | 19 | -3 | 1 | 94 | 88 | 6 |
| 1 | -4 | 12 | 89 | 61 | 6 | -19 | -3 | 2 | 92 | 126 | 7 |
| -3 | -4 | 13 | 83 | 96 | 6 | -18 | -3 | 2 | 107 | 116 | 5 |
| -2 | -4 | 13 | 92 | 100 | 6 | -17 | -3 | 2 | 145 | 155 | 4 |
| 1 | -4 | 13 | 92 | 117 | 7 | -16 | -3 | 2 | 106 | 122 | 5 |
| 2 | -4 | 13 | 150 | 219 | 5 | -15 | -3 | 2 | 78 | 75 | 6 |
| 1 | -3 | 0 | 365 | 266 | 2 | -14 | -3 | 2 | 173 | 136 | 4 |
| 2 | -3 | 0 | 758 | 623 | 3 | -13 | -3 | 2 | 276 | 275 | 3 |
| 4 | -3 | 0 | 113 | 86 | 3 | -12 | -3 | 2 | 195 | 198 | 3 |
| 5 | -3 | 0 | 76 | 52 | 4 | -11 | -3 | 2 | 71 | 29 | 6 |
| 6 | -3 | 0 | 65 | 32 | 4 | -10 | -3 | 2 | 217 | 191 | 3 |
| 7 | -3 | 0 | 155 | 158 | 3 | -9 | -3 | 2 | 160 | 132 | 3 |
| 11 | -3 | 0 | 307 | 278 | 3 | -6 | -3 | 2 | 489 | 359 | 2 |
| 13 | -3 | 0 | 316 | 290 | 3 | -5 | -3 | 2 | 306 | 275 | 2 |
| 14 | -3 | 0 | 156 | 160 | 4 | -4 | -3 | 2 | 229 | 200 | 2 |
| 18 | -3 | 0 | 135 | 94 | 4 | -3 | -3 | 2 | 357 | 300 | 2 |
| -19 | -3 | 1 | 158 | 154 | 4 | -2 | -3 | 2 | 176 | 174 | 2 |
| -18 | -3 | 1 | 133 | 116 | 5 | -1 | -3 | 2 | 106 | 130 | 3 |
| -17 | -3 | 1 | 190 | 186 | 4 | 0 | -3 | 2 | 286 | 250 | 2 |
| -16 | -3 | 1 | 286 | 246 | 3 | 2 | -3 | 2 | 82 | 57 | 3 |
| -15 | -3 | 1 | 303 | 295 | 3 | 5 | -3 | 2 | 208 | 193 | 2 |
| -14 | -3 | 1 | 70 | 50 | 6 | 6 | -3 | 2 | 64 | 9 | 5 |
| -13 | -3 | 1 | 289 | 277 | 3 | 7 | -3 | 2 | 385 | 316 | 2 |

Values of 10*Fobs and 10*Fcalc

| h | k | l | Fobs | Fcalc | Í(F) | h | k | l | Fobs | Fcalc | Í(F) |
|---|---|---|------|-------|------|---|---|---|------|-------|------|
| 8 | -3 | 2 | 132 | 84 | 3 | 7 | -3 | 4 | 132 | 145 | 3 |
| 9 | -3 | 2 | 225 | 177 | 3 | 8 | -3 | 4 | 209 | 242 | 3 |
| 10 | -3 | 2 | 121 | 94 | 4 | 10 | -3 | 4 | 215 | 172 | 3 |
| 14 | -3 | 2 | 127 | 69 | 4 | 11 | -3 | 4 | 180 | 193 | 3 |
| 15 | -3 | 2 | 94 | 110 | 5 | 12 | -3 | 4 | 166 | 142 | 4 |
| 18 | -3 | 2 | 98 | 98 | 6 | 13 | -3 | 4 | 175 | 185 | 4 |
| -19 | -3 | 3 | 116 | 125 | 5 | 17 | -3 | 4 | 136 | 113 | 5 |
| -15 | -3 | 3 | 214 | 202 | 3 | 18 | -3 | 4 | 69 | 63 | 7 |
| -14 | -3 | 3 | 75 | 61 | 6 | -18 | -3 | 5 | 82 | 67 | 7 |
| -13 | -3 | 3 | 107 | 61 | 5 | -17 | -3 | 5 | 269 | 259 | 4 |
| -12 | -3 | 3 | 366 | 323 | 3 | -16 | -3 | 5 | 122 | 134 | 5 |
| -11 | -3 | 3 | 146 | 124 | 4 | -14 | -3 | 5 | 129 | 134 | 4 |
| -8 | -3 | 3 | 324 | 303 | 2 | -13 | -3 | 5 | 274 | 250 | 3 |
| -4 | -3 | 3 | 70 | 30 | 4 | -12 | -3 | 5 | 242 | 232 | 3 |
| -3 | -3 | 3 | 772 | 686 | 3 | -11 | -3 | 5 | 598 | 598 | 3 |
| -2 | -3 | 3 | 270 | 234 | 2 | -10 | -3 | 5 | 268 | 236 | 3 |
| -1 | -3 | 3 | 203 | 223 | 2 | -8 | -3 | 5 | 302 | 312 | 3 |
| 0 | -3 | 3 | 136 | 153 | 3 | -7 | -3 | 5 | 250 | 238 | 3 |
| 1 | -3 | 3 | 339 | 325 | 2 | -6 | -3 | 5 | 313 | 281 | 2 |
| 2 | -3 | 3 | 586 | 541 | 2 | -5 | -3 | 5 | 248 | 176 | 2 |
| 3 | -3 | 3 | 546 | 467 | 2 | -4 | -3 | 5 | 608 | 540 | 2 |
| 4 | -3 | 3 | 652 | 488 | 2 | -3 | -3 | 5 | 195 | 104 | 3 |
| 5 | -3 | 3 | 470 | 417 | 2 | -2 | -3 | 5 | 756 | 704 | 3 |
| 7 | -3 | 3 | 540 | 523 | 2 | -1 | -3 | 5 | 106 | 167 | 3 |
| 8 | -3 | 3 | 94 | 116 | 4 | 0 | -3 | 5 | 263 | 188 | 2 |
| 9 | -3 | 3 | 89 | 57 | 4 | 1 | -3 | 5 | 285 | 207 | 2 |
| 10 | -3 | 3 | 399 | 348 | 3 | 2 | -3 | 5 | 163 | 192 | 3 |
| 11 | -3 | 3 | 245 | 225 | 3 | 3 | -3 | 5 | 61 | 31 | 5 |
| 12 | -3 | 3 | 441 | 458 | 3 | 4 | -3 | 5 | 122 | 128 | 3 |
| 13 | -3 | 3 | 363 | 328 | 3 | 5 | -3 | 5 | 456 | 367 | 2 |
| 15 | -3 | 3 | 177 | 140 | 4 | 6 | -3 | 5 | 180 | 156 | 3 |
| -17 | -3 | 4 | 204 | 207 | 4 | 8 | -3 | 5 | 90 | 55 | 4 |
| -16 | -3 | 4 | 93 | 74 | 6 | 9 | -3 | 5 | 99 | 59 | 4 |
| -15 | -3 | 4 | 126 | 116 | 4 | 10 | -3 | 5 | 354 | 327 | 3 |
| -14 | -3 | 4 | 136 | 133 | 4 | 11 | -3 | 5 | 135 | 107 | 4 |
| -12 | -3 | 4 | 191 | 163 | 3 | 13 | -3 | 5 | 168 | 165 | 4 |
| -11 | -3 | 4 | 249 | 257 | 3 | 14 | -3 | 5 | 162 | 164 | 4 |
| -8 | -3 | 4 | 82 | 53 | 4 | -17 | -3 | 6 | 72 | 88 | 7 |
| -6 | -3 | 4 | 94 | 118 | 3 | -15 | -3 | 6 | 108 | 116 | 5 |
| -5 | -3 | 4 | 380 | 359 | 2 | -13 | -3 | 6 | 145 | 131 | 4 |
| -4 | -3 | 4 | 171 | 156 | 2 | -12 | -3 | 6 | 75 | 72 | 6 |
| -3 | -3 | 4 | 262 | 195 | 2 | -11 | -3 | 6 | 88 | 85 | 5 |
| -2 | -3 | 4 | 168 | 115 | 2 | -9 | -3 | 6 | 132 | 110 | 4 |
| 0 | -3 | 4 | 411 | 361 | 2 | -7 | -3 | 6 | 137 | 111 | 3 |
| 1 | -3 | 4 | 309 | 256 | 2 | -6 | -3 | 6 | 307 | 279 | 3 |
| 3 | -3 | 4 | 232 | 112 | 2 | -5 | -3 | 6 | 113 | 98 | 3 |
| 5 | -3 | 4 | 249 | 181 | 2 | -4 | -3 | 6 | 388 | 295 | 2 |
| 6 | -3 | 4 | 134 | 80 | 3 | -3 | -3 | 6 | 57 | 134 | 6 |

| h | k | l | Fobs | Fcalc | Í(F) | h | k | l | Fobs | Fcalc | Í(F) |
|---|---|---|------|-------|------|---|---|---|------|-------|------|
| 0 | -3 | 6 | 114 | 51 | 3 | 9 | -3 | 8 | 181 | 132 | 4 |
| 1 | -3 | 6 | 143 | 72 | 3 | 11 | -3 | 8 | 236 | 309 | 4 |
| 2 | -3 | 6 | 152 | 198 | 3 | 12 | -3 | 8 | 140 | 107 | 5 |
| 3 | -3 | 6 | 237 | 243 | 3 | 14 | -3 | 8 | 189 | 169 | 4 |
| 5 | -3 | 6 | 153 | 138 | 3 | -13 | -3 | 9 | 199 | 206 | 4 |
| 6 | -3 | 6 | 224 | 174 | 3 | -12 | -3 | 9 | 319 | 339 | 3 |
| 7 | -3 | 6 | 205 | 194 | 3 | -11 | -3 | 9 | 148 | 140 | 4 |
| 8 | -3 | 6 | 140 | 143 | 3 | -10 | -3 | 9 | 437 | 452 | 3 |
| 9 | -3 | 6 | 149 | 160 | 3 | -9 | -3 | 9 | 279 | 274 | 3 |
| 12 | -3 | 6 | 145 | 101 | 4 | -8 | -3 | 9 | 429 | 424 | 3 |
| 13 | -3 | 6 | 154 | 156 | 4 | -7 | -3 | 9 | 197 | 177 | 3 |
| 14 | -3 | 6 | 100 | 68 | 6 | -6 | -3 | 9 | 76 | 69 | 5 |
| 15 | -3 | 6 | 122 | 153 | 5 | -5 | -3 | 9 | 76 | 65 | 5 |
| -17 | -3 | 7 | 103 | 103 | 6 | -4 | -3 | 9 | 357 | 367 | 3 |
| -16 | -3 | 7 | 70 | 71 | 7 | -3 | -3 | 9 | 98 | 84 | 4 |
| -15 | -3 | 7 | 77 | 101 | 6 | -2 | -3 | 9 | 350 | 333 | 3 |
| -11 | -3 | 7 | 332 | 337 | 3 | -1 | -3 | 9 | 161 | 170 | 3 |
| -10 | -3 | 7 | 89 | 73 | 5 | 1 | -3 | 9 | 255 | 272 | 3 |
| -7 | -3 | 7 | 357 | 378 | 3 | 2 | -3 | 9 | 340 | 376 | 3 |
| -6 | -3 | 7 | 226 | 261 | 3 | 5 | -3 | 9 | 180 | 158 | 3 |
| -4 | -3 | 7 | 231 | 189 | 3 | 6 | -3 | 9 | 192 | 209 | 4 |
| -3 | -3 | 7 | 615 | 543 | 2 | 7 | -3 | 9 | 161 | 216 | 4 |
| 0 | -3 | 7 | 125 | 110 | 4 | 9 | -3 | 9 | 93 | 50 | 5 |
| 1 | -3 | 7 | 218 | 199 | 3 | 10 | -3 | 9 | 152 | 134 | 4 |
| 2 | -3 | 7 | 227 | 193 | 3 | 14 | -3 | 9 | 204 | 218 | 4 |
| 4 | -3 | 7 | 151 | 153 | 3 | -14 | -3 | 10 | 82 | 81 | 6 |
| 5 | -3 | 7 | 577 | 523 | 3 | -12 | -3 | 10 | 92 | 67 | 6 |
| 6 | -3 | 7 | 92 | 99 | 5 | -11 | -3 | 10 | 118 | 152 | 5 |
| 7 | -3 | 7 | 269 | 277 | 3 | -9 | -3 | 10 | 130 | 136 | 5 |
| 8 | -3 | 7 | 81 | 89 | 5 | -7 | -3 | 10 | 99 | 69 | 4 |
| 11 | -3 | 7 | 200 | 198 | 3 | -4 | -3 | 10 | 187 | 172 | 3 |
| 12 | -3 | 7 | 256 | 288 | 4 | -2 | -3 | 10 | 168 | 146 | 3 |
| 13 | -3 | 7 | 327 | 307 | 3 | 0 | -3 | 10 | 64 | 18 | 7 |
| 14 | -3 | 7 | 121 | 157 | 5 | 2 | -3 | 10 | 94 | 56 | 5 |
| 16 | -3 | 7 | 92 | 98 | 6 | 3 | -3 | 10 | 109 | 107 | 5 |
| -12 | -3 | 8 | 77 | 61 | 6 | 4 | -3 | 10 | 136 | 78 | 4 |
| -10 | -3 | 8 | 348 | 338 | 3 | 7 | -3 | 10 | 117 | 171 | 5 |
| -6 | -3 | 8 | 85 | 124 | 5 | -13 | -3 | 11 | 135 | 163 | 5 |
| -5 | -3 | 8 | 116 | 143 | 4 | -12 | -3 | 11 | 179 | 173 | 4 |
| -4 | -3 | 8 | 86 | 33 | 5 | -11 | -3 | 11 | 174 | 201 | 4 |
| -2 | -3 | 8 | 226 | 241 | 3 | -10 | -3 | 11 | 128 | 136 | 5 |
| 1 | -3 | 8 | 83 | 81 | 5 | -9 | -3 | 11 | 86 | 92 | 6 |
| 2 | -3 | 8 | 79 | 84 | 5 | -8 | -3 | 11 | 130 | 164 | 5 |
| 3 | -3 | 8 | 296 | 268 | 3 | -7 | -3 | 11 | 141 | 166 | 4 |
| 4 | -3 | 8 | 89 | 69 | 5 | -6 | -3 | 11 | 73 | 71 | 6 |
| 5 | -3 | 8 | 89 | 68 | 5 | -5 | -3 | 11 | 78 | 69 | 6 |
| 7 | -3 | 8 | 107 | 104 | 4 | -4 | -3 | 11 | 65 | 85 | 7 |
| 8 | -3 | 8 | 213 | 176 | 3 | -2 | -3 | 11 | 222 | 255 | 3 |

Values of 10*Fobs and 10*Fcalc

| h | k | l | Fobs | Fcalc | Í(F) | h | k | l | Fobs | Fcalc | Í(F) |
|---|---|---|------|-------|------|---|---|---|------|-------|------|
| -1 | -3 | 11 | 140 | 110 | 4 | -10 | -2 | 1 | 149 | 121 | 3 |
| 0 | -3 | 11 | 155 | 148 | 4 | -9 | -2 | 1 | 341 | 317 | 2 |
| 2 | -3 | 11 | 121 | 165 | 4 | -8 | -2 | 1 | 504 | 428 | 2 |
| 3 | -3 | 11 | 90 | 129 | 5 | -7 | -2 | 1 | 321 | 304 | 2 |
| 5 | -3 | 11 | 330 | 322 | 3 | -6 | -2 | 1 | 109 | 104 | 2 |
| 9 | -3 | 11 | 161 | 162 | 4 | -4 | -2 | 1 | 230 | 168 | 2 |
| 10 | -3 | 11 | 148 | 146 | 5 | -3 | -2 | 1 | 573 | 480 | 2 |
| 11 | -3 | 11 | 87 | 77 | 6 | -2 | -2 | 1 | 744 | 642 | 3 |
| -11 | -3 | 12 | 93 | 106 | 7 | -1 | -2 | 1 | 240 | 202 | 2 |
| -10 | -3 | 12 | 165 | 132 | 5 | 0 | -2 | 1 | 116 | 55 | 2 |
| -8 | -3 | 12 | 192 | 194 | 4 | 1 | -2 | 1 | 65 | 29 | 3 |
| -4 | -3 | 12 | 124 | 85 | 5 | 2 | -2 | 1 | 574 | 505 | 2 |
| -1 | -3 | 12 | 82 | 93 | 6 | 3 | -2 | 1 | 593 | 567 | 2 |
| 3 | -3 | 12 | 81 | 116 | 6 | 4 | -2 | 1 | 547 | 400 | 2 |
| 8 | -3 | 12 | 79 | 87 | 7 | 5 | -2 | 1 | 291 | 309 | 2 |
| 9 | -3 | 12 | 73 | 67 | 7 | 6 | -2 | 1 | 195 | 167 | 2 |
| -9 | -3 | 13 | 236 | 284 | 4 | 7 | -2 | 1 | 394 | 349 | 2 |
| -7 | -3 | 13 | 73 | 106 | 7 | 8 | -2 | 1 | 159 | 175 | 2 |
| -4 | -3 | 13 | 113 | 125 | 5 | 10 | -2 | 1 | 525 | 425 | 2 |
| -3 | -3 | 13 | 168 | 220 | 4 | 11 | -2 | 1 | 383 | 334 | 2 |
| -2 | -3 | 13 | 67 | 81 | 7 | 12 | -2 | 1 | 332 | 355 | 3 |
| 0 | -3 | 13 | 166 | 193 | 4 | 13 | -2 | 1 | 286 | 251 | 3 |
| 1 | -3 | 13 | 184 | 185 | 4 | 15 | -2 | 1 | 379 | 346 | 3 |
| 3 | -3 | 13 | 77 | 135 | 7 | 16 | -2 | 1 | 88 | 60 | 5 |
| 4 | -3 | 13 | 140 | 142 | 5 | 18 | -2 | 1 | 150 | 150 | 4 |
| 5 | -3 | 13 | 98 | 112 | 6 | -19 | -2 | 2 | 179 | 165 | 4 |
| 6 | -3 | 13 | 190 | 207 | 4 | -18 | -2 | 2 | 109 | 74 | 5 |
| -5 | -3 | 14 | 75 | 104 | 7 | -16 | -2 | 2 | 96 | 83 | 5 |
| -2 | -3 | 14 | 105 | 166 | 6 | -15 | -2 | 2 | 110 | 98 | 4 |
| 0 | -2 | 0 | 246 | 248 | 2 | -14 | -2 | 2 | 371 | 347 | 3 |
| 1 | -2 | 0 | 1197 | 922 | 4 | -13 | -2 | 2 | 151 | 144 | 4 |
| 2 | -2 | 0 | 358 | 269 | 1 | -11 | -2 | 2 | 216 | 210 | 3 |
| 3 | -2 | 0 | 678 | 637 | 2 | -10 | -2 | 2 | 189 | 133 | 2 |
| 4 | -2 | 0 | 284 | 250 | 2 | -9 | -2 | 2 | 527 | 480 | 2 |
| 5 | -2 | 0 | 496 | 374 | 2 | -8 | -2 | 2 | 614 | 517 | 2 |
| 7 | -2 | 0 | 102 | 107 | 3 | -7 | -2 | 2 | 250 | 201 | 2 |
| 8 | -2 | 0 | 49 | 7 | 4 | -6 | -2 | 2 | 98 | 91 | 3 |
| 11 | -2 | 0 | 133 | 122 | 3 | -3 | -2 | 2 | 154 | 156 | 2 |
| 13 | -2 | 0 | 405 | 410 | 3 | -2 | -2 | 2 | 103 | 91 | 2 |
| 14 | -2 | 0 | 402 | 379 | 3 | -1 | -2 | 2 | 360 | 306 | 2 |
| 17 | -2 | 0 | 76 | 89 | 6 | 0 | -2 | 2 | 267 | 218 | 2 |
| 18 | -2 | 0 | 178 | 169 | 4 | 1 | -2 | 2 | 520 | 427 | 2 |
| -20 | -2 | 1 | 130 | 101 | 5 | 2 | -2 | 2 | 217 | 219 | 2 |
| -19 | -2 | 1 | 212 | 201 | 4 | 4 | -2 | 2 | 214 | 143 | 2 |
| -16 | -2 | 1 | 66 | 47 | 6 | 5 | -2 | 2 | 62 | 58 | 4 |
| -14 | -2 | 1 | 138 | 102 | 4 | 6 | -2 | 2 | 490 | 375 | 2 |
| -12 | -2 | 1 | 279 | 209 | 3 | 7 | -2 | 2 | 310 | 273 | 2 |
| -11 | -2 | 1 | 104 | 101 | 4 | 8 | -2 | 2 | 540 | 480 | 2 |

Values of 10*Fobs and 10*Fcalc

| h | k | l | Fobs | Fcalc | Í(F) | h | k | l | Fobs | Fcalc | Í(F) |
|---|---|---|------|-------|------|---|---|---|------|-------|------|
| 9 | -2 | 2 | 304 | 281 | 2 | 1 | -2 | 4 | 63 | 100 | 4 |
| 12 | -2 | 2 | 264 | 250 | 3 | 2 | -2 | 4 | 478 | 326 | 2 |
| 14 | -2 | 2 | 340 | 308 | 3 | 3 | -2 | 4 | 1018 | 891 | 4 |
| 17 | -2 | 2 | 149 | 100 | 4 | 4 | -2 | 4 | 585 | 449 | 2 |
| 18 | -2 | 2 | 192 | 167 | 4 | 5 | -2 | 4 | 643 | 506 | 2 |
| -15 | -2 | 3 | 180 | 179 | 3 | 6 | -2 | 4 | 53 | 47 | 5 |
| -13 | -2 | 3 | 477 | 435 | 3 | 7 | -2 | 4 | 98 | 52 | 3 |
| -11 | -2 | 3 | 476 | 469 | 2 | 8 | -2 | 4 | 160 | 121 | 3 |
| -10 | -2 | 3 | 66 | 39 | 4 | 9 | -2 | 4 | 228 | 192 | 2 |
| -9 | -2 | 3 | 267 | 188 | 2 | 10 | -2 | 4 | 232 | 197 | 3 |
| -8 | -2 | 3 | 91 | 71 | 3 | 11 | -2 | 4 | 133 | 153 | 3 |
| -7 | -2 | 3 | 91 | 100 | 3 | 12 | -2 | 4 | 183 | 157 | 3 |
| -6 | -2 | 3 | 335 | 305 | 2 | 14 | -2 | 4 | 487 | 466 | 3 |
| -5 | -2 | 3 | 61 | 50 | 4 | 15 | -2 | 4 | 154 | 180 | 4 |
| -4 | -2 | 3 | 821 | 720 | 3 | -19 | -2 | 5 | 72 | 92 | 7 |
| -3 | -2 | 3 | 190 | 134 | 2 | -17 | -2 | 5 | 128 | 105 | 4 |
| -2 | -2 | 3 | 118 | 118 | 2 | -16 | -2 | 5 | 172 | 176 | 4 |
| -1 | -2 | 3 | 137 | 85 | 2 | -13 | -2 | 5 | 171 | 163 | 4 |
| 0 | -2 | 3 | 549 | 404 | 2 | -12 | -2 | 5 | 297 | 261 | 3 |
| 1 | -2 | 3 | 87 | 78 | 3 | -11 | -2 | 5 | 176 | 145 | 3 |
| 2 | -2 | 3 | 368 | 277 | 2 | -10 | -2 | 5 | 323 | 317 | 3 |
| 3 | -2 | 3 | 272 | 279 | 2 | -9 | -2 | 5 | 50 | 65 | 6 |
| 4 | -2 | 3 | 187 | 132 | 2 | -8 | -2 | 5 | 62 | 71 | 5 |
| 5 | -2 | 3 | 888 | 684 | 3 | -7 | -2 | 5 | 92 | 89 | 3 |
| 6 | -2 | 3 | 541 | 436 | 2 | -6 | -2 | 5 | 282 | 233 | 2 |
| 7 | -2 | 3 | 95 | 55 | 3 | -5 | -2 | 5 | 241 | 168 | 2 |
| 8 | -2 | 3 | 67 | 18 | 4 | -4 | -2 | 5 | 223 | 168 | 2 |
| 9 | -2 | 3 | 178 | 170 | 3 | -3 | -2 | 5 | 139 | 106 | 2 |
| 10 | -2 | 3 | 223 | 197 | 3 | -2 | -2 | 5 | 68 | 73 | 3 |
| 11 | -2 | 3 | 368 | 342 | 3 | -1 | -2 | 5 | 228 | 148 | 2 |
| 13 | -2 | 3 | 274 | 243 | 3 | 0 | -2 | 5 | 576 | 416 | 2 |
| 15 | -2 | 3 | 308 | 306 | 3 | 1 | -2 | 5 | 494 | 382 | 2 |
| 16 | -2 | 3 | 82 | 96 | 6 | 2 | -2 | 5 | 485 | 383 | 2 |
| 18 | -2 | 3 | 127 | 141 | 5 | 3 | -2 | 5 | 172 | 152 | 2 |
| 19 | -2 | 3 | 120 | 123 | 5 | 5 | -2 | 5 | 568 | 530 | 2 |
| -19 | -2 | 4 | 133 | 137 | 5 | 6 | -2 | 5 | 120 | 89 | 3 |
| -18 | -2 | 4 | 111 | 111 | 5 | 7 | -2 | 5 | 63 | 91 | 4 |
| -15 | -2 | 4 | 78 | 67 | 5 | 11 | -2 | 5 | 253 | 268 | 3 |
| -13 | -2 | 4 | 681 | 642 | 3 | 12 | -2 | 5 | 200 | 231 | 3 |
| -11 | -2 | 4 | 193 | 152 | 3 | 13 | -2 | 5 | 450 | 416 | 3 |
| -9 | -2 | 4 | 403 | 367 | 2 | 15 | -2 | 5 | 124 | 96 | 5 |
| -7 | -2 | 4 | 142 | 138 | 2 | 16 | -2 | 5 | 163 | 197 | 4 |
| -6 | -2 | 4 | 287 | 270 | 2 | -18 | -2 | 6 | 164 | 172 | 4 |
| -5 | -2 | 4 | 130 | 100 | 2 | -17 | -2 | 6 | 180 | 164 | 4 |
| -4 | -2 | 4 | 260 | 187 | 2 | -16 | -2 | 6 | 97 | 74 | 5 |
| -2 | -2 | 4 | 236 | 205 | 2 | -15 | -2 | 6 | 80 | 63 | 6 |
| -1 | -2 | 4 | 762 | 659 | 3 | -13 | -2 | 6 | 222 | 208 | 3 |
| 0 | -2 | 4 | 464 | 292 | 2 | -12 | -2 | 6 | 187 | 190 | 3 |

Values of 10*Fobs and 10*Fcalc

| h | k | l | Fobs | Fcalc | Í(F) | h | k | l | Fobs | Fcalc | Í(F) |
|---|---|---|------|-------|------|---|---|---|------|-------|------|
| -11 | -2 | 6 | 103 | 87 | 4 | 17 | -2 | 7 | 113 | 125 | 5 |
| -10 | -2 | 6 | 157 | 158 | 3 | -16 | -2 | 8 | 73 | 59 | 7 |
| -8 | -2 | 6 | 72 | 50 | 5 | -15 | -2 | 8 | 101 | 110 | 5 |
| -6 | -2 | 6 | 314 | 302 | 2 | -13 | -2 | 8 | 227 | 243 | 3 |
| -5 | -2 | 6 | 434 | 375 | 2 | -12 | -2 | 8 | 171 | 174 | 4 |
| -4 | -2 | 6 | 221 | 138 | 2 | -11 | -2 | 8 | 218 | 226 | 3 |
| -3 | -2 | 6 | 124 | 69 | 3 | -10 | -2 | 8 | 204 | 219 | 3 |
| -2 | -2 | 6 | 334 | 302 | 2 | -9 | -2 | 8 | 239 | 245 | 3 |
| -1 | -2 | 6 | 503 | 412 | 2 | -8 | -2 | 8 | 129 | 127 | 4 |
| 0 | -2 | 6 | 758 | 610 | 3 | -6 | -2 | 8 | 153 | 129 | 3 |
| 1 | -2 | 6 | 320 | 249 | 2 | -5 | -2 | 8 | 341 | 302 | 3 |
| 2 | -2 | 6 | 240 | 232 | 2 | -4 | -2 | 8 | 259 | 197 | 3 |
| 3 | -2 | 6 | 189 | 154 | 2 | -2 | -2 | 8 | 75 | 63 | 4 |
| 4 | -2 | 6 | 270 | 236 | 2 | -1 | -2 | 8 | 107 | 135 | 3 |
| 5 | -2 | 6 | 66 | 27 | 4 | 0 | -2 | 8 | 447 | 378 | 2 |
| 6 | -2 | 6 | 244 | 173 | 2 | 2 | -2 | 8 | 83 | 52 | 4 |
| 7 | -2 | 6 | 201 | 223 | 3 | 3 | -2 | 8 | 294 | 314 | 3 |
| 8 | -2 | 6 | 127 | 79 | 3 | 4 | -2 | 8 | 274 | 255 | 3 |
| 9 | -2 | 6 | 303 | 254 | 3 | 7 | -2 | 8 | 321 | 321 | 3 |
| 10 | -2 | 6 | 216 | 187 | 3 | 8 | -2 | 8 | 141 | 157 | 4 |
| 11 | -2 | 6 | 103 | 115 | 5 | 12 | -2 | 8 | 295 | 302 | 3 |
| 12 | -2 | 6 | 200 | 236 | 3 | 13 | -2 | 8 | 96 | 30 | 5 |
| 13 | -2 | 6 | 86 | 90 | 5 | 14 | -2 | 8 | 160 | 163 | 4 |
| 15 | -2 | 6 | 84 | 84 | 6 | 15 | -2 | 8 | 240 | 311 | 4 |
| 16 | -2 | 6 | 194 | 200 | 4 | 16 | -2 | 8 | 102 | 95 | 6 |
| 17 | -2 | 6 | 183 | 159 | 4 | -15 | -2 | 9 | 117 | 106 | 5 |
| -18 | -2 | 7 | 174 | 171 | 4 | -12 | -2 | 9 | 137 | 128 | 4 |
| -17 | -2 | 7 | 148 | 140 | 4 | -11 | -2 | 9 | 314 | 311 | 3 |
| -14 | -2 | 7 | 180 | 194 | 4 | -9 | -2 | 9 | 76 | 43 | 5 |
| -13 | -2 | 7 | 247 | 230 | 3 | -8 | -2 | 9 | 180 | 193 | 3 |
| -12 | -2 | 7 | 70 | 77 | 6 | -7 | -2 | 9 | 195 | 181 | 3 |
| -11 | -2 | 7 | 369 | 375 | 3 | -5 | -2 | 9 | 138 | 112 | 3 |
| -10 | -2 | 7 | 246 | 265 | 3 | -3 | -2 | 9 | 117 | 50 | 4 |
| -8 | -2 | 7 | 231 | 207 | 3 | -2 | -2 | 9 | 196 | 203 | 3 |
| -7 | -2 | 7 | 222 | 223 | 3 | 0 | -2 | 9 | 309 | 270 | 3 |
| -6 | -2 | 7 | 252 | 236 | 2 | 1 | -2 | 9 | 284 | 220 | 3 |
| -4 | -2 | 7 | 395 | 384 | 2 | 3 | -2 | 9 | 140 | 212 | 4 |
| 0 | -2 | 7 | 137 | 95 | 3 | 7 | -2 | 9 | 186 | 177 | 3 |
| 5 | -2 | 7 | 149 | 74 | 3 | 10 | -2 | 9 | 119 | 110 | 5 |
| 6 | -2 | 7 | 87 | 115 | 4 | 11 | -2 | 9 | 201 | 216 | 4 |
| 7 | -2 | 7 | 67 | 129 | 5 | 12 | -2 | 9 | 82 | 78 | 6 |
| 8 | -2 | 7 | 107 | 43 | 4 | 13 | -2 | 9 | 162 | 181 | 4 |
| 9 | -2 | 7 | 171 | 137 | 3 | 14 | -2 | 9 | 196 | 195 | 4 |
| 10 | -2 | 7 | 147 | 112 | 4 | -14 | -2 | 10 | 169 | 176 | 4 |
| 11 | -2 | 7 | 132 | 117 | 4 | -13 | -2 | 10 | 113 | 126 | 5 |
| 12 | -2 | 7 | 91 | 131 | 5 | -12 | -2 | 10 | 184 | 202 | 4 |
| 14 | -2 | 7 | 159 | 122 | 4 | -9 | -2 | 10 | 114 | 99 | 5 |
| 15 | -2 | 7 | 170 | 142 | 4 | -8 | -2 | 10 | 132 | 97 | 4 |

Values of 10*Fobs and 10*Fcalc

| h | k | l | Fobs | Fcalc | Í(F) | h | k | l | Fobs | Fcalc | Í(F) |
|---|---|---|------|-------|------|---|---|---|------|-------|------|
| -6 | -2 | 10 | 73 | 112 | 5 | 3 | -2 | 13 | 118 | 93 | 5 |
| -5 | -2 | 10 | 62 | 44 | 6 | 4 | -2 | 13 | 136 | 140 | 5 |
| -4 | -2 | 10 | 239 | 200 | 3 | 5 | -2 | 13 | 69 | 55 | 7 |
| -2 | -2 | 10 | 179 | 188 | 3 | 6 | -2 | 13 | 168 | 228 | 4 |
| -1 | -2 | 10 | 64 | 70 | 6 | -6 | -2 | 14 | 68 | 65 | 8 |
| 0 | -2 | 10 | 146 | 137 | 4 | -5 | -2 | 14 | 79 | 85 | 6 |
| 2 | -2 | 10 | 75 | 106 | 6 | -3 | -2 | 14 | 107 | 145 | 6 |
| 3 | -2 | 10 | 350 | 359 | 3 | -1 | -2 | 14 | 136 | 164 | 5 |
| 4 | -2 | 10 | 109 | 102 | 4 | 0 | -2 | 14 | 69 | 73 | 7 |
| 5 | -2 | 10 | 79 | 100 | 5 | 4 | -2 | 14 | 116 | 121 | 5 |
| 6 | -2 | 10 | 79 | 63 | 5 | 5 | -2 | 14 | 87 | 93 | 6 |
| 8 | -2 | 10 | 239 | 236 | 3 | 1 | -1 | 0 | 754 | 597 | 2 |
| 9 | -2 | 10 | 147 | 106 | 4 | 2 | -1 | 0 | 198 | 194 | 1 |
| 12 | -2 | 10 | 99 | 62 | 6 | 3 | -1 | 0 | 1193 | 976 | 3 |
| 13 | -2 | 10 | 201 | 226 | 4 | 4 | -1 | 0 | 1494 | 1217 | 3 |
| -12 | -2 | 11 | 184 | 179 | 4 | 5 | -1 | 0 | 903 | 695 | 3 |
| -11 | -2 | 11 | 180 | 220 | 4 | 6 | -1 | 0 | 333 | 297 | 2 |
| -10 | -2 | 11 | 80 | 113 | 6 | 7 | -1 | 0 | 296 | 244 | 2 |
| -9 | -2 | 11 | 207 | 187 | 4 | 8 | -1 | 0 | 480 | 405 | 2 |
| -7 | -2 | 11 | 144 | 166 | 4 | 9 | -1 | 0 | 590 | 476 | 2 |
| -5 | -2 | 11 | 219 | 196 | 3 | 10 | -1 | 0 | 359 | 279 | 2 |
| -4 | -2 | 11 | 374 | 365 | 3 | 11 | -1 | 0 | 195 | 154 | 3 |
| -1 | -2 | 11 | 190 | 209 | 3 | 12 | -1 | 0 | 68 | 89 | 5 |
| 1 | -2 | 11 | 274 | 281 | 3 | 13 | -1 | 0 | 265 | 204 | 3 |
| 2 | -2 | 11 | 105 | 104 | 5 | 14 | -1 | 0 | 577 | 469 | 3 |
| 5 | -2 | 11 | 94 | 136 | 5 | 15 | -1 | 0 | 137 | 92 | 4 |
| 6 | -2 | 11 | 207 | 231 | 4 | 18 | -1 | 0 | 192 | 160 | 4 |
| 8 | -2 | 11 | 114 | 127 | 5 | 19 | -1 | 0 | 209 | 176 | 4 |
| 9 | -2 | 11 | 84 | 71 | 6 | -20 | -1 | 1 | 90 | 98 | 6 |
| 11 | -2 | 11 | 92 | 120 | 6 | -19 | -1 | 1 | 90 | 80 | 5 |
| -12 | -2 | 12 | 152 | 160 | 5 | -17 | -1 | 1 | 79 | 80 | 6 |
| -11 | -2 | 12 | 122 | 175 | 5 | -16 | -1 | 1 | 141 | 127 | 4 |
| -9 | -2 | 12 | 80 | 62 | 6 | -15 | -1 | 1 | 100 | 92 | 4 |
| -8 | -2 | 12 | 139 | 156 | 4 | -14 | -1 | 1 | 102 | 67 | 4 |
| -6 | -2 | 12 | 176 | 177 | 4 | -10 | -1 | 1 | 220 | 161 | 2 |
| -5 | -2 | 12 | 164 | 176 | 4 | -9 | -1 | 1 | 215 | 170 | 2 |
| -4 | -2 | 12 | 88 | 80 | 5 | -8 | -1 | 1 | 44 | 4 | 5 |
| 0 | -2 | 12 | 151 | 143 | 4 | -5 | -1 | 1 | 260 | 148 | 2 |
| 1 | -2 | 12 | 128 | 184 | 4 | -4 | -1 | 1 | 1152 | 935 | 4 |
| 4 | -2 | 12 | 252 | 275 | 3 | -3 | -1 | 1 | 315 | 203 | 1 |
| 8 | -2 | 12 | 130 | 129 | 5 | -1 | -1 | 1 | 721 | 584 | 2 |
| 9 | -2 | 12 | 91 | 76 | 6 | 0 | -1 | 1 | 772 | 589 | 2 |
| -9 | -2 | 13 | 164 | 158 | 4 | 1 | -1 | 1 | 74 | 44 | 2 |
| -8 | -2 | 13 | 161 | 188 | 4 | 2 | -1 | 1 | 463 | 375 | 2 |
| -6 | -2 | 13 | 113 | 127 | 5 | 3 | -1 | 1 | 118 | 114 | 2 |
| -4 | -2 | 13 | 82 | 85 | 6 | 4 | -1 | 1 | 111 | 71 | 2 |
| -2 | -2 | 13 | 109 | 129 | 5 | 5 | -1 | 1 | 664 | 575 | 2 |
| 1 | -2 | 13 | 84 | 138 | 7 | 6 | -1 | 1 | 251 | 184 | 2 |

Values of 10*Fobs and 10*Fcalc

| h | k | l | Fobs | Fcalc | Í(F) | h | k | l | Fobs | Fcalc | Í(F) |
|---|---|---|------|-------|------|---|---|---|------|-------|------|
| 7 | -1 | 1 | 211 | 183 | 2 | -13 | -1 | 3 | 214 | 187 | 3 |
| 8 | -1 | 1 | 56 | 41 | 4 | -9 | -1 | 3 | 583 | 395 | 2 |
| 9 | -1 | 1 | 296 | 181 | 2 | -8 | -1 | 3 | 214 | 168 | 2 |
| 11 | -1 | 1 | 400 | 358 | 2 | -7 | -1 | 3 | 72 | 60 | 3 |
| 12 | -1 | 1 | 153 | 155 | 3 | -6 | -1 | 3 | 49 | 50 | 4 |
| 13 | -1 | 1 | 356 | 275 | 3 | -5 | -1 | 3 | 181 | 164 | 2 |
| 14 | -1 | 1 | 201 | 172 | 3 | -4 | -1 | 3 | 261 | 227 | 2 |
| 15 | -1 | 1 | 75 | 114 | 6 | -3 | -1 | 3 | 101 | 58 | 2 |
| 17 | -1 | 1 | 256 | 289 | 3 | -2 | -1 | 3 | 69 | 60 | 2 |
| 20 | -1 | 1 | 86 | 78 | 6 | -1 | -1 | 3 | 102 | 157 | 2 |
| -19 | -1 | 2 | 165 | 120 | 4 | 0 | -1 | 3 | 157 | 170 | 2 |
| -18 | -1 | 2 | 240 | 226 | 3 | 1 | -1 | 3 | 838 | 670 | 3 |
| -16 | -1 | 2 | 64 | 123 | 7 | 2 | -1 | 3 | 224 | 206 | 2 |
| -14 | -1 | 2 | 76 | 33 | 5 | 3 | -1 | 3 | 181 | 154 | 2 |
| -13 | -1 | 2 | 325 | 298 | 3 | 4 | -1 | 3 | 308 | 241 | 2 |
| -11 | -1 | 2 | 179 | 169 | 3 | 5 | -1 | 3 | 344 | 211 | 2 |
| -10 | -1 | 2 | 101 | 68 | 3 | 6 | -1 | 3 | 750 | 614 | 3 |
| -9 | -1 | 2 | 575 | 466 | 2 | 7 | -1 | 3 | 247 | 156 | 2 |
| -8 | -1 | 2 | 1202 | 924 | 4 | 9 | -1 | 3 | 683 | 547 | 2 |
| -7 | -1 | 2 | 205 | 187 | 2 | 10 | -1 | 3 | 235 | 158 | 2 |
| -6 | -1 | 2 | 820 | 613 | 3 | 11 | -1 | 3 | 196 | 202 | 3 |
| -5 | -1 | 2 | 707 | 534 | 3 | 12 | -1 | 3 | 210 | 221 | 3 |
| -4 | -1 | 2 | 476 | 296 | 2 | 14 | -1 | 3 | 94 | 72 | 5 |
| -3 | -1 | 2 | 381 | 266 | 1 | 15 | -1 | 3 | 124 | 112 | 4 |
| -2 | -1 | 2 | 291 | 302 | 1 | 17 | -1 | 3 | 115 | 133 | 5 |
| -1 | -1 | 2 | 654 | 556 | 2 | 18 | -1 | 3 | 81 | 74 | 6 |
| 0 | -1 | 2 | 684 | 2027 | 2 | -19 | -1 | 4 | 76 | 74 | 6 |
| 1 | -1 | 2 | 1202 | 926 | 3 | -17 | -1 | 4 | 125 | 111 | 4 |
| 2 | -1 | 2 | 173 | 111 | 1 | -13 | -1 | 4 | 368 | 318 | 3 |
| 3 | -1 | 2 | 924 | 676 | 3 | -12 | -1 | 4 | 178 | 137 | 3 |
| 4 | -1 | 2 | 949 | 755 | 3 | -11 | -1 | 4 | 167 | 122 | 3 |
| 5 | -1 | 2 | 629 | 554 | 2 | -10 | -1 | 4 | 759 | 631 | 3 |
| 6 | -1 | 2 | 161 | 135 | 2 | -9 | -1 | 4 | 577 | 481 | 2 |
| 7 | -1 | 2 | 102 | 70 | 3 | -8 | -1 | 4 | 363 | 317 | 2 |
| 8 | -1 | 2 | 102 | 107 | 3 | -6 | -1 | 4 | 333 | 281 | 2 |
| 9 | -1 | 2 | 1019 | 755 | 4 | -5 | -1 | 4 | 665 | 568 | 2 |
| 10 | -1 | 2 | 539 | 439 | 2 | -4 | -1 | 4 | 310 | 303 | 2 |
| 14 | -1 | 2 | 309 | 299 | 3 | -1 | -1 | 4 | 791 | 636 | 3 |
| 15 | -1 | 2 | 65 | 51 | 6 | 0 | -1 | 4 | 977 | 795 | 3 |
| 16 | -1 | 2 | 185 | 198 | 3 | 1 | -1 | 4 | 451 | 385 | 2 |
| 17 | -1 | 2 | 97 | 64 | 5 | 2 | -1 | 4 | 242 | 177 | 2 |
| 18 | -1 | 2 | 139 | 133 | 4 | 3 | -1 | 4 | 212 | 220 | 2 |
| 19 | -1 | 2 | 76 | 107 | 7 | 4 | -1 | 4 | 393 | 269 | 2 |
| -20 | -1 | 3 | 93 | 90 | 6 | 5 | -1 | 4 | 505 | 370 | 2 |
| -17 | -1 | 3 | 89 | 138 | 5 | 6 | -1 | 4 | 438 | 330 | 2 |
| -16 | -1 | 3 | 141 | 145 | 4 | 7 | -1 | 4 | 275 | 232 | 2 |
| -15 | -1 | 3 | 159 | 184 | 4 | 8 | -1 | 4 | 426 | 334 | 2 |
| -14 | -1 | 3 | 127 | 145 | 4 | 10 | -1 | 4 | 68 | 83 | 4 |

Values of 10*Fobs and 10*Fcalc

| h | k | l | Fobs | Fcalc | Í(F) | h | k | l | Fobs | Fcalc | Í(F) |
|---|---|---|------|-------|------|---|---|---|------|-------|------|
| 12 | -1 | 4 | 389 | 346 | 3 | -3 | -1 | 6 | 121 | 92 | 2 |
| 13 | -1 | 4 | 161 | 105 | 3 | -2 | -1 | 6 | 181 | 187 | 2 |
| 14 | -1 | 4 | 111 | 74 | 4 | -1 | -1 | 6 | 387 | 323 | 2 |
| 15 | -1 | 4 | 108 | 142 | 5 | 0 | -1 | 6 | 620 | 466 | 2 |
| 16 | -1 | 4 | 170 | 154 | 4 | 1 | -1 | 6 | 1150 | 925 | 4 |
| 17 | -1 | 4 | 258 | 219 | 4 | 2 | -1 | 6 | 356 | 283 | 2 |
| 18 | -1 | 4 | 283 | 267 | 4 | 3 | -1 | 6 | 469 | 418 | 2 |
| -19 | -1 | 5 | 65 | 77 | 7 | 4 | -1 | 6 | 193 | 176 | 2 |
| -16 | -1 | 5 | 96 | 113 | 5 | 5 | -1 | 6 | 152 | 142 | 2 |
| -12 | -1 | 5 | 187 | 170 | 3 | 6 | -1 | 6 | 131 | 84 | 3 |
| -11 | -1 | 5 | 132 | 133 | 3 | 7 | -1 | 6 | 224 | 174 | 2 |
| -10 | -1 | 5 | 262 | 245 | 2 | 8 | -1 | 6 | 239 | 189 | 3 |
| -9 | -1 | 5 | 74 | 55 | 4 | 9 | -1 | 6 | 560 | 458 | 2 |
| -8 | -1 | 5 | 163 | 157 | 2 | 11 | -1 | 6 | 66 | 18 | 6 |
| -7 | -1 | 5 | 197 | 175 | 2 | 12 | -1 | 6 | 287 | 245 | 3 |
| -6 | -1 | 5 | 271 | 185 | 2 | 13 | -1 | 6 | 323 | 255 | 3 |
| -5 | -1 | 5 | 526 | 453 | 2 | 14 | -1 | 6 | 274 | 263 | 3 |
| -4 | -1 | 5 | 95 | 108 | 3 | 15 | -1 | 6 | 103 | 128 | 5 |
| -3 | -1 | 5 | 236 | 239 | 2 | 16 | -1 | 6 | 101 | 114 | 5 |
| -2 | -1 | 5 | 218 | 187 | 2 | -19 | -1 | 7 | 90 | 105 | 6 |
| -1 | -1 | 5 | 383 | 367 | 2 | -16 | -1 | 7 | 231 | 259 | 4 |
| 0 | -1 | 5 | 378 | 315 | 2 | -14 | -1 | 7 | 108 | 120 | 4 |
| 1 | -1 | 5 | 507 | 429 | 2 | -12 | -1 | 7 | 75 | 59 | 6 |
| 2 | -1 | 5 | 169 | 103 | 2 | -11 | -1 | 7 | 184 | 174 | 3 |
| 3 | -1 | 5 | 314 | 216 | 2 | -10 | -1 | 7 | 135 | 131 | 3 |
| 4 | -1 | 5 | 601 | 424 | 2 | -9 | -1 | 7 | 250 | 204 | 3 |
| 5 | -1 | 5 | 478 | 385 | 2 | -6 | -1 | 7 | 93 | 98 | 3 |
| 6 | -1 | 5 | 201 | 239 | 2 | -5 | -1 | 7 | 257 | 238 | 2 |
| 9 | -1 | 5 | 319 | 258 | 2 | -4 | -1 | 7 | 224 | 219 | 2 |
| 11 | -1 | 5 | 162 | 140 | 3 | -3 | -1 | 7 | 214 | 140 | 2 |
| 12 | -1 | 5 | 129 | 131 | 4 | -2 | -1 | 7 | 337 | 235 | 2 |
| 13 | -1 | 5 | 149 | 136 | 4 | -1 | -1 | 7 | 248 | 214 | 2 |
| 14 | -1 | 5 | 190 | 163 | 3 | 0 | -1 | 7 | 80 | 44 | 4 |
| 15 | -1 | 5 | 187 | 196 | 4 | 1 | -1 | 7 | 385 | 303 | 2 |
| 17 | -1 | 5 | 151 | 163 | 4 | 2 | -1 | 7 | 118 | 110 | 3 |
| -19 | -1 | 6 | 153 | 142 | 5 | 4 | -1 | 7 | 179 | 156 | 2 |
| -17 | -1 | 6 | 182 | 198 | 4 | 5 | -1 | 7 | 128 | 103 | 3 |
| -14 | -1 | 6 | 422 | 390 | 3 | 8 | -1 | 7 | 84 | 79 | 5 |
| -13 | -1 | 6 | 393 | 376 | 3 | 9 | -1 | 7 | 245 | 226 | 3 |
| -12 | -1 | 6 | 71 | 89 | 5 | 10 | -1 | 7 | 79 | 95 | 5 |
| -11 | -1 | 6 | 81 | 92 | 5 | 11 | -1 | 7 | 161 | 156 | 3 |
| -10 | -1 | 6 | 223 | 215 | 3 | 12 | -1 | 7 | 133 | 141 | 4 |
| -9 | -1 | 6 | 391 | 356 | 2 | 14 | -1 | 7 | 125 | 125 | 4 |
| -8 | -1 | 6 | 462 | 358 | 2 | 17 | -1 | 7 | 75 | 56 | 7 |
| -7 | -1 | 6 | 310 | 276 | 2 | -18 | -1 | 8 | 196 | 189 | 4 |
| -6 | -1 | 6 | 119 | 92 | 3 | -16 | -1 | 8 | 122 | 147 | 5 |
| -5 | -1 | 6 | 438 | 370 | 2 | -14 | -1 | 8 | 180 | 176 | 4 |
| -4 | -1 | 6 | 388 | 336 | 2 | -13 | -1 | 8 | 342 | 322 | 3 |

Values of 10*Fobs and 10*Fcalc

| h | k | l | Fobs | Fcalc | Í(F) | h | k | l | Fobs | Fcalc | Í(F) |
|---|---|---|------|-------|------|---|---|---|------|-------|------|
| -11 | -1 | 8 | 210 | 199 | 3 | -7 | -1 | 10 | 141 | 113 | 4 |
| -10 | -1 | 8 | 140 | 136 | 4 | -6 | -1 | 10 | 428 | 422 | 3 |
| -9 | -1 | 8 | 280 | 249 | 3 | -5 | -1 | 10 | 311 | 301 | 3 |
| -8 | -1 | 8 | 144 | 133 | 3 | -3 | -1 | 10 | 100 | 112 | 4 |
| -7 | -1 | 8 | 88 | 93 | 4 | -2 | -1 | 10 | 111 | 91 | 4 |
| -6 | -1 | 8 | 503 | 465 | 2 | -1 | -1 | 10 | 426 | 404 | 3 |
| -5 | -1 | 8 | 337 | 291 | 2 | 0 | -1 | 10 | 361 | 372 | 3 |
| -4 | -1 | 8 | 126 | 119 | 3 | 1 | -1 | 10 | 549 | 491 | 3 |
| -3 | -1 | 8 | 221 | 200 | 2 | 2 | -1 | 10 | 529 | 503 | 3 |
| -2 | -1 | 8 | 124 | 148 | 3 | 3 | -1 | 10 | 62 | 109 | 7 |
| -1 | -1 | 8 | 528 | 513 | 2 | 4 | -1 | 10 | 166 | 157 | 3 |
| 0 | -1 | 8 | 338 | 303 | 2 | 5 | -1 | 10 | 71 | 51 | 6 |
| 3 | -1 | 8 | 377 | 305 | 2 | 6 | -1 | 10 | 80 | 83 | 5 |
| 4 | -1 | 8 | 613 | 542 | 2 | 7 | -1 | 10 | 210 | 205 | 3 |
| 5 | -1 | 8 | 369 | 329 | 3 | 8 | -1 | 10 | 81 | 79 | 5 |
| 6 | -1 | 8 | 173 | 140 | 3 | 9 | -1 | 10 | 64 | 45 | 6 |
| 7 | -1 | 8 | 79 | 114 | 5 | 10 | -1 | 10 | 216 | 225 | 4 |
| 8 | -1 | 8 | 134 | 98 | 4 | 11 | -1 | 10 | 93 | 66 | 5 |
| 9 | -1 | 8 | 327 | 279 | 3 | 12 | -1 | 10 | 187 | 198 | 4 |
| 10 | -1 | 8 | 91 | 75 | 5 | 13 | -1 | 10 | 67 | 52 | 8 |
| 11 | -1 | 8 | 125 | 152 | 4 | -14 | -1 | 11 | 90 | 117 | 6 |
| 12 | -1 | 8 | 194 | 198 | 3 | -8 | -1 | 11 | 191 | 162 | 3 |
| 15 | -1 | 8 | 72 | 95 | 7 | -6 | -1 | 11 | 129 | 140 | 4 |
| 16 | -1 | 8 | 81 | 86 | 6 | -4 | -1 | 11 | 135 | 156 | 4 |
| -13 | -1 | 9 | 107 | 77 | 5 | -3 | -1 | 11 | 124 | 154 | 4 |
| -12 | -1 | 9 | 79 | 99 | 6 | -1 | -1 | 11 | 168 | 150 | 4 |
| -11 | -1 | 9 | 130 | 122 | 4 | 0 | -1 | 11 | 222 | 169 | 3 |
| -8 | -1 | 9 | 142 | 103 | 4 | 1 | -1 | 11 | 187 | 163 | 3 |
| -7 | -1 | 9 | 135 | 124 | 4 | 2 | -1 | 11 | 235 | 275 | 3 |
| -6 | -1 | 9 | 71 | 84 | 5 | 8 | -1 | 11 | 107 | 97 | 5 |
| -5 | -1 | 9 | 244 | 250 | 3 | 10 | -1 | 11 | 173 | 176 | 4 |
| -3 | -1 | 9 | 272 | 260 | 3 | -12 | -1 | 12 | 76 | 87 | 6 |
| -2 | -1 | 9 | 61 | 118 | 5 | -11 | -1 | 12 | 69 | 72 | 7 |
| -1 | -1 | 9 | 68 | 88 | 5 | -10 | -1 | 12 | 185 | 199 | 4 |
| 1 | -1 | 9 | 300 | 331 | 3 | -9 | -1 | 12 | 136 | 154 | 5 |
| 4 | -1 | 9 | 306 | 277 | 3 | -8 | -1 | 12 | 107 | 112 | 5 |
| 5 | -1 | 9 | 222 | 200 | 3 | -6 | -1 | 12 | 120 | 100 | 4 |
| 8 | -1 | 9 | 221 | 239 | 3 | -3 | -1 | 12 | 74 | 77 | 6 |
| 11 | -1 | 9 | 155 | 161 | 4 | -2 | -1 | 12 | 253 | 290 | 3 |
| 13 | -1 | 9 | 83 | 60 | 6 | -1 | -1 | 12 | 147 | 176 | 4 |
| 14 | -1 | 9 | 149 | 137 | 5 | 2 | -1 | 12 | 152 | 153 | 4 |
| -16 | -1 | 10 | 196 | 214 | 4 | 3 | -1 | 12 | 187 | 194 | 4 |
| -15 | -1 | 10 | 88 | 80 | 6 | 5 | -1 | 12 | 112 | 141 | 5 |
| -14 | -1 | 10 | 87 | 104 | 6 | 7 | -1 | 12 | 142 | 131 | 4 |
| -12 | -1 | 10 | 79 | 84 | 6 | 8 | -1 | 12 | 232 | 244 | 4 |
| -11 | -1 | 10 | 207 | 210 | 3 | 9 | -1 | 12 | 100 | 98 | 6 |
| -10 | -1 | 10 | 270 | 288 | 3 | 10 | -1 | 12 | 74 | 95 | 7 |
| -8 | -1 | 10 | 61 | 82 | 6 | -5 | -1 | 13 | 162 | 165 | 4 |

Values of 10*Fobs and 10*Fcalc

| h | k | l | Fobs | Fcalc | Í(F) | h | k | l | Fobs | Fcalc | Í(F) |
|---|---|---|------|-------|------|---|---|---|------|-------|------|
| 1 | -1 | 13 | 75 | 103 | 6 | -3 | 0 | 2 | 475 | 385 | 2 |
| 2 | -1 | 13 | 108 | 144 | 5 | -2 | 0 | 2 | 347 | 970 | 1 |
| 5 | -1 | 13 | 122 | 136 | 5 | -1 | 0 | 2 | 524 | 390 | 2 |
| -9 | -1 | 14 | 144 | 193 | 5 | 0 | 0 | 2 | 302 | 260 | 1 |
| -6 | -1 | 14 | 252 | 305 | 4 | 1 | 0 | 2 | 297 | 288 | 1 |
| -2 | -1 | 14 | 96 | 99 | 5 | 2 | 0 | 2 | 115 | 98 | 1 |
| -1 | -1 | 14 | 67 | 77 | 7 | 3 | 0 | 2 | 853 | 703 | 3 |
| 1 | -1 | 14 | 119 | 99 | 5 | 4 | 0 | 2 | 570 | 420 | 2 |
| 2 | -1 | 14 | 111 | 145 | 5 | 5 | 0 | 2 | 805 | 691 | 3 |
| 3 | -1 | 14 | 312 | 330 | 4 | 6 | 0 | 2 | 311 | 270 | 2 |
| 4 | -1 | 14 | 115 | 152 | 5 | 7 | 0 | 2 | 56 | 71 | 4 |
| 2 | -1 | 15 | 88 | 124 | 7 | 8 | 0 | 2 | 953 | 779 | 3 |
| 2 | 0 | 0 | 661 | 592 | 2 | 9 | 0 | 2 | 210 | 201 | 2 |
| 3 | 0 | 0 | 1020 | 873 | 3 | 10 | 0 | 2 | 204 | 187 | 2 |
| 4 | 0 | 0 | 252 | 131 | 1 | 11 | 0 | 2 | 97 | 77 | 3 |
| 5 | 0 | 0 | 384 | 393 | 1 | 12 | 0 | 2 | 256 | 187 | 3 |
| 6 | 0 | 0 | 635 | 539 | 2 | 13 | 0 | 2 | 919 | 756 | 3 |
| 7 | 0 | 0 | 512 | 354 | 2 | 14 | 0 | 2 | 410 | 320 | 3 |
| 8 | 0 | 0 | 1450 | 1038 | 5 | 16 | 0 | 2 | 72 | 73 | 5 |
| 9 | 0 | 0 | 847 | 629 | 3 | 18 | 0 | 2 | 275 | 230 | 3 |
| 10 | 0 | 0 | 301 | 265 | 2 | 19 | 0 | 2 | 150 | 113 | 4 |
| 11 | 0 | 0 | 427 | 406 | 2 | -19 | 0 | 4 | 203 | 171 | 4 |
| 12 | 0 | 0 | 375 | 346 | 2 | -18 | 0 | 4 | 76 | 93 | 6 |
| 13 | 0 | 0 | 122 | 132 | 4 | -16 | 0 | 4 | 120 | 150 | 4 |
| 15 | 0 | 0 | 329 | 316 | 3 | -14 | 0 | 4 | 429 | 391 | 3 |
| 16 | 0 | 0 | 134 | 159 | 4 | -13 | 0 | 4 | 228 | 209 | 3 |
| 17 | 0 | 0 | 216 | 141 | 4 | -12 | 0 | 4 | 166 | 144 | 3 |
| 18 | 0 | 0 | 412 | 351 | 3 | -11 | 0 | 4 | 142 | 171 | 3 |
| 19 | 0 | 0 | 200 | 165 | 4 | -10 | 0 | 4 | 515 | 428 | 2 |
| 20 | 0 | 0 | 115 | 114 | 5 | -9 | 0 | 4 | 292 | 279 | 2 |
| -2 | 0 | 1 | 59 | 0 | 2 | -8 | 0 | 4 | 1312 | 1020 | 4 |
| -1 | 0 | 1 | 39 | 0 | 2 | -7 | 0 | 4 | 1005 | 715 | 3 |
| 0 | 0 | 1 | 51 | 0 | 1 | -5 | 0 | 4 | 53 | 105 | 4 |
| -20 | 0 | 2 | 97 | 96 | 6 | -4 | 0 | 4 | 64 | 85 | 3 |
| -19 | 0 | 2 | 152 | 109 | 4 | -2 | 0 | 4 | 526 | 503 | 2 |
| -18 | 0 | 2 | 98 | 86 | 5 | -1 | 0 | 4 | 460 | 323 | 2 |
| -17 | 0 | 2 | 133 | 127 | 4 | 0 | 0 | 4 | 862 | 2427 | 3 |
| -14 | 0 | 2 | 175 | 163 | 3 | 3 | 0 | 4 | 550 | 319 | 2 |
| -13 | 0 | 2 | 165 | 154 | 3 | 4 | 0 | 4 | 643 | 526 | 2 |
| -12 | 0 | 2 | 345 | 259 | 2 | 6 | 0 | 4 | 239 | 170 | 2 |
| -11 | 0 | 2 | 375 | 328 | 2 | 7 | 0 | 4 | 425 | 317 | 2 |
| -10 | 0 | 2 | 586 | 452 | 2 | 8 | 0 | 4 | 135 | 160 | 3 |
| -9 | 0 | 2 | 305 | 252 | 2 | 9 | 0 | 4 | 1345 | 1063 | 4 |
| -8 | 0 | 2 | 140 | 102 | 2 | 12 | 0 | 4 | 92 | 141 | 4 |
| -7 | 0 | 2 | 459 | 351 | 2 | 13 | 0 | 4 | 408 | 365 | 3 |
| -6 | 0 | 2 | 1079 | 818 | 3 | 14 | 0 | 4 | 198 | 156 | 3 |
| -5 | 0 | 2 | 567 | 1585 | 2 | 15 | 0 | 4 | 106 | 106 | 5 |
| -4 | 0 | 2 | 712 | 2069 | 2 | 16 | 0 | 4 | 260 | 268 | 3 |

Values of 10*Fobs and 10*Fcalc

| h | k | l | Fobs | Fcalc | Í(F) | h | k | l | Fobs | Fcalc | Í(F) |
|---|---|---|------|-------|------|---|---|---|------|-------|------|
| -19 | 0 | 6 | 151 | 167 | 4 | 1 | 0 | 8 | 1673 | 1447 | 5 |
| -18 | 0 | 6 | 251 | 241 | 4 | 2 | 0 | 8 | 1076 | 922 | 4 |
| -17 | 0 | 6 | 250 | 251 | 4 | 5 | 0 | 8 | 346 | 367 | 2 |
| -16 | 0 | 6 | 170 | 195 | 4 | 7 | 0 | 8 | 312 | 241 | 3 |
| -15 | 0 | 6 | 87 | 73 | 5 | 8 | 0 | 8 | 528 | 492 | 3 |
| -13 | 0 | 6 | 184 | 167 | 3 | 9 | 0 | 8 | 814 | 738 | 3 |
| -12 | 0 | 6 | 334 | 294 | 3 | 10 | 0 | 8 | 125 | 140 | 5 |
| -11 | 0 | 6 | 386 | 373 | 3 | 13 | 0 | 8 | 124 | 123 | 4 |
| -10 | 0 | 6 | 331 | 284 | 2 | 15 | 0 | 8 | 75 | 81 | 6 |
| -8 | 0 | 6 | 183 | 216 | 3 | -16 | 0 | 10 | 79 | 116 | 7 |
| -7 | 0 | 6 | 107 | 90 | 3 | -15 | 0 | 10 | 279 | 313 | 4 |
| -6 | 0 | 6 | 640 | 566 | 2 | -14 | 0 | 10 | 229 | 223 | 4 |
| -5 | 0 | 6 | 903 | 777 | 3 | -13 | 0 | 10 | 156 | 159 | 4 |
| -4 | 0 | 6 | 823 | 687 | 3 | -12 | 0 | 10 | 73 | 52 | 6 |
| -3 | 0 | 6 | 100 | 123 | 3 | -11 | 0 | 10 | 251 | 269 | 3 |
| -2 | 0 | 6 | 159 | 141 | 2 | -10 | 0 | 10 | 159 | 180 | 4 |
| -1 | 0 | 6 | 552 | 429 | 2 | -9 | 0 | 10 | 287 | 265 | 3 |
| 0 | 0 | 6 | 561 | 487 | 2 | -7 | 0 | 10 | 172 | 216 | 3 |
| 1 | 0 | 6 | 224 | 174 | 2 | -6 | 0 | 10 | 146 | 150 | 4 |
| 2 | 0 | 6 | 290 | 207 | 2 | -5 | 0 | 10 | 217 | 199 | 3 |
| 3 | 0 | 6 | 83 | 54 | 3 | -4 | 0 | 10 | 290 | 273 | 3 |
| 4 | 0 | 6 | 381 | 363 | 2 | -3 | 0 | 10 | 74 | 75 | 5 |
| 5 | 0 | 6 | 623 | 548 | 2 | -2 | 0 | 10 | 385 | 387 | 3 |
| 6 | 0 | 6 | 94 | 61 | 3 | -1 | 0 | 10 | 430 | 393 | 3 |
| 7 | 0 | 6 | 79 | 37 | 4 | 0 | 0 | 10 | 165 | 152 | 3 |
| 8 | 0 | 6 | 105 | 107 | 3 | 1 | 0 | 10 | 319 | 336 | 3 |
| 9 | 0 | 6 | 442 | 371 | 2 | 2 | 0 | 10 | 240 | 211 | 3 |
| 10 | 0 | 6 | 155 | 170 | 3 | 3 | 0 | 10 | 592 | 549 | 3 |
| 11 | 0 | 6 | 135 | 129 | 4 | 4 | 0 | 10 | 697 | 663 | 3 |
| 12 | 0 | 6 | 312 | 244 | 3 | 5 | 0 | 10 | 293 | 270 | 3 |
| 13 | 0 | 6 | 371 | 328 | 3 | 6 | 0 | 10 | 136 | 181 | 4 |
| 16 | 0 | 6 | 78 | 58 | 6 | 7 | 0 | 10 | 90 | 109 | 5 |
| -18 | 0 | 8 | 117 | 98 | 5 | 9 | 0 | 10 | 231 | 233 | 3 |
| -17 | 0 | 8 | 140 | 143 | 5 | 12 | 0 | 10 | 106 | 121 | 5 |
| -16 | 0 | 8 | 163 | 197 | 4 | 13 | 0 | 10 | 187 | 163 | 4 |
| -15 | 0 | 8 | 112 | 75 | 5 | 14 | 0 | 10 | 137 | 138 | 5 |
| -14 | 0 | 8 | 272 | 273 | 3 | -13 | 0 | 12 | 96 | 118 | 6 |
| -11 | 0 | 8 | 108 | 99 | 5 | -6 | 0 | 12 | 521 | 569 | 3 |
| -10 | 0 | 8 | 725 | 714 | 3 | -2 | 0 | 12 | 296 | 277 | 3 |
| -9 | 0 | 8 | 454 | 422 | 3 | -1 | 0 | 12 | 472 | 467 | 3 |
| -8 | 0 | 8 | 444 | 360 | 3 | 1 | 0 | 12 | 443 | 448 | 3 |
| -7 | 0 | 8 | 779 | 672 | 3 | 2 | 0 | 12 | 635 | 700 | 3 |
| -6 | 0 | 8 | 344 | 306 | 2 | 3 | 0 | 12 | 341 | 340 | 3 |
| -5 | 0 | 8 | 260 | 275 | 2 | 4 | 0 | 12 | 78 | 86 | 6 |
| -4 | 0 | 8 | 379 | 371 | 2 | 6 | 0 | 12 | 145 | 159 | 4 |
| -2 | 0 | 8 | 175 | 208 | 2 | 8 | 0 | 12 | 106 | 95 | 5 |
| -1 | 0 | 8 | 286 | 253 | 2 | 10 | 0 | 12 | 158 | 168 | 4 |
| 0 | 0 | 8 | 441 | 330 | 2 | 11 | 0 | 12 | 199 | 234 | 4 |

Values of 10*Fobs and 10*Fcalc

| h | k | l | Fobs | Fcalc | Í(F) | h | k | l | Fobs | Fcalc | Í(F) |
|---|---|---|------|-------|------|---|---|---|------|-------|------|
| - | - | - | ---- | ----- | ---- | - | - | - | ---- | ----- | ---- |
| -10 | 0 | 14 | 203 | 295 | 4 | | | | | | |
| -9 | 0 | 14 | 82 | 106 | 7 | | | | | | |
| -6 | 0 | 14 | 93 | 106 | 6 | | | | | | |
| -5 | 0 | 14 | 130 | 157 | 5 | | | | | | |
| 0 | 0 | 14 | 127 | 168 | 5 | | | | | | |
| 2 | 0 | 14 | 165 | 183 | 4 | | | | | | |
| 6 | 0 | 14 | 67 | 60 | 7 | | | | | | |
| 7 | 0 | 14 | 87 | 105 | 6 | | | | | | |

# Bibliography

Block, E. "Reaction of Organic Sulfur Compounds." Ed. A.T.
    Blonquist and H.H. Wasserman. New York: Academic Press
    Inc., 1978.

Durst, T. Comprehensive Organic Chemistry. Ed. D. Jones. Vol.
    3. London: Perg. Press, 1977.

Glusker, Jenny P., and Kenneth N. Trueblood. Crystal
    Structure Analysis A Primer. New York: Oxford University
    Press, 1985.

Hawthorne, M.P., Journal of American Chemical Society. 82,
    1960.

Henry, N.F.M., and K. Longsdale, eds. International Tables for
    X-ray Crystallography. Kynoch Press, 1952.

Hoggs, D.R., Int. Rev. Sci., Organic Chemistry Ser., 1975.
    pp. 267-268.

Kharasch, M.S., G. Stampa and W. Nudenberg. Journal of
    Organic Chemistry. 18, 1973, pp. 575

Muhundam M., Ph.D. Thesis, Dept. of Chemistry, S.V.
    University, Tirupati, India.

Strating, J. "Organic Sulfur Compounds." Vol. 1. Ed. N.
    Khrasch. London: Perg. Press, 1961. p. 146.

Szmant, H.H., and G.A. Brost. Journal of American Chemical
    Society. 73, 1951.

Truce, W.E., T.C. Klinger and W.W. Brand. "Sulfones and
    Sulfoxides." Ed. S.Oae. New York: Plenum Press, 1977.
    p. 171.

VITA


Tommie Heltcel

Candidate for the Degree of

Bachelor of Science

and

Completion of

McCabe Honors Program


Thesis:    THE CRYSTALLINE STRUCTURE OF MM3, A DERIVATIVE OF
                                DAPSONE

Major:     Chemistry/Mathematics

Biographical Information:

   Personal Data:  Born in Guthrie, Oklahoma, July 17, 1969,
   the son of Louis V. and Roberta Heltcel

Education:  Graduation from Guthrie High School, Guthrie,
   Oklahoma, in May 1987;  will complete requirements for
   Bachelor of Science degree at Langston University in May 1994,
   having also completed all requirements in the
   E. P. McCabe Honors Program.