Crystal and molecular structure of calcium 1-naphthyl phosphate trihydrate
by Chi-Tang Li

A thesis submitted to the Graduate Faculty in partial fulfillment of the requirements for the degree of DOCTOR OF PHILOSOPHY in ' \ Chemistry
Montana State University


Abstract:
The crystal and molecular structure of calcium 1-naphthyl, phosphate has been solved by x-ray diffraction methods. This crystal has the following lattice parameter: a=7.244±0.002Å α=84°19'±3' Z=2 b=8.994±0.003Å β=78°32'±2' D0=1.503 g/ml c=18.725±0.004Å γ=88°52'±4' Dc=1.508 g/ml Diffraction intensities were measured visually, corrected by the size factor, Lorentz and polarization factors, and the absorption factor. Intensity statistics showed that the crystal had the. symmetry of Pl.

The structure was solved with a three dimensional Patterson function, minimum function, and three dimensional Fourier synthesis. Least-squares refinements, which included first individual isotropic then anisotropic temperature factors were carried out. The final residue factor (R-factor) is 10.3% for 1724 observed reflections. The phosphate groups are distorted tetrahedrons. The four phosphate oxygens are bonded in the following manner. One oxygen is bonded to the naphthyl group, another oxygen is bonded to a hydrogen, the other two oxygens are coordinated to two calcium atoms which are related to each other by an inversion center. The neighboring phosphate groups are joined, together by hydrogen bonding between two oxygens, one of which has a.hydrogen on it. Each calcium is coordinated to seven oxygens, four of which are contributed by four nearby phosphate groups, the other three from three surrounding water molecules. The calcium and the seven coordination oxygens are arranged in a distorted pentagonal bipyramid.

The pentagonal angles of O-Ca-O have the range of 67.4° to 78.6°, with the average of 72.4° (the theoretical pentagonal angle being 72°). Naphthyl groups are distorted planes. In the naphthyl groups, that side which is closest to the two nearby naphthyl groups has the shortest c-c distance of I.30 and 1.31Å. The bond distances and angles are as below: P-0: 1.47 to 1.59 with the average of 1.53Å O-P-O angle: 103 to 117 with the average of 109 degrees C-C: 1.30 to 1.48 with the average of I.38Å C-C-C angle: 116 to 125 with the average of 120 degrees The molecules are held together by strong hydrogen bonding and van der Waals forces. The successful solution of the structure has confirmed a new indexing method developed by the author. New derivations are included for each of the following formulas of equations: 1. Wolf-Bragg equation 2. Equi-inclination Weissenberg index-checking formula 3. Sin^2 θ equation for triclinic symmetry or higher 4. Triclinci interplanar spacing equation 5. Clarified forms of the x-ray Fourier synthesis equations

# CRYSTAL AND MOLECULAR STRUCTURE OF CALCIUM 1-NAPHTHYL PHOSPHATE TRIHYDRATE

by

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A thesis submitted to the Graduate Faculty in partial fulfillment of the requirements for the degree

of

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in

Chemistry

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## ABSTRACT

The crystal and molecular structure of calcium 1-naphthyl phosphate has been solved by x-ray diffraction methods. This crystal has the following lattice parameter:

| | | |
|---|---|---|
| $a=7.244\pm0.002$Å | $b=8.994\pm0.003$Å | $C=18.725\pm0.004$Å |
| $\alpha=84°19'\pm3'$ | $\beta=78°32'\pm2'$ | $\gamma=88°52'\pm4'$ |
| $Z=2$ | $D_o=1.503$ g/ml | $D_c=1.508$ g/ml |

Diffraction intensities were measured visually, corrected by the size factor, Lorentz and polarization factors, and the absorption factor. Intensity statistics showed that the crystal had the symmetry of $P\bar{1}$. The structure was solved with a three dimensional Patterson function, minimum function, and three dimensional Fourier synthesis. Least-squares refinements, which included first individual isotropic then anisotropic temperature factors were carried out. The final residue factor (R-factor) is 10.3% for 1724 observed reflections.

The phosphate groups are distorted tetrahedrons. The four phosphate oxygens are bonded in the following manner. One oxygen is bonded to the naphthyl group, another oxygen is bonded to a hydrogen, the other two oxygens are coordinated to two calcium atoms which are related to each other by an inversion center. The neighboring phosphate groups are joined together by hydrogen bonding between two oxygens, one of which has a hydrogen on it. Each calcium is coordinated to seven oxygens, four of which are contributed by four nearby phosphate groups, the other three from three surrounding water molecules. The calcium and the seven coordination oxygens are arranged in a distorted pentagonal bipyramid. The pentagonal angles of O-Ca-O have the range of 67.4° to 78.6°, with the average of 72.4° (the theoretical pentagonal angle being 72°). Naphthyl groups are distorted planes. In the naphthyl groups, that side which is closest to the two nearby naphthyl groups has the shortest c-c distance of 1.30 and 1.31Å. The bond distances and angles are as below:

P-O: 1.47 to 1.59 with the average of 1.53Å
O-P-O angle: 103 to 117 with the average of 109 degrees
C-C: 1.30 to 1.48 with the average of 1.38Å
C-C-C angle: 116 to 125 with the average of 120 degrees

The molecules are held together by strong hydrogen bonding and van der Waals forces.

The successful solution of the structure has confirmed a new indexing method developed by the author. New derivations are included for each of the following formulas or equations:

1. Wolf-Bragg equation
2. Equi-inclination Weissenberg index-checking formula
3. $\sin^2\theta$ equation for triclinic symmetry or higher
4. Triclinci interplanar spacing equation
5. Clarified forms of the x-ray Fourier synthesis equations

# SECTION I

## INTRODUCTION

Organic phosphates play a very important role in biological processes. The variety of the manifestations and functions of organic phosphate esters in living systems is indeed amazing. "There is hardly anything that goes on in the (living) cell in which esters of phosphoric acid, in one form or another, are not involved at some stage." (23) Two examples are cited below to illustrate the importance of organic phosphates in biological systems. (a) Deoxyribonucleic acid (DNA) which contains many organic phosphate groups, plays a key role in the storage and transport of genetic information. Crick and Watson (11) proposed an ingenious double-helix model for DNA which fits remarkably well all the facts known at the present time, and for this work, they were awarded a Nobel prize in 1962. (b) Adenosine 3',5' cyclic phosphate is a factor stimulating the conversion of inactive glycogen phosphorylase to the active form in tissue preparations. An understanding of the complicated functions of these and other organic phosphates requires basic and precise structural knowledge. The complexity of many of the substances present in living systems makes them, at least for the present, unsuitable for x-ray diffraction studies. However, a variety of simpler organic phosphates are known, and few of their structures have been determined. Although these substances may not actually be present in living systems, the basic structures should not be very much different from those in more complex molecules. Thus, solution of simpler structures will assist in present understanding as well as making solution of structures for more complex substances

easier in the future.

Calcium 1-naphthyl phosphate was chosen for this structural study, because (a) it is very easy to obtain a good single crystal for x-ray work; (b) calcium and phosphorus atoms are fairly large suggesting use of the heavy atom method to solve the crystal structure; (c) this crystal is triclinic. Since I have worked out a method for indexing triclinic crystals as well as an index-checking method, I wanted to gain experience in using this method, even though triclinic crystals present problems not usually present in crystals of higher symmetry.

Despite the importance of knowledge of the detailed structure of organic phosphates for understanding their varied functions, relatively few structures have been accurately determined.

These few organic phosphates whose structures have been determined precisely are described briefly as below.

1. Dibenzyl phosphoric acid, $(C_6H_5CH_2)_2PO_4H$, was studied by Dunitz and Rollett (15). This crystal had the following lattice parameters:

   Monoclinic with $a=20.287\pm0.040$Å $b=5.709\pm0.010$Å

   $c=12.648\pm0.020$Å $\beta=103°13'\pm0°10'$

   $Z=4$, space group of $P2_1/a$

   The final R was 11.0% for 2471 general observed reflections.

   Bond distances and angles are summarized below:

   For phosphate groups:

   P-O (in Å)

   Range 1.469 to 1.566

Average 1.531

P-OR 1.566 & 1.545

P-OH 1.545

O-P-O (in degree)

Range 103.8 to 117.2

Average 109.3

Angle between longest & shortest P-O 103.8 (min.)

Angle between 2 very short P-O 117.2 (max.)

P-O-C (oxygen on ester bond) 122.3 & 118.8

For benzene ring:

C-C (in Å)

Range 1.340 to 1.407

Average 1.378

C-C-C angle (in degree)

Range 118.5 to 121.9

Average 120.0

For close approaches between pairs of atoms indirectly covalently linked:

O-O from 2.444 to 2.573Å

O-C from 3.030 to 3.393Å

2. Calcium Thymidylate, $C_{10}H_{13}O_8N_2CaP^{\circ}6H_2O$, was studied by Trueblood, Horn & Luzzati (34). This crystal had the following lattice parameters:

Monoclinic with $a=14.40\pm0.02$Å $b=6.87\pm0.01$Å

$c=9.181\pm0.01$Å $\beta=90°58'\pm3'$

Z=2, space group of $P2_1$

The final R was 11.6% for 1575 general observed reflections.

The entire structure is held together by the Ca-O bonds and a complex network of hydrogen bonds.

For phosphate group:

P-O (in Å)

| | |
|---|---|
| Range | 1.474 to 1.587 |
| Average | 1.515 |
| P-OR | 1.587 |
| P-O. . .Ca | 1.486 & 1.514 |

O-P-O (in degree)

| | |
|---|---|
| Range | 102.1 to 118.4 |
| Average | 109.3 |
| Angle between longest & shortest P-O | 102.1 (min.) |
| Angle between two very short P-O | 118.4 (max.) |

P-O-C (ester oxygen) 118.8°

C-O ($PO_4$) 1.472A

For calcium coordination:

The environment of Ca ion is a distorted pentagonal bipyramid. Calcium coordination number is seven with four phosphate oxygens (from three different molecules) and one water molecule lying approximately in a plane and two waters on a line through the calcium nearly perpendicular to this plane.

O-O (in Å)

| | |
|---|---|
| Range | 2.29 to 2.65 |
| Average | 2.42 |

O-Ca-O angle (in degree)

| | |
|---|---|
| Range | 57 to 80 |
| Average | 72 |

3. 2-Amino-Ethanol Phosphate, $NH_3^+-CH_2-CH_2-O-PO_3H^-$, was studied by Kraut (24). This crystal had the following lattice parameters:

Monoclinic with $a=9.04\pm0.02$Å $b=7.75\pm0.02$Å

$c=8.86\pm0.02$Å $\beta=102^\circ 27' \pm 8'$

$Z=4$, space group of $P2_1/c$

The final R was 6.5% for 1000 observed general reflections. Bond distances and angles for phosphate group are summarized below:

P-O (in Å)

| | |
|---|---|
| Range | 1.493 to 1.591 |
| Average | 1.536 |
| P-OR | 1.591 |
| P-OH | 1.557 |

Two of the oxygens on the phosphate group were reported to be attached by double bonds (1.493 & 1.503Å)

O-P-O (in degree)

| | |
|---|---|
| Range | 103.9 to 117.4 |
| Average | 109.4 |
| Angle between longest & shortest P-O | 103.9 (min.) |
| Angle between two very short P-O | 117.4 (max.) |

P-O-C (oxygen on ester bond) 118.7°

C-O ($PO_4$) 1.429Å

4. Adenosine-5'-phosphate, $C_{10}H_{14}O_7N_5P$, was studied by Kraut & Jensen (25). This crystal had the following lattice parameters:

Monoclinic with a=12.77±0.92Å b=11.82±0.02Å

c=4.882±0.01Å $\beta$=92°24'±5'

Z=2, space group of $P2_1$

The final R was 6.8% for 1197 general observed reflections. Bond distances and angles for phosphate groups are summarized below:

P-O (in Å)

| | |
|---|---|
| Range | 1.514 to 1.610 |
| Average | 1.546 |
| P-OR | 1.610 |
| P-OH | 1.566 |

O-P-O (in degree)

| | |
|---|---|
| Range | 105.7 to 118.2 |
| Average | 109.4 |
| Angle between longest & shortest P-O | 105.7°(min.) |
| Angle between two very short P-O | 118.2°(max.) |
| P-O-C (oxygen on ester bond) | 114.7° |
| C-O ($PO_4$) | 1.475Å |

The following organic phosphates have been solved with either limited data or by projections. No descriptions of these structures is made here. They are mentioned only by title.

1. "Crystal and Molecular Structure of Cytidylic Acid" by Alver &

Furberg (2)

2. "The Crystal Structure of Ba-Ribose-5-Phosphate" by Furberg & Mostad (16)

3. "The Crystal Structure of Triphenyl Phosphate" by Davies & Stanley (13)

4. "The Crystal Structure of Ba-Phenyl Phosphate" by Svetich & Caughlan (33)

## SECTION II

## EXPERIMENTAL WORK

### Preparation and identification of calcium 1-naphthyl phosphate

Calcium 1-naphthyl phosphate was purchased from Aldrich Chemical Company, Inc. in the form of a crystalline powder. It was purchased as Ca $C_{10}H_7PO_4 \cdot H_2O$, however chemical analysis and solution of the crystal structure have shown it to be $Ca(C_{10}H_7HPO_4)_2 \cdot 3H_2O$. To confirm the structure analysis, this compound was analyzed for calcium and phosphorus. In addition, infrared spectra were taken of the original powder and the crystals used for the structure analysis, in order to confirm that the two were identical compounds. These are shown in Fig. 1 and 2.

Calcium was determined with a Beckman Flame Quartz Spectrophotometer (Model DU) by comparing with a standard calcium solution. Phosphorus was determined by colorimetric analysis on a Beckman model B spectrophotometer by comparing with a standard phosphorus compound. Details of the analysis are included in Appendix A.

The results of the analysis, together with the comparison with the two possible structural formulas are listed in the following table. An examination of the table clearly indicates that the compound is $Ca(C_{10}H_7HPO_4)_2 \cdot 3H_2O$.

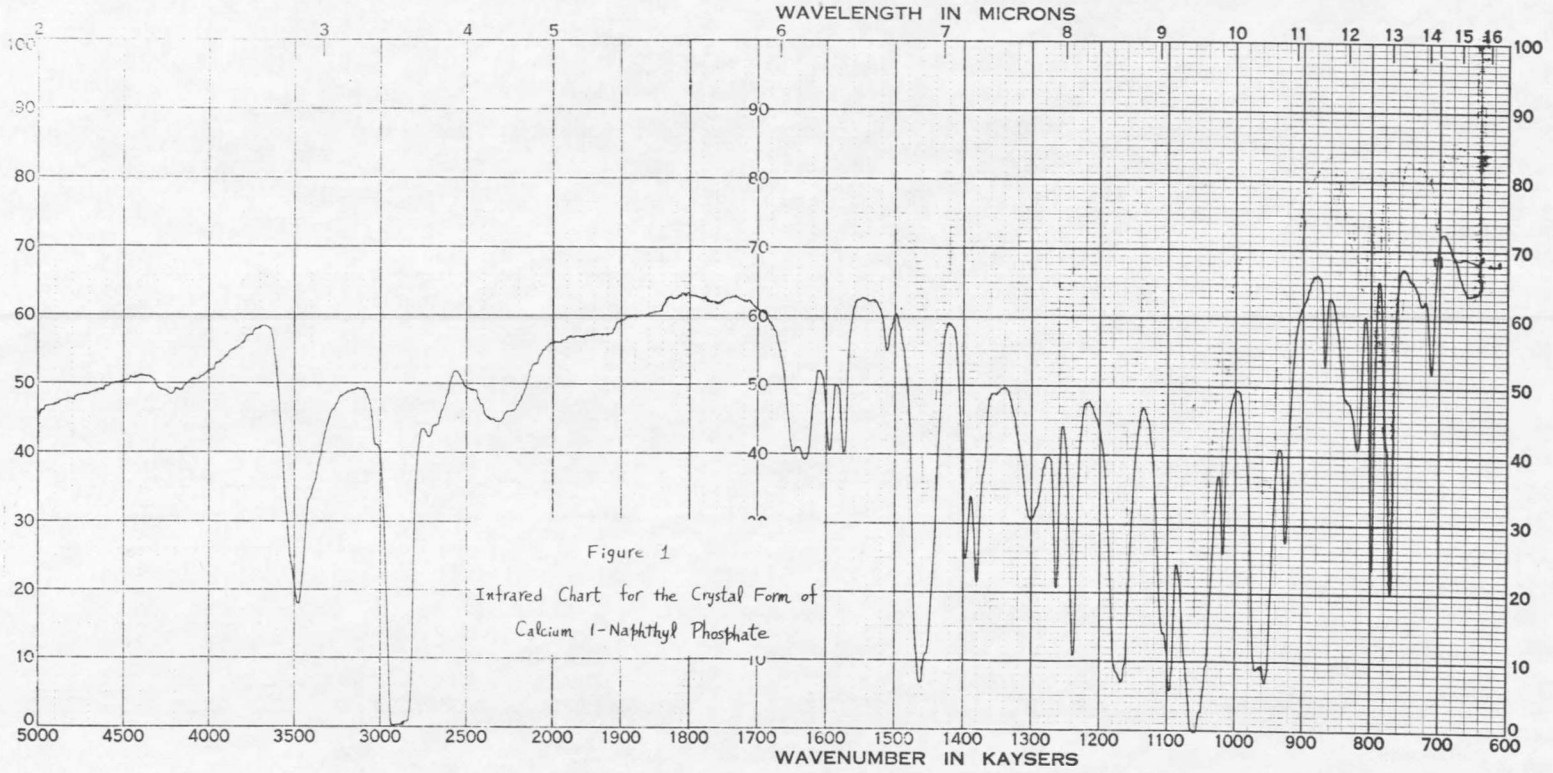



Figure 1

Infrared Chart for the Crystal Form of Calcium 1-Naphthyl Phosphate

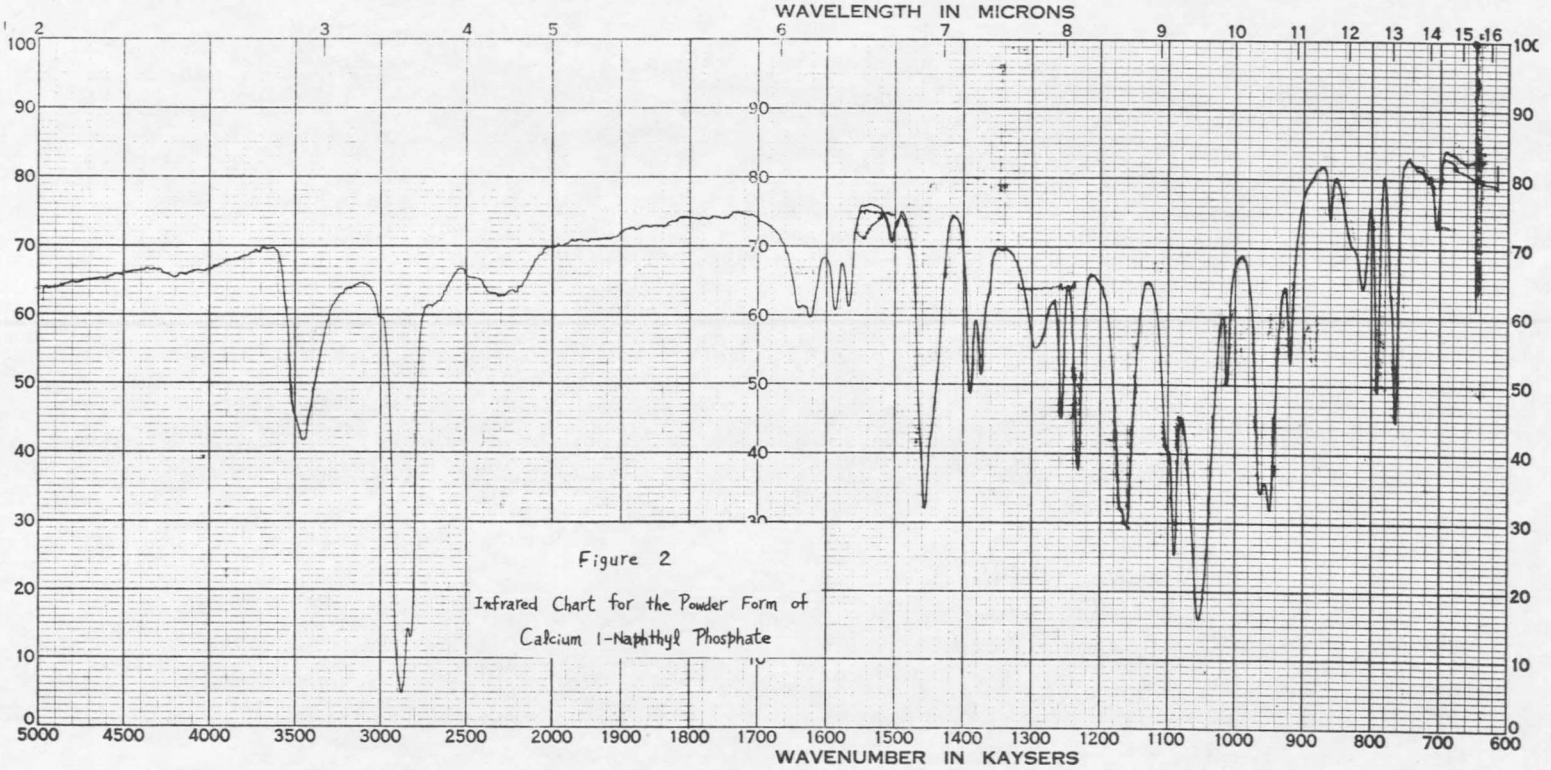



Figure 2

Infrared Chart for the Powder Form of Calcium 1-Naphthyl Phosphate

Table I. Chemical Analysis Results

| | Sample Analysis | $Ca(C_{10}H_7HPO_4)_2 \cdot 3H_2O$ | $CaC_{10}H_7PO_4 \cdot H_2O$ |
|---|---|---|---|
| % Ca | 7.916 | 7.416 | 14.320 |
| ppm of Ca when 0.1977 gm sample diluted to 500 ml | 31.3 | 29.3 | 56.6 |
| % P | 11.103 | 11.463 | 11.053 |
| ppm of P when 0.1977 gm sample diluted to 500 ml | 43.9 | 45.3 | 43.7 |
| Atomic ratio P/Ca | 1.83 | 2.0 | 1.0 |

Water was found to be the best solvent for obtaining good crystals, even though the solubility in water is very samll. A saturated solution at room temperature was prepared, and slow evaporation at this temperature produced good single crystals. The crystal used for this x-ray work had the following approximate dimensions determined with the microscope: 1.3 x 0.216 x 0.125 $mm^3$.

The density was determined by the floatation method, where carbon tetrachloride diluted with ether was used as the substrate.

| Test no. | Density g/ml |
|---|---|
| 1 | 1.5027 |
| 2 | 1.5037 |

The x-ray diffraction data was obtained from Weissenberg and precession cameras, using copper radiation ($\lambda_{av}$=1.5418Å with nickel filter). A

Phillips generater type no. 12045 B/3 series no. 57-677 and Phillips copper tube were used. Both the Weissenberg and precession cameras were Supper instruments. The Weissenberg camera (Model E of Charles Supply Company's product) has a diameter of 57.3 mm and the precession camera has a magnification factor of 60, i.e., the distance of the film to the crystal is 60 mm. Kodak medical no screen x-ray film was used. For details of film processing, see Appendix B.

Integrated photographs of three films in the camera were taken for all Weissenberg levels. Since the crystal was a triclinic, the goniometer head setting are different for precession photographs than for Weissenberg photographs. After the crystal was aligned, two integrated precession pictures (hko and okl) were taken. These pictures were used chiefly for scaling the different Weissenberg levels to a common base.

Since there are some unique features in determining the unit cell constants and indexing the photographs, these are treated in Sections 3 and 4. Intensity data were collected as described below.

Intensities of indexed photographs were obtained by visual comparsion with a standard scale. The graded intensity scale was prepared in the following manner. Three film strips were put in a metal cassette in the same manner as the three films in the Weissenberg camera. The metal cassette was wrapped in a lead shield except for a small hole in the middle. The distance of metal cassette from x-ray source was 62.5 inches while the height of the small hole from ground was 49 inches. The copper x-ray tube was operated at 35 kv and 10 ma. The metal cassette was exposed to nickel-filtered copper radiation at the following time interval: 5, 10, 15, 20, 25,

30, 35, 40, 45, 50, 55, 60, 65, 70, 75, 80, 85, 90, 95, 100, 105, 110, 115, and 120 seconds. After each exposure, the film strips were moved up a few millimeters. The film strips were developed in the same manner as the integrated films and at the same time as the films for which the intensity scale is to be used. A scale was selected in the following manner and used for all the Weissenberg photographs. The darkest spot on the scale was darker than any x-ray spots on the third film (the lightest one), while the lightest spot on the scale was lighter than any spot on the third film.

Three films of the same level are called A, B, C according to the order of darkness. A is the darkest while C the lightest. Each film was read against the same scale. For many reflections there were three readings for each spot. The average ratios of A/B and A/C for each level were found. By means of these ratios, B and C films were scaled to the same level as A film. Some of the three readings were rejected for the following reason. Both ends of the scale are generally less accurate, especially the dark end due to non-linear relation between energy and optical density of film. If one such reading differed by 40% or more from the rest readings, it was rejected. Two persons were hired to read the films. Their readings on the whole were in reasonable agreement. When they were reading the same films, six readings were recorded for each spot. The average intensity for each spot was obtained by taking the average of the six readings. If the highest and lowest readings among the six differ by more than 25%, a re-check was done by the author.

## SECTION III

## DETERMINATION OF THE LATTICE PARAMETERS

The formulas described in this section for determining the unit cell constants are generally applicable for crystals of triclinic symmetry or higher.

This method describes use of oscillation, Weissenberg and precession photographs to obtain all the lattice parameters for a triclinic crystal. The crystal is assumed to be mounted on its b axis in the following treatment.

From oscillation photographs, the film coordinate $y_n$ for the $n^{th}$ level can be easily measured. If $r_F$ is the film radius,

$$b=n\lambda(1+(r_F/y_n)^2)^{1/2}$$

This form of the equation is derived very simply in the following way. It is shown in Fig. 3a, b, c the simple sketches of the geometrical configurations for taking the oscillation photograph. The normalized reciprocal lattice is always dimensionless. When the unit reciprocal lattice is multiplied by the film radius $r_F$, the sphere of reflection will fit the film exactly and the Fig. 3b is converted into Fig. 3c which is quite meaningful. In Fig. 3c, since the triangle OMP is similar to the triangle ONB, we have

$$r_F/r_F d^*_{ono}=(r_F^2+y_n^2)^{1/2}/y_n$$

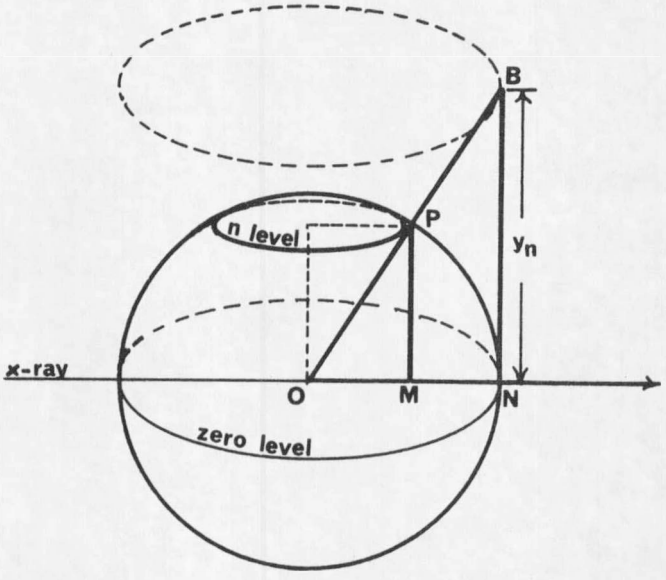
$$1/d^*_{ono}=(1+(r_F/y_n)^2)^{1/2}$$

since $d^*_{ono}=nd^*_{olo}=n\lambda/b$

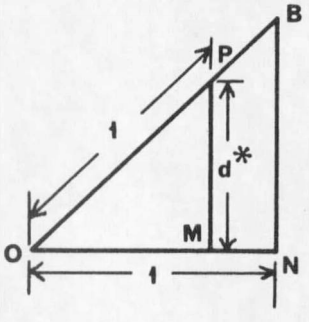
thus $b/n\lambda=(1+(r_F/y_n)^2)^{1/2}$

or $b=n\lambda(1+(r_F/y_n)^2)^{1/2}$

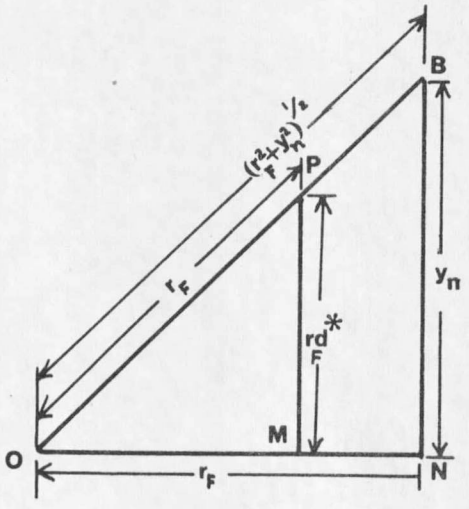
From the zero level Weissenberg photograph, the interplanar spacing of $d_{100}$ and $d_{001}$ and the cell edge of a and c can be found as below.




a.




b.




c.

Figure 3 Derivation for the oscillation formula

$$a=d_{100}/\sin\beta^{*}\sin\gamma=d_{100}/\sin\beta\sin\gamma^{*}$$

$$d_{100}=n\lambda/2\sin\theta_{noo}$$

For a camera of diameter 57.3 mm, $\theta_{noo}=x_{noo}$ where $x_{noo}$ is the vertical distance from the spot noo to the center line of the film.

If the film translation is 0.5 mm per degree crystal rotation

$$\beta^{*}=2z_{(a^{*}c^{*})}$$

where z is the horizontal distance in mm between the two axes a* and c*.

$\beta^{*}$ can also be calculated by using the Wolf-Bragg equation (19). For the hol zone, the Wolf-Bragg equation takes the following form:

$$4\sin^{2}\theta_{hol}=h^{2}a^{*2}+l^{2}c^{*2}+2hlc^{*}a^{*}\cos\beta^{*}$$

For Weissenberg camera of diameter 57.3 mm

$$\theta_{hol}=x_{hol}$$

$$\cos\beta^{*}=\left(4\sin^{2}x_{hol}-h^{2}a^{*2}-l^{2}c^{*2}\right)/2hla^{*}c^{*}$$

where $a^{*}=\lambda/d_{100}$

$c^{*}=\lambda/d_{001}$

Zero level precession photograph may also be used for calculation axial distances and angles.

The interplanar spacing and the cell edge are given by

$$a=d_{100}/\sin\beta^{*}\sin\gamma=d_{100}/\sin\beta\sin\gamma^{*}$$

$$d_{100}=n\lambda/a^{*}_{noo}=60n\lambda/a^{*\prime}_{noo}$$

$a^{*\prime}_{noo}$ is the acutal length (in mm) measured from the point noo to the origin point on the precession picture. It is understood that the reciprocal lattice has been magnified sixty times by the precession camera (the distance from the film to the crystal is 60 mm).

The interaxial angle may be calculated either by direct measurement or

from the Wolf-Bragg equation.

(1) By direct measurement: Since the precession photograph is an undistorted picture of the reciprocal lattice, the $\alpha^*$ angle can be determined by the direct measurement of the angle between the axes of b* and c* on the b*c* precession photograph.

(2) By the using of Wolf-Bragg equation: For example, consider the b*c* precession photograph. The Wolf-Bragg equation corresponding to this has the following form.

$$\sin^2\theta_{okl}=\tfrac{1}{4}(k^2b^{*2}+l^2c^{*2}+2klb^*c^*\cos\alpha^*)$$

From the Bragg's law

$$\sin\theta_{okl}=(\lambda/d_{okl})/2=\sigma_{okl}/2$$

or $$\sin^2\theta_{okl}=\sigma_{okl}^2/4$$

thus $$\sigma^2_{okl}=k^2b^{*2}+l^2c^{*2}+2klb^*c^*\cos\alpha^*$$

$$\cos\alpha^*=(\sigma_{okl}^2-k^2b^{*2}-l^2c^{*2})/2klb^*c^*$$

where $\sigma_{okl}$ is the relative distance from the origin to the point okl.

Thus from the methods described above, the unit cell constants can be calculated.

The standard deviation is used here as a measure of precision. The estimated standard deviation (s. d.) per single determination is calculated by the following formula,

$$s.d.=((d_1^2+d_2^2+\ldots\ldots+d_n^2)/(n-1))^{1/2}$$

where d is the deviation of each single measurement from the mean, and n is the number of determinations made.

The estimated standard deviation of the mean (S. D.) is the estimated standard deviation of a single determination divided by the square of the

number of determinations.

$$S.D. = s.d./n^{1/2}$$

1. Oscillation photograph

$r_F = 28.45$ mm ( checked against Nacl)

$\lambda = 1.5418$Å

Table II. Determination of Cell Edge from Oscillation Data

| n | $y_n$(mm) | $r_F/y_n$ | $(r_F/y_n)^2$ | $n(1+(r_F/y_n)^2)^{1/2}$ | b | %error |
|---|---|---|---|---|---|---|
| 1 | 4.95 | 5.748 | 33.040 | 5.834 | 8.996 | 0.022 |
| 2 | 10.39 | 2.738 | 7.498 | 5.830 | 8.989 | 0.055 |
| 3 | 17.08 | 1.666 | 2.775 | 5.829 | 8.987 | 0.077 |
| 4 | 26.85 | 1.060 | 1.123 | 5.828 | 8.986 | 0.089 |
| 5 | 47.0 | 0.605 | 0.366 | 5.844 | 9.010 | 0.066 |
| | | | | | Mean= $8.994 \pm 0.003$Å | |

Standard deviation for a single determination=0.007Å

Standard deviation of the mean =0.003Å

2. Zero level Weissenberg photograph

$$\gamma = (360/2\pi r_F)x$$

$r_F = 28.45$ mm

$$\gamma = 2.014x$$

For zero level

$$\gamma = 2\theta$$

thus $\theta = 1.007x$

$$d_{hol} = \lambda / 2\sin\theta_{hol} = \lambda / 2\sin(1.007x)$$

Table III. Determination of $d_{001}$ from Zero Level Weissenberg Photograph

| ool | $x_{ool}$ (mm) | $\theta_{ool}$ | $\sin\theta_{ool}$ | $d_{ool}$ | $d_{ool}$ | error% |
|---|---|---|---|---|---|---|
| 4 | 9.65 | 9.72 | 0.16878 | 4.5675 | 18.270 | 0.027 |
| 5 | 12.10 | 12.18 | 0.21128 | 3.6487 | 18.244 | 0.114 |
| 6 | 14.55 | 14.65 | 0.25291 | 3.0481 | 18.288 | 0.125 |
| 8 | 19.60 | 19.74 | 0.33764 | 2.2832 | 18.266 | 0.005 |
| 9 | 22.15 | 22.31 | 0.37959 | 2.0309 | 18.278 | 0.071 |
| 10 | 24.80 | 24.97 | 0.42209 | 1.8264 | 18.264 | 0.005 |
| 11 | 27.45 | 27.64 | 0.46390 | 1.6618 | 18.082 | 0.028 |
| 12 | 30.25 | 30.46 | 0.50692 | 1.5208 | 18.249 | 0.088 |
| 13 | 33.05 | 33.28 | 0.54872 | 1.4049 | 18.264 | 0.005 |
| 14 | 35.95 | 36.20 | 0.59061 | 1.3053 | 18.274 | 0.049 |
| 16 | 42.20 | 42.50 | 0.67559 | 1.1411 | 18.258 | 0.038 |
| 17 | 45.60 | 45.92 | 0.71833 | 1.0732 | 18.244 | 0.114 |
| 18 | 49.10 | 49.44 | 0.75970 | 1.0147 | 18.265 | 0.000 |

Mean=18.265$\pm$0.004A

Standard deviation for a single determination=0.013Å

Standard deviation of the mean =0.004Å

Table IV. Determination of $d_{100}$ from Zero Level Weissenberg Photograph

| hoo | $x_{hoo}$ (mm) | $\theta_{hoo}$ | $\sin\theta_{hoo}$ | $d_{hoo}$ | $d_{loo}$ | error% |
|---|---|---|---|---|---|---|
| 1 | 6.20 | 6.24 | 0.10870 | 7.0920 | 7.0920 | 0.094 |
| 2 | 12.45 | 12.54 | 0.21712 | 3.5505 | 7.1013 | 0.037 |
| 3 | 18.88 | 19.01 | 0.32575 | 2.3665 | 7.0995 | 0.011 |
| 4 | 25.55 | 25.73 | 0.43413 | 1.7757 | 7.1028 | 0.058 |
| 7 | 49.15 | 49.49 | 0.76041 | 1.0138 | 7.0966 | 0.030 |
| 8 | 59.88 | 60.30 | 0.86863 | 0.88749 | 7.0999 | 0.017 |

Mean=7.0987±0.0017A

Standard deviation for a single determination=0.0039Å

Standard deviation of the mean =0.0017Å

For $\beta$ * angle

$$\cos\beta^* = (4\sin^2\theta_{hol} - h^2a^{*2} - l^2c^{*2})/2hla^*c^*$$

$$\theta_{hol} = 1.007x_{hol}$$

$$a^* = \lambda/d_{100} = 1.5418/7.0987 = 0.21719$$

$$c^* = \lambda/d_{001} = 1.5418/18.265 = 0.084413$$

$$a^{*2} = 4.71715\times10^{-2}$$

$$c^{*2} = 0.71256\times10^{-2}$$

$$2a^*c^* = 3.66674\times10^{-2}$$

Table V. Determination of $\beta^*$ Angle from Zero Level Weissenberg Photograph

| hol | $x_{hol}$ | $\theta_{hol}$ | $\sin\theta_{hol}$ | $4\sin^2\theta_{hol}$ | $\cos\beta^*$ | $\beta^*$ | error% |
|---|---|---|---|---|---|---|---|
| 1014 | 35.15 | 35.04 | 0.57928 | 1.34226 | -0.19778 | 101°24' | 0.01 |
| 3010 | 28.5 | 28.70 | 0.48022 | 0.92244 | -0.19515 | 101°16' | 0.15 |
| 404 | 25.5 | 25.68 | 0.43312 | 0.75037 | -0.20178 | 101°38' | 0.22 |
| 5010 | 28.0 | 38.27 | 0.61932 | 1.53423 | -0.19506 | 101°15' | 0.16 |
| 708 | 49.9 | 50.25 | 0.76884 | 2.36444 | -0.19626 | 101°19' | 0.10 |
| 807 | 58.85 | 59.26 | 0.85949 | 2.95489 | -0.20124 | 101°36' | 0.18 |
| | | | | | | Mean=101°25'$\pm$7' | |

Standard deviation for a single determination=0.279°

Standard deviation of the mean =0.113°

3. Precession photograph

Since the precession camera was not calibrated with Nacl, the precision of the cell constants determined from the zero level precession photographs is uncertain. Only the $\alpha^*$ and $\gamma^*$ angles which can not be obtained from the oscillation and zero level Weissenberg photographs are used.

$\gamma^*$ angle

From the a*b* precession photograph, $\gamma^*$ angle is found to be 90°.

$\alpha^*$ angle

$$\cos\alpha^* = (\sigma_{okl}^2 - k^2b^{*2} - l^2c^{*2})/2klb^*c^*$$

Table VI. Determination of $\alpha^*$ Angle from Zero level Precession Photograph

| Distance Measured | $2\sigma_{okl}$ | $\sigma_{okl}$ | $\cos\alpha^*$ | $\alpha^*$ | error% |
|---|---|---|---|---|---|
| $0\bar{2}2-02\bar{2}$ | 47.0 | 23.5 | -0.09527 | 95°28' | 0.10 |
| $0\bar{2}3-02\bar{3}$ | 52.8 | 26.4 | -0.09669 | 95°33' | 0.01 |
| $0\bar{2}4-02\bar{4}$ | 59.75 | 29.88 | -0.09905 | 95°41' | 0.14 |
| $0\bar{2}5-02\bar{5}$ | 67.4 | 33.7 | -0.09774 | 95°37' | 0.04 |
| $0\bar{2}6-02\bar{6}$ | 75.55 | 37.78 | -0.09601 | 95°31' | 0.06 |
| | | | | Mean=95°34'±5' | |

Standard deviation for a single measurement=0.172°

Standard deviation of the mean =0.077°

4. Calculation

The cell constants obtained from the different x-ray pictures are summarized as below.

$b=8.994\text{Å}$

$d_{100}=7.0987\fallingdotseq 7.099\text{Å}$

$d_{001}=18.265\text{Å}$

$\alpha^*=95°34'$

$\beta^*=101°25'$

$\gamma^*=90°$

To calculate the interaxial angles in the direct cell, we proceed as follow (6).

$$\cos\alpha = (\cos\beta^* \cos\gamma^* - \cos\alpha^*)/\sin\beta^* \sin\gamma^*$$

$$\alpha = 84°19'$$

Similarly,

$$\beta = 78°32'$$

$$\gamma = 88°52'$$

$$a = d_{100}/\sin\gamma^* \sin\beta = 7.099/0.98004 = 7.244\text{Å}$$

$$b = 8.994\text{Å}$$

$$c = d_{001}/\sin\beta \sin\alpha^* = 18.265/(0.98004)(0.99528) = 18.725\text{Å}$$

In summary

$a = 7.244 \pm 0.002$Å  $b = 8.994 \pm 0.003$Å  $c = 18.725 \pm 0.004$Å

$\alpha = 84°19' \pm 3'$  $\beta = 78°32' \pm 2'$  $\gamma = 88°52' \pm 4'$

Let V be the unit cell volume

$$V = abc \sin\alpha \sin\beta \sin\gamma^*$$

$$= (7.244)(8.994)(18.725)(0.99508)(0.98004)$$

$$= (65.153)(18.261)$$

$$= 1{,}189.8\text{Å}^3$$

For $Ca(C_{10}H_7HPO_4)_2 \cdot 3H_2O$

Molecular weight = 540.426

Density = 1.5031 g/ml

Molecular volume = $540.426/(1.5031)(0.6023)$

$= 540.426/0.90531$

$= 596.9\text{Å}^3$

Number of molecules per unit cell = $1{,}189.8/596.9$

$= 1.993$

Let $D_o$ and $D_c$ be observed and calculated density respectively.

$D_o = 1.503$ g/ml

$D_c = 1.503\ (2/1.993)$

$= 1.508$ g/ml

## SECTION IV

## INDEXING THE TRICLINIC EQUI-INCLINATION WEISSENBERG X-RAY PHOTOGRAPH AND A METHOD OF CHECKING

Usually, x-ray diffraction photographs taken by the equi-inclination Weissenberg method can be indexed routinely. However, for triclinic crystals, certain problems arise in the indexing and it is worth while examining the methods used here.

It is not difficult to index the zero level triclinic Weissenberg photograph. Problems start when we try to index the upper level triclinic equi-inclination Weissenberg pictures. This is because the reciprocal lattice axial lines of a triclinic crystals do not show up as straight lines on the upper equi-inclination Weissenberg photographs. The method outlined here offers not only the correct indexing but also the unique choice of unit cell.

For the triclinic system, since there is no symmetry except possibly an inversion center, a primitive cell is always chosen. There are many ways to choose a primitive cell in a triclinic lattice. Given the three translations of the primitive cell edges x, y, z and the three axial labels a, b, and c, there are six ways of fixing a, i.e., x, -x, y, -y, z, and -z. If a is assigned as x or -x, there are four ways to fix b, that is y, -y, z and -z. Then, if a right hand coordinate system is chosen, c is automatically fixed. Thus, there are a total of twenty-four possible ways of fixing labels to the translations. Balashov (3,4) devised some rules, which will theoretically lead to a unique choice.

Balashov's method:

1. Select a primitive cell having the smallest volume.

2. Let $c > b > a$

This rule follows Buerger's convention (6). Usually, this will lead to $a^* > b^* > c^*$. Donnay and Nowacki (14) suggested a different order-convention; $b > a > c$. The reason they prefer c as the shortest axis is that crystals ordinarily grow so that they are elongated parallel to the shortest translations and the choice of c for the shortest translation causes the crystal to look like a vertical column. On the other hand, the Buerger's convention $c > b > a$ has the following advantages as indicated by Balashov (2); (a) It is convenient for tabulation purposes (b) It can be used for tetragonal and hexagonal crystals, where (in contrast to the orthorhombic system) the c and a axes are fixed by symmetry convention, the ratio c/a is greater than unity, i.e., c is greater than a which violated Donnay's convention.

3. Let $\alpha, \beta, \gamma$ be homogeneous, that is, all obtuse or all acute.

The ordinary procedure of doing this is first to choose $\alpha^*$, $\beta^*, \gamma^*$ all acute. If $\alpha, \beta, \gamma$ do not turn out all obtuse, adjust $\alpha^*$, $\beta^*$, or $\gamma^*$ (by taking their supplement) until $\alpha, \beta, \gamma$ are all acute. Some people prefer that all $\alpha, \beta, \gamma$ be non-acute. To convert all acute angles to all obtuse ones, the Delaunay Reduction (20) may be used. The Delaunay Reduction gives the cell which has the three interaxial angles ($\alpha, \beta, \gamma$) all non-acute, and within the limits imposed by this condition, the three translations a, b, c the shortest possible. The Delaunay Reduction is based on the following principles: the reciprocal of an

obtuse parallepiped is an acute one and usually vice versa.

To show that the Balashov's method leads to an unique choice of unit cell, proceed as follows.

Fig. 4 a, b shows the general arrangement of three axial lables a, b, c and the interaxial angles $\alpha, \beta, \gamma$, as well as the projection of c axis on ab plane.

If the projection of c-axis or z lies in the MxN zone, i.e., on the positive x side of the perpendicular to x as shaded, angle xoz or $\beta$ is acute.

Similarly, if the projection of z lies in the TyS zone, i.e., on the positive y side of the perpendicular to y as shaded, angle yoz or $\alpha$ is acute.

Since $xyz_1$ rotated 180 degree equal to $\bar{x}\bar{y}z_3$

$xyz_2$ rotated 180 degree equal to $\bar{x}\bar{y}z_4$

there are only two kinds of triclinic crystals, i.e., axial system like $xyz_1$ (type 1) and $xyz_2$ (type 2).

Type 1: $xyz_1$

$\alpha$ or yoz is acute

$\beta$ or xoz is acute

$\gamma$ or xoy is acute

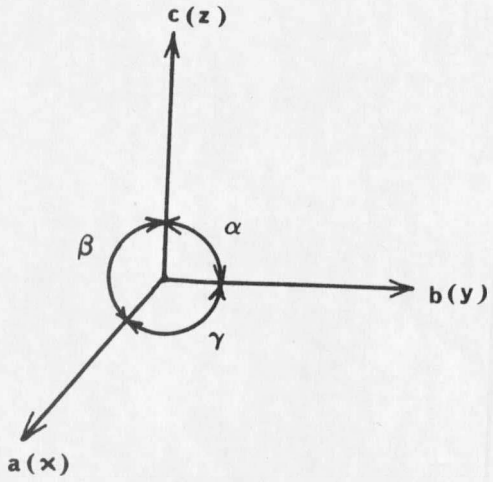
Type 2: $xyz_2$

$\alpha$ or yoz is acute

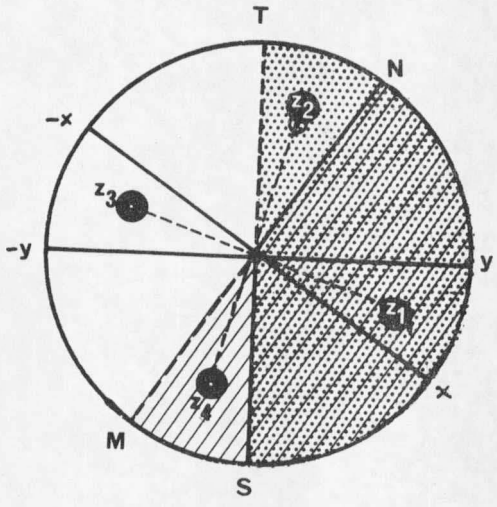
$\beta$ or xoz is obtuse

$\gamma$ or xoy is acute

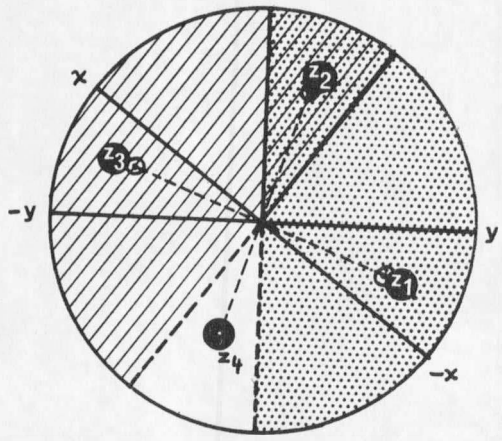
We can have different representations of the triclinic crystal




a.




b.




c.

Figure 4 Illustration of the unique choice for the unit cell

by different combinations of acute and obtuse angles.

For example, if a is changed from plus x to minus x, the character of $\beta$ and $\gamma$ changes from acute to obtuse or vice versa, as shown in Fig. 4 c.

Type 1: $\bar{x}yz_1$

$\alpha$ or yoz is acute

$\beta$ or xoz is obtuse

$\gamma$ or xoy is obtuse

Type 2: $\bar{x}yz_2$

$\alpha$ or yoz is acute

$\beta$ or xoz is acute

$\gamma$ or xoy is obtuse

Following the same procedure, we can have all the possible arrangements of a, b, c and the angle characters as listed in the following table. (table in Buerger (7) with corrections)

Table VII. Possible Sets of Interaxial Angles in the Triclinic System

Type 1 crystal

| Orientation | cos | Type of Coordinate System | Designation of Representation | |
|---|---|---|---|---|
| abc is $xyz_1$ | + + + | R | 1R | Normal |
| abc is $\bar{x}yz_1$ | + - - | L | 3L | |
| abc is $\bar{x}\bar{y}z_1$ | - - + | R | 2R | |
| abc is $x\bar{y}z_1$ | - + - | L | 4L | |
| abc is $\bar{x}\bar{y}\bar{z}_1$ | + + + | L | 1L | Normal |
| abc is $\bar{x}y\bar{z}_1$ | + - - | R | 3R | |
| abc is $xy\bar{z}_1$ | - - + | L | 2L | |

| Orientation | cos | Type of Coordinate System | Designation of Representation | | |
|---|---|---|---|---|---|
| abc is $\bar{x}y\bar{z}_1$ | - + - | R | 4R | | |
| | | Type 2 Crystal | | | |
| abc is $xyz_2$ | + - + | R | 1R | | |
| abc is $\bar{x}yz_2$ | + + - | L | | 3L | |
| abc is $\bar{x}\bar{y}z_2$ | - + + | R | 2R | | |
| abc is $x\bar{y}z_2$ | - - - | L | | 4L | Normal |
| abc is $\bar{x}\bar{y}\bar{z}_2$ | + - + | L | | 1L | |
| abc is $x\bar{y}\bar{z}_2$ | + + - | R | 3R | | |
| abc is $xy\bar{z}_2$ | - + + | L | | 2L | |
| abc is $\bar{x}y\bar{z}_2$ | - - - | R | 4R | | Normal |

A crystal can be either one of the two crystal types and can not be both at the same time. Hence, once the type of coordinate system is chosen, there is only one case for the interaxial angles to be all acute or all obtuse. Balashov's method of letting $\alpha$ , $\beta$ , $\gamma$ be all obtuse or all acute is thus justified.

A suggested indexing method for the triclinic Weissenberg photographs:

In the equi-inclination Weissenberg method, the camera is so inclined that the direct x-ray beam and the diffracted beam are equally inclined to the layers of the reciprocal lattice. The equi-inclination keeps the reciprocal lattice rotation axis exactly on the circumference of the reflecting circle of the n-layer.

Certain indexing problems arise for triclinic crystals for which Weissenberg photographs are taken. It should be understood that x-ray

diffraction photographs provide a picture of the reciprocal lattice. For the ease of illustration, it is assumed that the crystal is mounted on b axis unless otherwise specified. The two reciprocal axes a* and c* will show up as straight lines on the zero Weissenberg photograph and the photograph is indexed in the normal manner. In indexing the upper level Weissenberg photographs for triclinic crystal, the reciprocal lines h10, h20 01ℓ, 02ℓ etc. no longer appear as straight lines. If any reciprocal lattice axial line e.g. hno, or onl passes through the rotation axis, a straight line will result on all the equi-inclination Weissenberg levels. This can occur if any upper level reciprocal lattice line projection on the zero level coincides with the a* or c*. For orthogonal systems this is always the case, for monoclinic systems it is the case if the crystal is mounted on b, but not so if mounted on a or c, and would only be accidentally the case for triclinic crystals. However, for any non-orthogonal crystal, a non-axial reciprocal lattice line may, on one level or another, accidentally pass through the rotation center, producing a straight line on the equi-inclination Weissenberg photograph. Thus, for triclinic crystal, usually no upper level reciprocal lattice line will pass through the rotation axis. The problem of indexing the triclinc upper level equi-inclination Weissenberg photographs is to recognize the reciprocal lattice lines. Assuming all the reciprocal lattice lines on the zero level are known, the easy way to do this is to project the upper levels onto the zero level. Fig. 5 a represents the zero level where the point O is the rotation center, the horizontal line passing through the rotation center is the c* axis

or ool line, and the line passing through the point O and making an angle $\beta^*$ with c* is a* axis or hoo line. All the upper level reciprocal lattice points oko must lie on the b* axis. The length and positions of the b* axis projection on the zero level a* c* plane can be calculated (For calculation, see next paragraph). The positions of the point oko corresponding to the $k^{th}$ level can thus be located. From oko, construct the $k^{th}$ level reciprocal lattice network hkl by drawing lines parallel to a* and c*. Consider the four reciprocal lattice lines sitting closest to the rotation center, O. These represent the four festoons next to the two straight axial lines of the zero level projected onto the $k^{th}$ level. The festoon at the right or left of a* projection corresponds to the right or left reciprocal lattice lines of a* in Fig. 5 a. The other two festoons can be identified in the same manner. Once these four festoon (the reciprocal lattice lines) have been indexed properly, there is no problem indexing the other reciprocal lattice points. An illustration of these procedures is shown in Fig. 5.

A calculation for the length and location of the axial projection:

First obtain all the reciprocal lattice cell constants a*, b*, c* and $\alpha^*, \beta^*, \gamma^*$. From these, the reciprocal lattice unit cell is constructed as shown in Fig. 6 where three axes meet at the point O, and OA, OB, OC represent the unit length of a*, b* and c* respectively. Then, in the BOC plane (b* c* plane), draw BN perpendicular to OC. From B, draw line BM perpendicular to the plane AOC (a* C* plane). Connect NM and OM. From the geometrical relation, we have

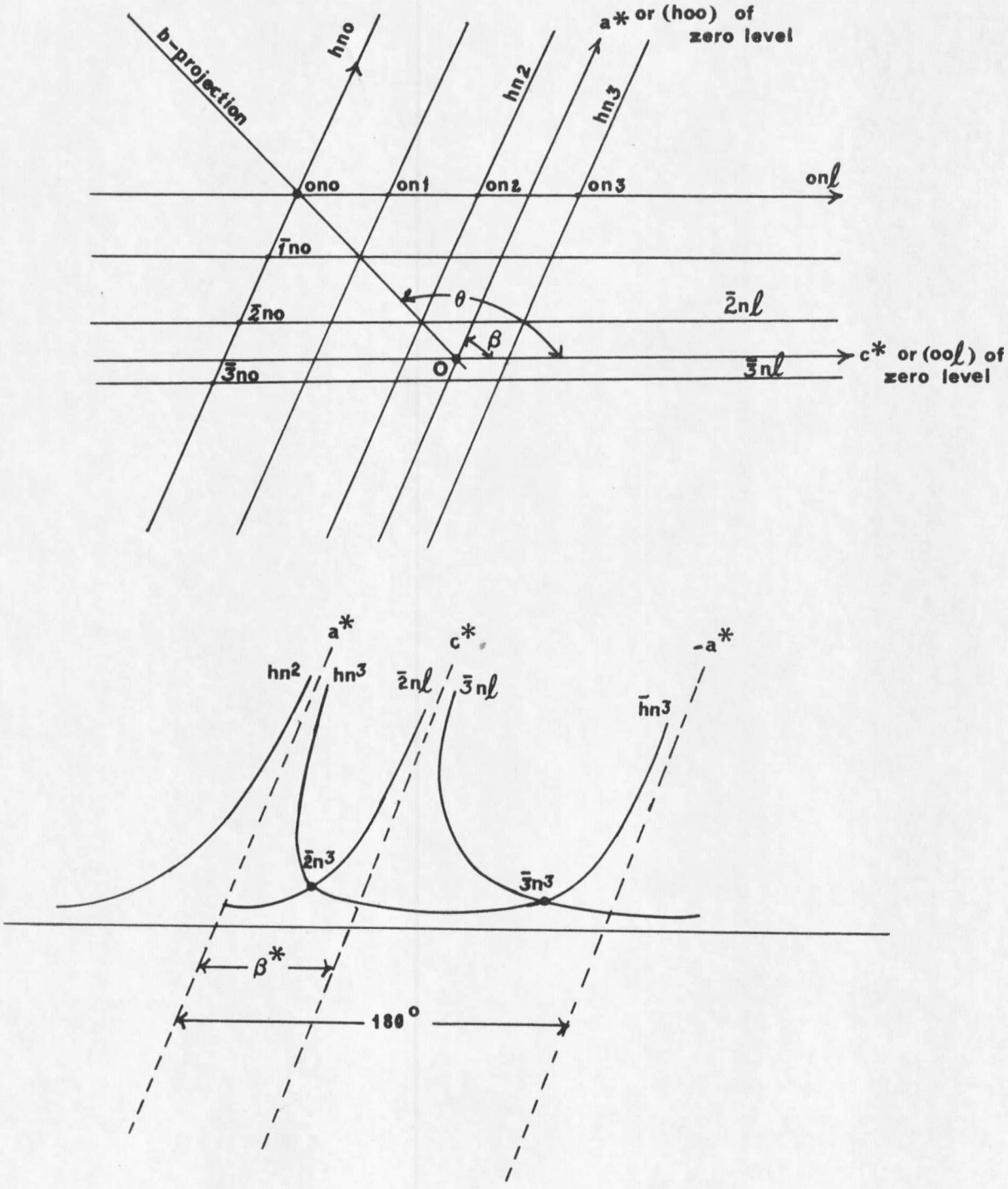



Figure 5 An illustration of the indexing procedures

$ON = b^* \cos\alpha^*$

$BN = b^* \sin\alpha^*$

Angle BNM = $180-\gamma$ (for derivation, see Buerger (6))

$BM = b^* \sin\alpha^* \sin\gamma$

$NM = -b^* \sin\alpha^* \cos\gamma$

$OM = b^*(1-\sin^2\alpha^* \sin^2\gamma)^{1/2}$

$\cos p = (ON^2+OM^2-MN^2)/2ON \cdot OM$

$= ((b^*\cos\alpha^*)^2+b^{*2}(1-\sin^2\alpha^* \sin^2\gamma)-(b^*\sin\alpha^*\cos\gamma)^2)/$

$2(b^*\cos\alpha^*)b^*(1-\sin^2\alpha^* \sin^2\gamma)^{1/2}$

Where OM is the unit length of b* projection on a* c* plane.

p is the location of b* projection on a*c* plane (the angle between b* projection and c*).

It is noted that the approximate location of b* projections can be determined as follows by the interaxial angles $\alpha^*$ and $\gamma^*$ only.

Table VIII. Determination of b*- Projection Location on a* c* Plane.

| Interaxial angles | | Quadrant where b* projection lies |
|---|---|---|
| acute | acute | 1 |
| obtuse | obtuse | 3 |
| acute | obtuse | 4 |
| obtuse | acute | 2 |

Index-checking method:

The index-checking method will serve as a check on proper

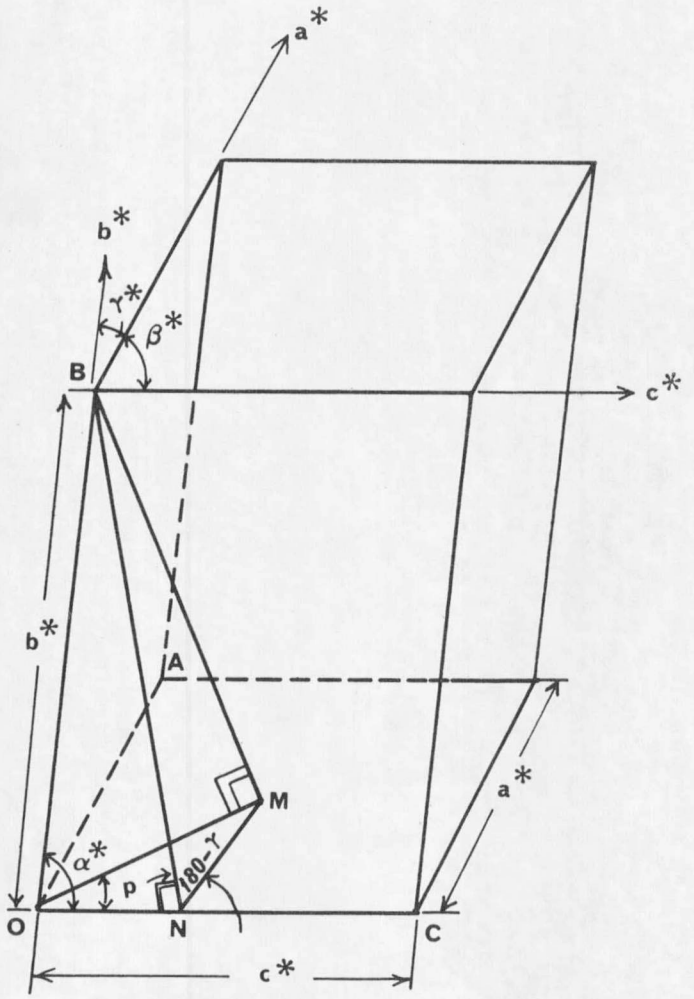



Figure 6 The calculation of b*-projection on a*c* plane

indexing of the equi-inclination Weissenberg photographs. The calculation of the vertical distance of the hkl reflection from the equator line, $x_{calc.}$ is compared with the measured distances $x_{obs.}$ If the percentage error (error%)

$$\text{Error \%} = (x_{obs.}-x_{calc.})/x_{obs.}$$

equal or less than 5%, a correct indexing is assumed.

Index-checking formulas:

For equi-inclination Weissenberg method

$$x_{calc.} = \tfrac{1}{2}\cos^{-1}(2(1-\sin^2\theta)/\cos^2\mu - 1)$$

Where $\mu$ is the angle of inclination

$\sin^2\theta$ may be calculated from Wolf-Bragg equation as below:

$$4\sin^2\theta_{hkl}=h^2a^{*2}+k^2b^{*2}+l^2c^{*2}+2hka^*b^*\cos\gamma^*+$$
$$2klb^*c^*\cos\alpha^*+2lhc^*a^*\cos\beta^*$$

Derivation of index-checking formulas:

a. Wolf-Bragg equation

Note: The Wolf-Bragg equation is not present in many standard reference books. I found this equation in a Russion journal (19,5), translated and sent to me by V. Balashov. Since I could not find a derivation for this equation in the literature, a derivation is included here.

A reciprocal lattice vector $\vec{\sigma}_{hkl}$ is a vector, drawn from the reciprocal lattice origin to the reciprocal lattice point hkl as shown in Fig. 7 a. It has three components ha*, kb*, and lc* along the three axial directions.

From the vector analysis, we have

$$\vec{\sigma}_{hkl}=h\vec{a}^*+k\vec{b}^*+l\vec{c}^*$$

$$\sigma^2_{hkl}=\vec{\sigma}_{hkl}\cdot\vec{\sigma}_{hkl}$$

$$=(h\vec{a}^*+k\vec{b}^*+l\vec{c}^*)\cdot(h\vec{a}^*+k\vec{b}^*+l\vec{c}^*)$$

$$=h^2a^{*2}+k^2b^{*2}+l^2c^{*2}+2hk\vec{a}^*\cdot\vec{b}^*+2kl\vec{b}^*\cdot\vec{c}^*+2hl\vec{a}^*\cdot\vec{c}^*$$

Since $\vec{a}^*\cdot\vec{b}^*=a^*b^*\cos\gamma^*$, $\vec{b}^*\cdot\vec{c}^*=b^*c^*\cos\alpha^*$,

$\vec{a}^*\cdot\vec{c}^*=a^*c^*\cos\beta^*$

$$\sigma^2_{hkl}=h^2a^{*2}+k^2b^{*2}+l^2c^{*2}+2hka^*b^*\cos\gamma^*+2klb^*c^*\cos\alpha^*$$
$$+2hla^*c^*\cos\beta^*$$

From Bragg's equation (Fig. 7b)

$$\lambda=2d_{hkl}\sin\theta_{hkl}$$

or $$4\sin^2\theta_{hkl}=(\lambda/d_{hkl})^2=\sigma^2_{hkl}$$

Combining the above equations, we have

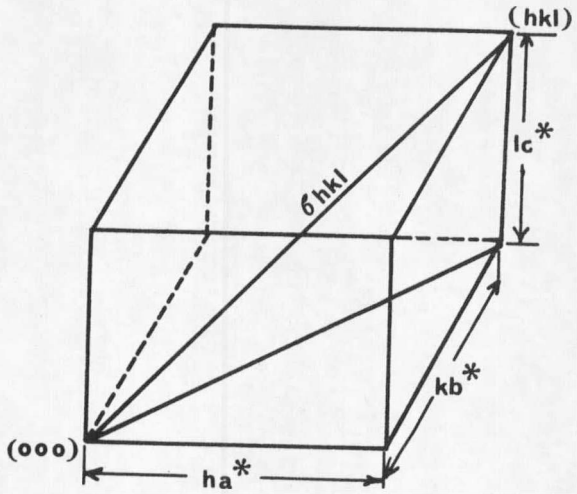
$$4\sin^2\theta_{hkl}=h^2a^{*2}+k^2b^{*2}+l^2c^{*2}+2hka^*c^*\cos\gamma^*$$
$$+2klb^*c^*\cos\alpha^*+2hla^*c^*\cos\beta^*$$

b. Equi-inclination Weissenberg index-checking formula

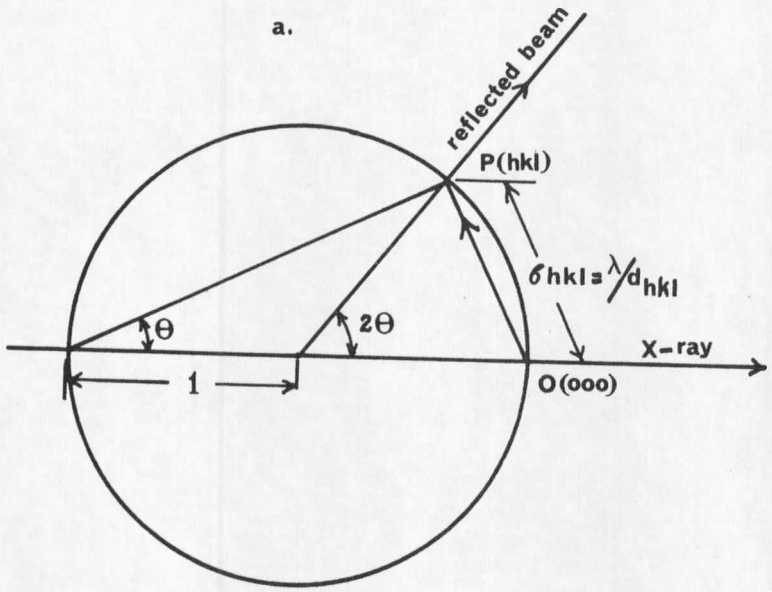
Fig. 8 a, b illustrates the equi-inclination method in three dimensions and the important part of the spherical surface diagram. The crystal is sitting at the center of a unit radius sphere (sphere of reflection). Since the angle (in radian) subtended from the center of a sphere or a circle is equal to the arc length divided by the radius and the radius of the sphere of reflection is unit,

$\widehat{PO}=2\theta$ $\qquad$ $\widehat{AB}=\gamma$

$\widehat{PA}=\chi$ $\qquad$ $\widehat{BO}=\mu$




a.




b.

Figure 7 Derivation of the Wolf-Bragg equation

Where $\Theta$ is the Bragg glancing angle

$\chi = \tan^{-1} y_n/r_F$, $y_n$ is the distance from $n^{th}$ level line to the center line in an oscillation picture, $r_F$ is the film radius.

$\gamma$ is the general reflection angle

$\mu$ is the inclination angle

Note that

Angle PAB=90 degree, Angle ABO=90 degree

Angle PAO=90 degree + Angle BAO

From the spherical geometry, the following equations are true:

(1) For right spherical triangle

$\cos c = \cos a \cos b$, $\sin A = \sin a / \sin c$

(2) For oblique spherical triangle

$\cos a = \cos b \cos c + \sin b \sin c \cos A$

Let $\overset{\frown}{AO}=y$, Angle BAO=z

Since ABO is a right spherical triangle (Angle ABO is 90 degree),

$$\cos y = \cos\mu \cos\gamma \quad \ldots\ldots\ldots\ldots\ldots\ldots (1)$$

or $\sin y = (1-\cos^2\mu \cos^2\gamma)^{1/2}$

$$\sin z = \sin\mu / \sin y$$

$$= \sin\mu / (1-\cos^2\mu \cos^2\gamma)^{1/2} \quad \ldots\ldots\ldots\ldots (2)$$

PAO is an oblique spherical triangle; thus

$$\cos 2\Theta = \cos\chi \cos y + \sin\chi \sin y \cos(90+z)$$

$$= \cos\chi \cos y - \sin\chi \sin y \sin z \quad \ldots\ldots\ldots\ldots (3)$$

Substituting equations (1) and (2) into equation (3),

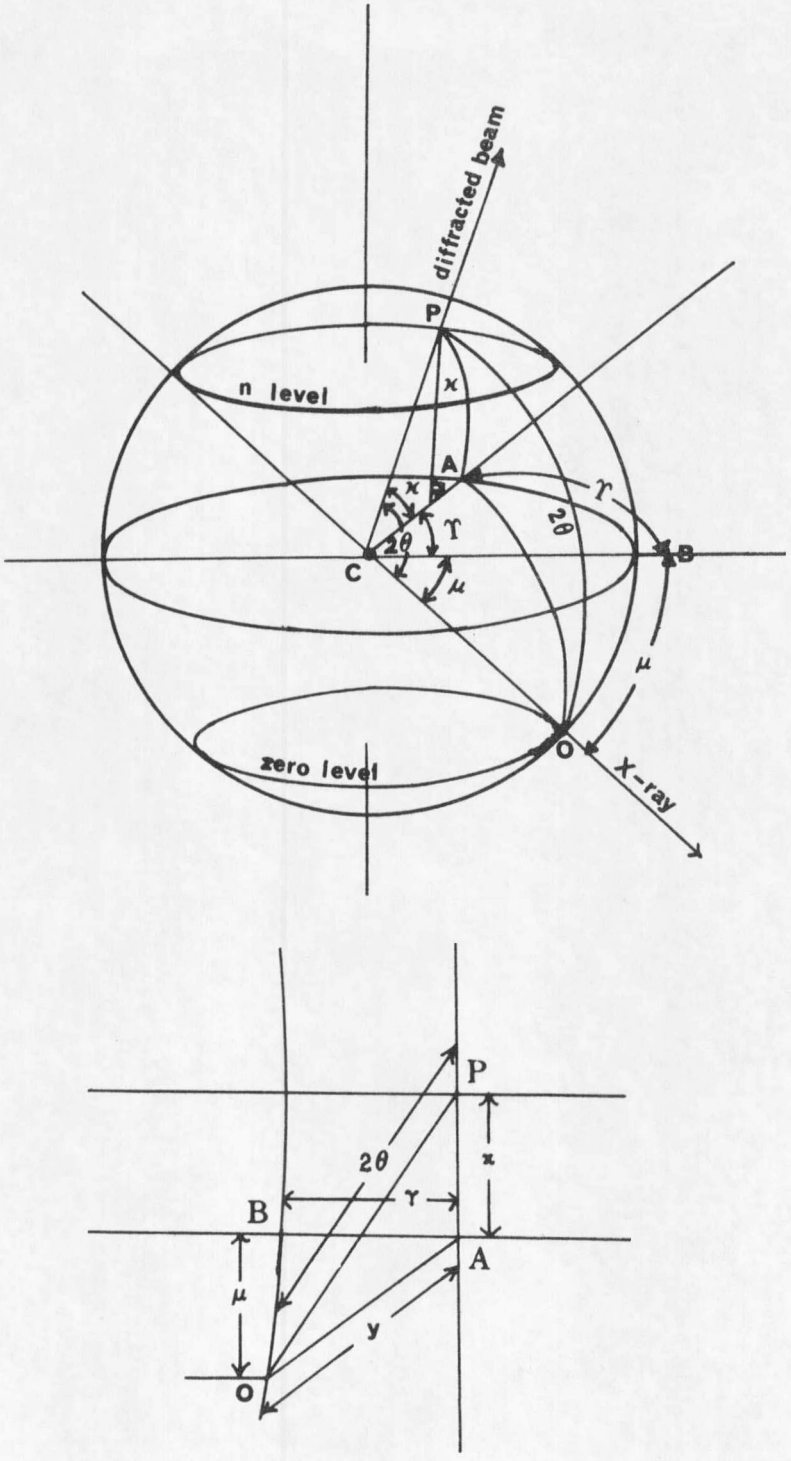



Figure 8 a. Illustration for equi-inclination Weissenberg method
b. The important spherical surface diagram

$$\cos 2\theta = \cos\chi \cos\mu \cos\gamma - \sin\chi \sin\gamma \sin\mu / \sin\gamma$$

$$= \cos\chi \cos\mu \cos\gamma - \sin\chi \sin\mu$$

For equi-inclination method

$$\chi = \mu$$

Thus, $\cos 2\theta = \cos^2\mu \cos\gamma - \sin^2\mu = \cos^2\mu \cos\gamma - 1 + \cos^2\mu$

$$= \cos^2\mu (1+\cos\gamma) - 1 \quad \ldots\ldots\ldots\ldots (4)$$

or $$\cos\gamma = \frac{1+\cos 2\theta}{\cos^2\mu} - 1$$

$$= \frac{1+1-2\sin^2\theta}{\cos^2\mu} - 1$$

$$= \frac{2(1-\sin^2\theta)}{\cos^2\mu} - 1$$

Therefore, $x = \gamma/2 = \frac{1}{2}\cos^{-1}(2(1-\sin^2\theta)/\cos^2\mu - 1)$

D. Application

The unique choice of unit cell and the indexing methods for the triclinic crystals are applied to the triclinic crystal of calcium 1-naphthyl phosphate $Ca(C_{10}H_7HPO_4)_2 \cdot 3H_2O$. The results which will, in turn, serve as an illustration of the above methods will be reported in the following sections.

1. Unique choice of unit cell for calcium 1-naphthyl phosphate.

A direct calculation from the oscillation, zero level Weissenberg, and precession photographs gives us the following cell constants.

$d_{100} = 7.099$ Å

$b = 8.994$ Å

$d_{001}=18.265\text{Å}$

$\alpha^*=95^\circ 34'$ or $84^\circ 26'$

$\beta^*=101^\circ 25'$ or $78^\circ 35'$

$\gamma^*=90^\circ$

Since $d_{100}$ and $d_{001}$ are not too far from a and c respectively, the Balashov's second rule i.e., $c>b>a$ is temporarily used to assign the above labels.

To see whether all angles $\alpha$, $\beta$, $\gamma$ are homogeneous, first take $\alpha^*$, $\beta^*$, $\gamma^*$ all acute.

$\alpha^*=84\ 26'$

$\beta^*=78\ 35'$

$\gamma^*=90^\circ$

Then, $\sin\alpha^*=0.99528$ $\cos\alpha^*=0.09700$

$\sin\beta^*=0.98021$ $\cos\beta^*=0.19794$

$\sin\gamma^*=1.0$ $\cos\gamma^*=0.0$

Thus, $$\cos\alpha=\frac{\cos\beta^*\cos\gamma^*-\cos\alpha^*}{\sin\beta^*\sin\gamma^*}$$

$\cos\alpha=(0-0.09700)/0.98021=-0.09896$

$\alpha=95^\circ 41'$

$\cos\beta=(\cos\alpha^*\cos\gamma^*-\cos\beta^*)/\sin\alpha^*\sin\gamma^*$

$=-0.19794/0.99528=-0.19888$

$\beta=101^\circ 28'$

$\cos\gamma=(\cos\alpha^*\cos\beta^*-\cos\gamma^*)/\sin\alpha^*\sin\beta^*$

$=(0.0970)(0.19794)/(0.99528)(0.98021)$

$=0.01920/0.97558$

$=0.01968$

$\gamma = 88^{\circ}52'$

Since $\alpha, \beta$ both are obtuse, while $\gamma$ is acute, they are not homogeneous. This rules out the possibility of their being all obtuse. To make them all acute, adjust $\alpha^*, \beta^*$ by taking supplements. It is not difficult to obtain the following:

$\alpha^* = 95^{\circ}34'$

$\beta^* = 101^{\circ}25'$

$\gamma^* = 90^{\circ}$

$\cos\alpha = 0.09896$

$\alpha = 84^{\circ}19'$

$\cos\beta = 0.19888$

$\beta = 78^{\circ}32'$

$\cos\gamma = 0.01968$

$\gamma = 88^{\circ}52'$

Thus all the angles $\alpha, \beta, \gamma$ are acute, and accordingly homogeneous. The constants a and c can now be obtained as follows:

$a = d_{100}/\sin\beta \sin\gamma^* = 7.099/0.98004 = 7.244\text{Å}$

$c = d_{100}/\sin\beta \sin\alpha^* = 18.265/(0.98004)(0.99528) = 18.725\text{Å}$

$b = 8.994\text{Å}$

It is apparent that $c > b > a$, which is the Balashov's second rule. From this, our temporary label $d_{100} > b > d_{100}$ is justified. Indexing the triclinic crystal of calcium 1-naphthyl phosphate

a. Determination of the axial direction on which upper levels lie

The Balashov's rules already determine the orientation of three axes a, b, c and the crystal is found to be mounted on b axis, although we are not certain of the direction of b*. This is determined by using right-hand coordinates. Fig. 9c shows the orientation of the film with respect to the camera and x-ray. The observer is standing at the position such that the x-ray is passing through the sphere of reflection from left to right and the rotation dial is in front of the observer. In the zero level picture, the axial labels a*, c* and their directions are already fixed by the Balashov's rules as in Fig. 9 a. This will, in turn, fix the axial labels and their directions in Fig. 9 b and c. In Fig. 9 b, a* c* is assumed to lie in a horizontal plane. When c* rotates toward a*, from the right-hand coordinate, the positive b* must be vertical above the plane, i.e., positive b* is away from rotation dial. Since upper levels lie in the directions away from rotation dial, they must mount in the positive b* direction.

b. Calculation of the length and location of the axial projection.

In the calculation of the axial projection length, we are concerned with the relative lengths of a*, b*, c* rather than the absolute lengths. For ease of calculation, the relative lengths of a*, b*, c* will be used. The cell constants found are listed below.

a=7.244Å  b=8.994Å  c=18.725Å

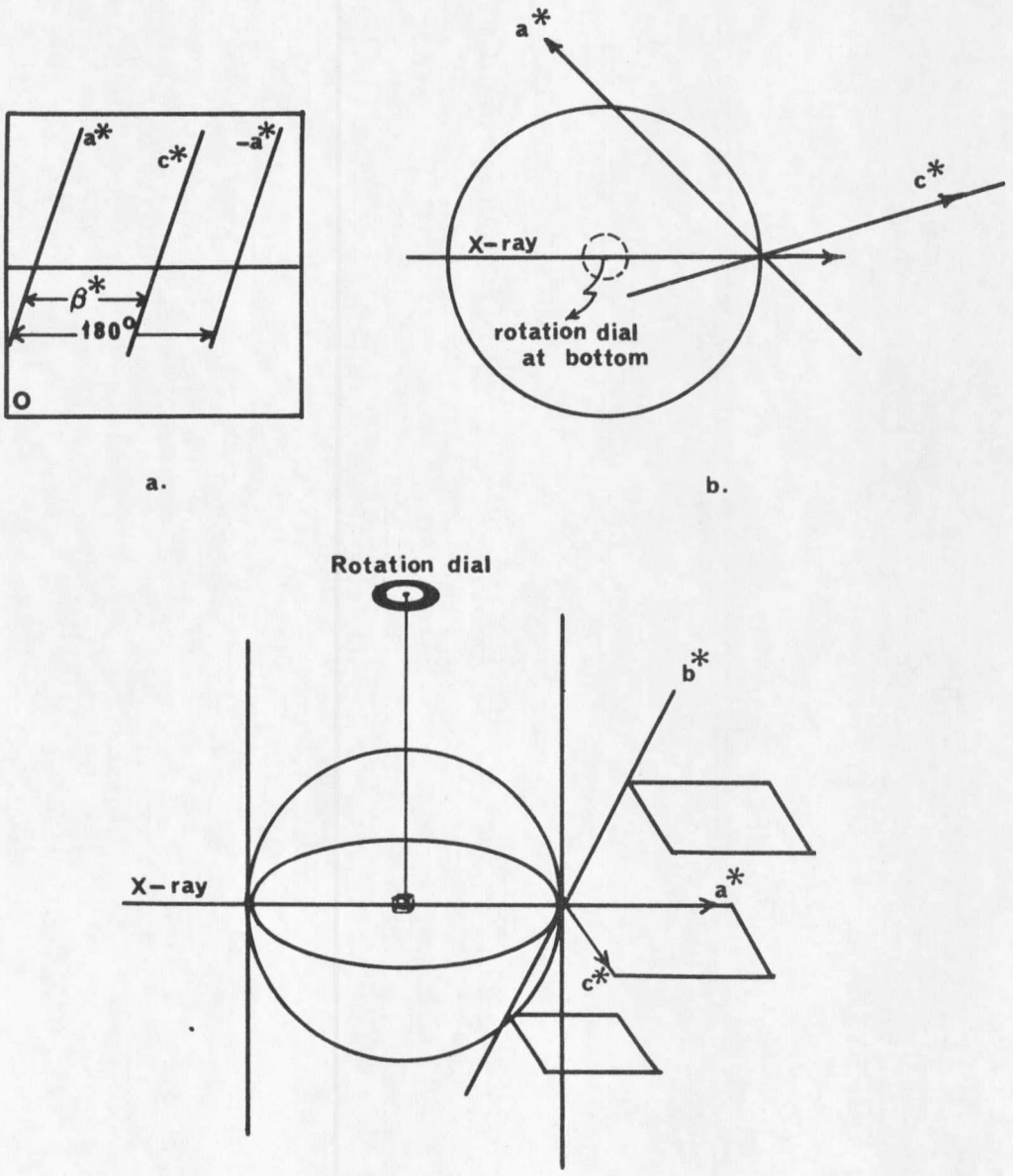



Figure 9 Orientation of film with respect to camera and x-ray

$\alpha = 84^\circ 19'$ $\beta = 78^\circ 32'$ $\gamma = 88^\circ 52'$

$d_{100} = 7.099\text{Å}$ $d_{010} = 8.950\text{Å}$ $d_{001} = 18.265\text{Å}$

$\alpha^* = 95^\circ 34'$ $\beta^* = 101^\circ 25'$ $\gamma^* = 90^\circ$

$a^* = \lambda/d_{100}$ $b^* = \lambda/d_{010}$ $c^* = \lambda/d_{001}$

$a^* : b^* : c^* = 1/d_{100} : 1/d_{010} : 1/d_{001} = 1/7.099 : 1/8.950 :$

$1/18.265 = 2.57 : 2.04 : 1$

Let $a^* = 2.57$ $b^* = 2.04$ $c^* = 1$

The b* projection $= OM$

$$= b^*(1-\sin^2\alpha^*\sin^2\gamma)^{1/2}$$

$$= 0.254$$

$$\cos p = ((b^*\cos\alpha^*)^2 + b^{*2}(1-\sin^2\alpha^*\sin^2\gamma) - (b^*\sin\alpha^*\cos\gamma)^2)/$$

$$2b^*\cos\alpha^* b^*(1-\sin^2\alpha^*\sin^2\gamma)^{1/2}$$

$$= -0.97867$$

$p = 180^\circ + 11^\circ 51' = 191^\circ 51'$ or $180^\circ - 11^\circ 51' = 168^\circ 9'$

The former value is in the third quadrant, while the latter value is in the second quadrant. $\alpha^*$ and $\gamma^*$ are used to determine the correct location for b* projection as discussed previously. Since $\alpha^*$ and $\gamma^*$ are both obtuse, the b* projection lies in the third quadrant. Hence, $p = 191^\circ 51'$.

Indexing the triclinic crystal of calcium 1-naphthyl phosphate:

The indexing of calcium 1-naphthyl phosphate is illustrated in Fig. 10 a, b, c, d. Two things are considered below.

a. Since the $\gamma^*$ angle is 90 degree, the reciprocal lattice axial line okl should appear as a straight line on each upper level. This was found to be the case except those okl lines were too weak

to see for k being odd due to the existence of a pseudo b-glide plane. The other reciprocal lattice axial line hko was not a straight line for all upper levels.

b. For fourth level, the h41 line shows up as a straight line on the film, because it happens to pass through the rotation axis.

Index-checking data:

For the checking of the indexing, I have written an IBM 1620 computer program (Fortran I). The results of the index-checking for calcium 1-naphthyl phosphate are listed in Table XXXV in appendix C. More than one thousand reflections have been checked and all gave percentage errors less than 5%. Thus, indexing is correct for this crystal. The successful solution of the structure further confirms the correct indexing of the equi-inclination photographs.

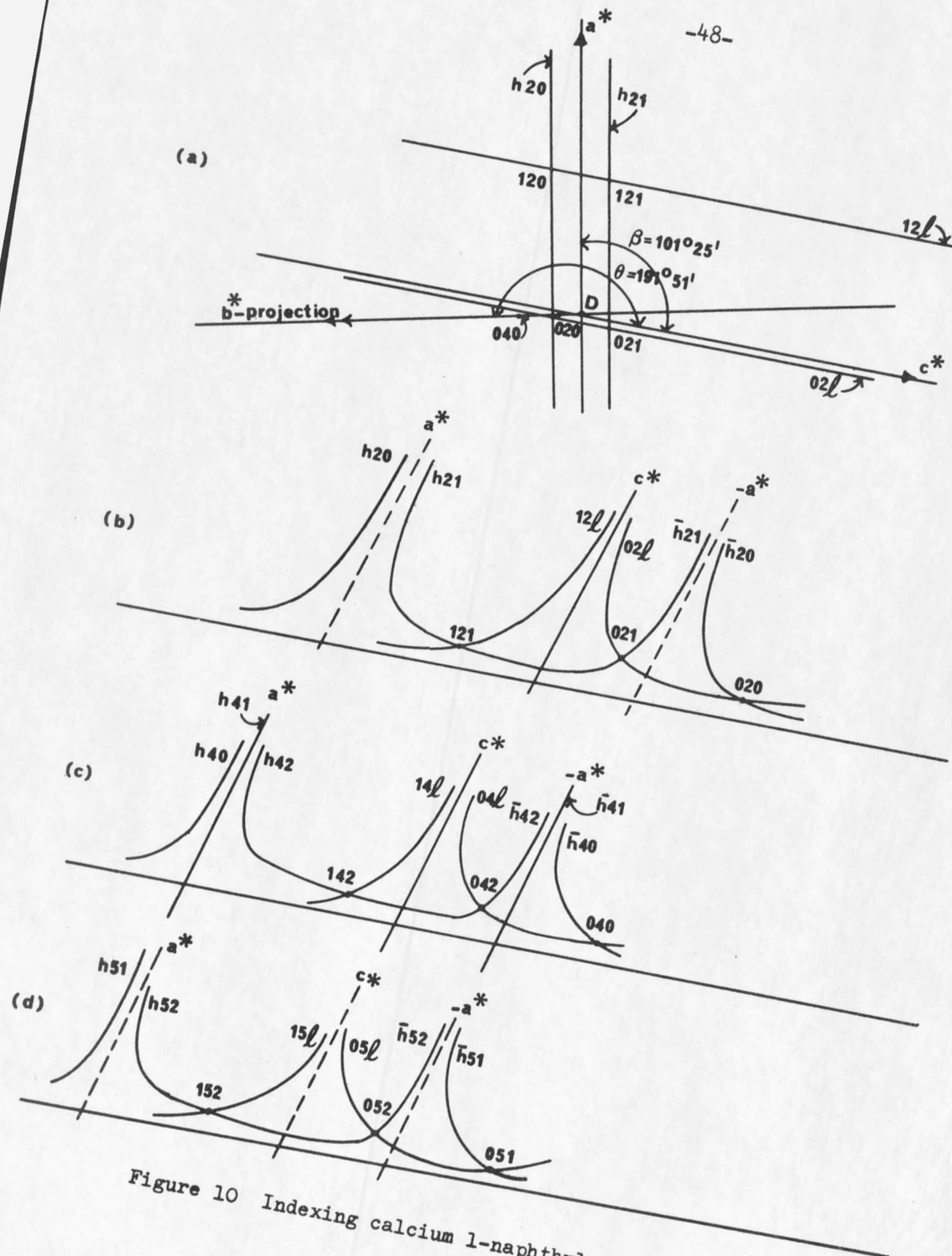



Figure 10 Indexing calcium 1-naphthyl phosphate

## SECTION V

## UNIQUE FEATURES OF DATA REDUCTION

### A. Scaling

The Weissenberg levels were scaled to a common basis (a) by precession photographs (b) by the Wilson plot.

(a) The integrated intensities of all the spots on the zero level precession photographs were read and corrected by the Lorentz and polarization factors. It was assumed that the x-ray spots on the precession pictures had more or less the same absorption correction as those of same index on the Weissenberg photographs. The precession intensities were compared with the corresponding Weissenberg intensities both of which were corrected for the Lorentz and polarization factors, and the Weissenberg intensities corrected for size factor. A constant ratio was obtained for each Weissenberg level. Each Weissenberg level was multiplied by its own ratio and thus scaled to a common basis.

(b) The Wilson plot method may be considered as a satisfactory scaling method, provided that the number of reflections in each Weissenberg level is sufficient for a good Wilson plot. This has particular advantage for very high Weissenberg levels where very few spots, if any, appear on the precession pictures (usually they give inaccurate intensities, since they may be too close to the edge of the film). Before the overall Wilson plot is calculated, the Weissenberg levels should be scaled approximately to a common basis. This can be done either by precession pictures or by the

exposure times of the photographs. Final adjustments of the scale factors may then be made by adjusting the individual Wilson plots to fit the over-all Wilson plot. An example of this is illustrated in Fig 11. In this figure, the upper straight line represents the overall Wilson plot, while the lower one is the Wilson plot of the fifth level. These two lines differ in vertical coordinate by 0.34. To scale the fifth level to the same basis, its vertical coordinate should add 0.34. This is equivalent to multiplying the $F^2$'s by $k=e^{0.34}=1.405$, or multiplying the F's by $k^{1/2}=1.185$.

B. Size correction

Size correction is an important factor in the visual estimation of x-ray reflection intensities from upper level Weissenberg photographs. Phillips (29,30), the first one who discussed this problem in great detail, derived the special W-function for such corrections. The following paragraph will discuss the cause of size variation briefly as well as the practical aspects of the direct application which is not quite clear in Phillips's articles.

1. Cause of size variation

The size variation in spot areas arises from the divergence of the x-ray beam incident upon the inclined crystal (the upper level Wessenberg photographs). The reflection spots on the upper level Weissenberg film are contracted or extended according to whether the film motion is in the same or the opposite direction as the spot growth.

2. Size correction equations

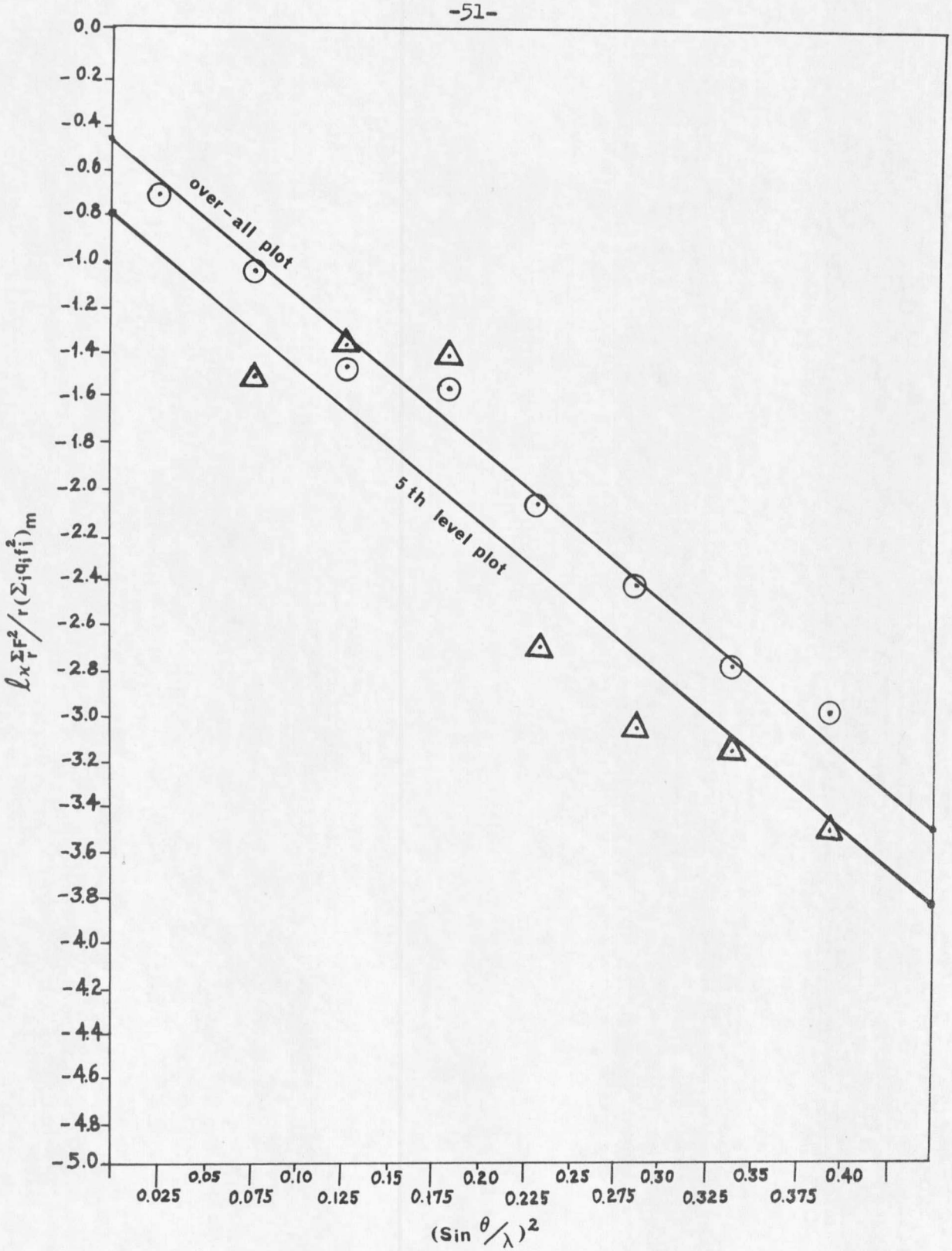



Figure 11 Scaling by the Wilson plot method

Assuming that the spot intensity is inversely proportional to the spot area,

$$I_m A=I_e(A+\Delta A)=I_c(A-\Delta A)$$

Where I represents the intensity, the subscript m refers to the mean value, e to the extended value, and c to the contracted one.

A represents the spot area before variation

$\Delta A$ represents the spot area variation.

It is this size correction that converts both $I_e$ and $I_c$ to $I_m$.

It should be noted that the above equations only hold for small variation in area.

It will be shown later that $I_m$ is the harmonic mean of $I_e$ and $I_c$, i.e.,

$$I_m=2I_eI_c/(I_e+I_c)$$

Since there may not be many equivalent spots appearing on both the top and bottom parts of the film, alternate ways to calculate $I_m$ must be used. These are

$$I_m=I_e(A+\Delta A)/A=I_eW$$

$$I_m=I_c(A-\Delta A)/A=I_c(2A-(A+\Delta A))/A=I_c(2-W)$$

a. Computation of W

The W-function of any reflection can be obtained from the reciprocal lattice coordinates and the W-plot derived and plotted by Phillips. The reciprocal lattice cylindrical coordinates for equi-inclination Weissenberg pictures can be seen from Fig. 12 as follows.

$$\zeta=2\sin\mu$$

$\xi = 2\cos\mu \sin x$

Where $\zeta, \xi$ are reciprocal lattice coordinates parallel and perpendicaular to the rotation axis respectively.

$\mu$ is the equi-inclination angle

x is the vertical distance from the spot to the center line of the film measured along the film.

b. Derivation of $I_m = 2I_e I_c/(I_e+I_c)$

Given $I_m A = I_e(A+\Delta A) = I_c(A-\Delta A)$

Collecting the common terms of A and $\Delta A$, we have

$$(I_e+I_c)\,\Delta A = (I_c-I_e)A$$

$$\Delta A = A(I_c-I_e)/(I_c+I_e)$$

$$I_m A = I_e(A+\Delta A) = I_e(A+A(I_c-I_e)/(I_c+I_e))$$

$$I_m = I_e(1+(I_c-I_e)/(I_c+I_e)) = 2I_c I_e/(I_c+I_e)$$

It has been mentioned earlier that the size correction equations

$$I_m A = I_e(A+\Delta A) = I_c(A-\Delta A)$$

hold only for small area variation. When a very large variation in area arises, e.g., for spots very close to the center line of the film, W may be greater than two. Then $I_m$ will become negative ($I_m = I_c(2-W)$), which is meaningless. For such a case, the corresponding precession intensity is used if available, or this reflection is not included at all.

C. Derivation of the general data reduction equations for triclinic crystal

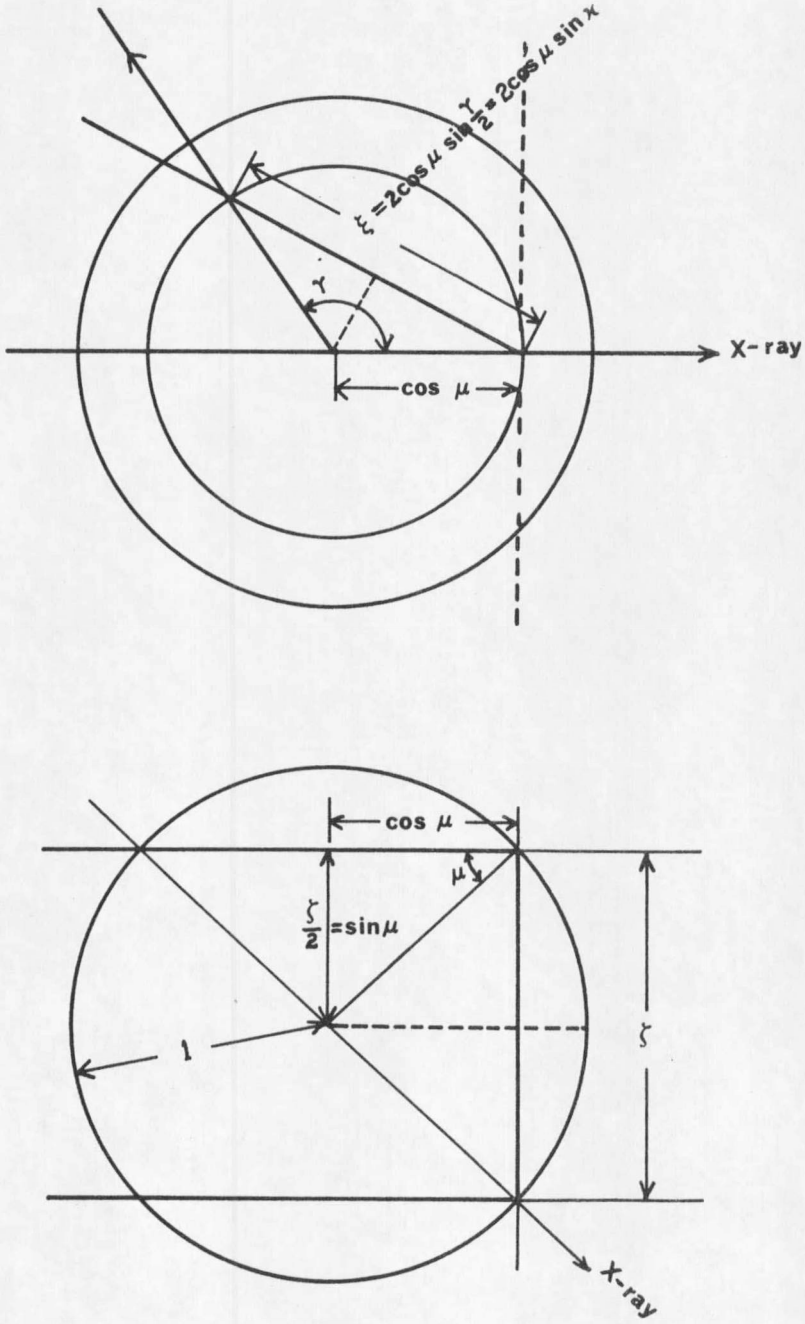



Figure 12 Reciprocal Lattice Cylindrical Coordinates for Equi-Inclination Weissenberg Photograph

Although the general equations stated below are found in many standard reference books, I was unable to find in the literature the derivations for these equations. I am therefore including the derivations in this dissertation.

The raw intensity data is reduced according to the following equation:

$$F=(I/A(LP))^{1/2}$$

where I is the raw intensity after proper scaling and correcting by the size factor

A is the absorption factor

Lp is the Lorentz and polarization factors

F is the structure factor

A, the absorption factor, will be discussed later in the section.

The polarization factor $p^{-1}$ (21) is

$$p^{-1}=2/(1+\cos^2 2\theta) \quad \ldots\ldots\ldots\ldots\ldots\ldots \quad (7)$$

This is a function of $\theta$ only. But the Lorentz factor $L^{-1}$ has different expressions for different x-ray methods. For equi-inclination Weissenberg method, the Lorentz factor (21) is

$$L^{-1}=\zeta\cos\theta=\cos^2\mu\,\sin\gamma$$

$$=\sin 2\theta(\sin^2\theta-\sin^2\mu)^{1/2}/\sin\theta \quad \ldots\ldots\ldots\ldots \quad (5)$$

It is interesting to see that the above three expressions for $L^{-1}$ can very easily be shown to be identical by the equi-inclination Weissenberg index-checking formula which I derived in Section 4. The index-checking formula for equi-inclination Weissenberg method is

$$\cos 2\theta=\cos^2\mu\,(1+\cos\gamma)-1 \quad \ldots\ldots\ldots\ldots\ldots \quad (4)$$

A different form can be obtained as follows.

$$2\cos^2\theta-1=\cos^2\mu\,(1+\cos\Upsilon)-1$$

$$2\cos^2\theta-1=\cos^2\mu\,(1+2\cos^2(\Upsilon/2)-1)-1$$

$$2\cos^2\theta=2\cos^2\mu\cos^2\Upsilon/2 \quad \ldots\ldots\ldots\ldots$$

$$\cos\theta=\cos\mu\cos\Upsilon/2 \quad \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots(6)$$

One of the forms of equation (5) is

$$L^{-1}=\xi\cos\theta=\cos^2\mu\sin\Upsilon$$

For the equi-inclination Weissenberg method,

$$\xi=2\cos\mu\sin\Upsilon/2$$

$$L^{-1}=\xi\cos\theta=2\cos\mu\sin(\Upsilon/2)\cos\theta$$

From equation (6)

$$\cos\theta=\cos\mu\cos\Upsilon/2$$

Thus, $L^{-1}=\xi\cos\theta=2\cos\mu\sin(\Upsilon/2)\cos\mu\cos\Upsilon/2$

$$=\cos^2\mu\sin\Upsilon$$

Another form of equation (5) is

$$L^{-1}=\xi\cos\theta=\sin2\theta(\sin^2\theta-\sin^2\mu)^{1/2}/\sin\theta$$

This can be simplified as follows:

$$\sin2\theta/\sin\theta=2\sin\theta\cos\theta/\sin\theta=2\cos\theta$$

$$\xi\cos\theta=2\cos\theta(\sin^2\theta-\sin^2\mu)^{1/2}$$

or $$\xi=2(\sin^2\theta-\sin^2\mu)^{1/2}$$

To show $\xi=2(\sin^2\theta-\sin^2\mu)^{1/2}$ proceed as follows:

$$\xi=2\cos\mu\sin\Upsilon/2$$

From equation (6)

$$\cos\theta=\cos\mu\cos\Upsilon/2$$

or $$\cos\Upsilon/2=\cos\theta/\cos\mu$$

$$\sin \gamma/2=(1-\cos^2 \gamma/2)^{1/2}=(1-\cos^2\theta/\cos^2\mu)^{1/2}$$

$$=(\cos^2\mu-\cos^2\theta)^{1/2}/\cos\mu$$

$$=(1-\sin^2\mu-1+\sin^2\theta)^{1/2}/\cos\mu$$

$$=(\sin^2\theta-\sin^2\mu)^{1/2}/\cos\mu$$

Thus, $\xi=2\cos\mu(\sin^2\theta-\sin^2\mu)^{1/2}/\cos\mu$

$$=2(\sin^2\theta-\sin^2\mu)^{1/2}$$

An expression for $\sin^2\theta$ for triclinic crystals is derived in the following.

$$p^{-1}=2/(1+\cos^2 2\theta) \quad \ldots\ldots\ldots\ldots\ldots\ldots \quad (7)$$

$$L^{-1}=2\cos\theta(\sin^2\theta-\sin^2\mu)^{1/2} \quad \ldots\ldots\ldots\ldots \quad (8)$$

Combining equations (7) and (8)

$$(Lp)^{-1}=4\cos\theta(\sin^2\theta-\sin^2\mu)^{1/2}/(1+\cos^2 2\theta)$$

From trigonometry: $\cos\theta=(1-\sin^2\theta)^{1/2}$

$$1+\cos^2 2\theta=1+(1-2\sin^2\theta)^2=(1-2\sin^2\theta+2\sin^4\theta)2$$

Then, $(Lp)^{-1}=2((1-\sin^2\theta)(\sin^2\theta-\sin^2\mu))^{1/2}/(1-2\sin^2\theta+2\sin^4\theta)$

where $\mu$ is the equi-inclination angle and is constant for each Weissenberg photograph, $\theta$ is the diffraction angle.

$\sin^2\theta$ can be calculated from cell constants a, b, c, $\alpha$, $\beta$, $\gamma$ by the following equation (Equation taken from Univ. of Washington Crystallographic computer write-ups for IBM 650 with correction.)

$$\sin^2\theta=h^2s_{11}+k^2s_{22}+l^2s_{33}+hks_{12}+hls_{13}+kls_{23}$$

Where $D=4a^2b^2c^2(1-\cos^2\alpha-\cos^2\beta-\cos^2\gamma+2\cos\alpha\cos\beta\cos\gamma)$

$$s_{11}=\lambda^2b^2c^2\sin^2\alpha/D$$

$$s_{22}=\lambda^2a^2c^2\sin^2\beta/D$$

$$s_{33}=\lambda^2a^2b^2\sin^2\gamma/D$$

$$s_{12}=2\lambda^2abc^2(\cos\alpha\cos\beta-\cos\gamma)/D$$

$$s_{13}=2\lambda^2ab^2c(\cos\alpha\cos\gamma-\cos\beta)/D$$

$$s_{23}=2\lambda^2a^2bc(\cos\beta\cos\gamma-\cos\alpha)/D$$

The above equation is general and can be used for any crystal system. This can be derived by either of the two following methods.

a. By the using of Wolf-Bragg equation

The Wolf-Bragg equation is (For derivation, see Section 4)

$$\sin^2\theta_{hkl}=h^2(a^{*2}/4)+k^2(b^{*2}/4)+l^2(c^{*2}/4)+hk(a^*b^*\cos\gamma^*/2)+kl(b^*c^*\cos\alpha^*/2)+hl(a^*C^*\cos\beta^*/2)$$

$$s_{11}=a^{*2}/4$$

But $a^*=\lambda/d_{100}$

To show $s_{11}=a^{*2}/4=\lambda^2/4d_{100}^2=\lambda^2b^2c^2\sin^2\alpha/4a^2b^2c^2(1-\cos^2\alpha-\cos^2\beta-\cos^2\gamma+2\cos\alpha\cos\beta\cos\gamma)$,

proceed as follows.

From Buerger (6):

$$V=abc\sin\alpha\sin\beta^*\sin\gamma$$

$$=abc(1-\cos^2\alpha-\cos^2\beta-\cos^2\gamma+2\cos\alpha\cos\beta\cos\gamma)^{1/2}$$

Then, $\sin\beta^*\sin\gamma=(1-\cos^2\alpha-\cos^2\beta-\cos^2\gamma-2\cos\alpha\cos\beta\cos\gamma)^{1/2}/\sin\alpha$

$$d_{100}=a\sin\beta^*\sin\gamma$$

$$d_{100}=a(1-\cos^2\alpha-\cos^2\beta-\cos^2\gamma+2\cos\alpha\cos\beta\cos\gamma)^{1/2}/\sin\alpha$$

$$(1/d_{100})^2=1/(a\sin\beta^*\sin\gamma)^2$$

$$=\sin^2\alpha/a^2(1-\cos^2\alpha-\cos^2\beta-\cos^2\gamma+2\cos\alpha\cos\beta\cos\gamma)$$

thus $$s_{11}=\lambda^2/4d^2_{100}=\frac{\lambda^2\sin^2\alpha}{4a^2(1-\cos^2\alpha-\cos^2\beta-\cos^2\gamma+2\cos\alpha\cos\beta\cos\gamma)}$$

$$=\frac{\lambda^2b^2c^2\sin^2\alpha}{4a^2b^2c^2(1-\cos^2\alpha-\cos^2\beta-\cos^2\gamma+2\cos\alpha\cos\beta\cos\gamma)}$$

$$=\lambda^2b^2c^2\sin^2\alpha/D$$

Similarly, $s_{22}=\lambda^2a^2c^2\sin^2\beta/D$, $s_{33}=\lambda^2a^2b^2\sin^2\gamma/D$

To show $s_{12}=2\lambda^2abc^2(\cos\alpha\cos\beta-\cos\gamma)/D$ as follows

From the Wolf-Bragg equation,

$$s_{12}=a^*b^*\cos\gamma^*/2$$

$$a^*=\lambda/d_{100}, \qquad b^*=\lambda/d_{010}$$

$$s_{12}=\lambda^2\cos\gamma^*/2d_{100}d_{010} \quad \ldots\ldots\ldots\ldots (9)$$

From the previous proof,

$$d_{100}=a(1-\cos^2\alpha-\cos^2\beta-\cos^2\gamma+2\cos\alpha\cos\beta\cos\gamma)^{1/2}/\sin\alpha$$

$$\ldots\ldots\ldots\ldots\ldots\ldots (10)$$

Similarly

$$d_{010}=b(1-\cos^2\alpha-\cos^2\beta-\cos^2\gamma+2\cos\alpha\cos\beta\cos\gamma)^{1/2}/$$

$$\sin\beta \ldots\ldots\ldots\ldots\ldots\ldots (11)$$

Also $$\cos\gamma^*=\frac{(\cos\alpha\cos\beta-\cos\gamma)}{\sin\alpha\sin\beta} \quad \ldots\ldots\ldots\ldots (12)$$

Substituting equations (10), (11), (12) into (9), we have

$$s_{12}=2\lambda^2abc^2(\cos\alpha\cos\beta-\cos\gamma)/4a^2b^2c^2(1-\cos^2\alpha$$
$$-\cos^2\beta-\cos^2\gamma+2\cos\alpha\cos\beta\cos\gamma)=2\lambda^2abc^2(\cos\alpha\cos\beta-\cos\gamma)/D$$

Similarly,

$$s_{13}=2\lambda^2ab^2c(\cos\alpha\cos\gamma-\cos\beta)/D$$

$$s_{23}=2\lambda^2a^2bc(\cos\beta\cos\gamma-\cos\alpha)/D$$

b. By using the triclinic interplanar spacing equation (equation (13)

to be derived later)

The equation (13) is

$$(1/d_{hkl})^2=(hA/a+kB/b+lC/c)/E$$

Where

$$A=\begin{vmatrix} h/a & \cos\gamma & \cos\beta \\ k/b & 1 & \cos\alpha \\ l/c & \cos\alpha & 1 \end{vmatrix} = h(1-\cos^2\alpha)/a-\cos\gamma(k/b-(l/c)\cos\alpha)+\cos\beta((k/b)\cos\alpha-l/c)$$

$$B=\begin{vmatrix} 1 & h/a & \cos\beta \\ \cos\gamma & k/b & \cos\alpha \\ \cos\beta & l/c & 1 \end{vmatrix} = (k/b-(l/c)\cos\alpha)-h/a(\cos\gamma-\cos\alpha\cos\beta)+\cos\beta((l/c)\cos\gamma-(k/b)\cos\beta)$$

$$C=\begin{vmatrix} 1 & \cos\gamma & h/a \\ \cos\gamma & 1 & k/b \\ \cos\beta & \cos\alpha & l/c \end{vmatrix} = (l/c-(k/b)\cos\alpha)-\cos\gamma((l/c)\cos\gamma-(k/b)\cos\beta)+h/a(\cos\alpha\cos\gamma-\cos\beta)$$

$$E=\begin{vmatrix} 1 & \cos\gamma & \cos\beta \\ \cos\gamma & 1 & \cos\alpha \\ \cos\beta & \cos\alpha & 1 \end{vmatrix} = 1-\cos^2\alpha-\cos^2\beta-\cos^2\gamma+2\cos\alpha\cos\beta\cos\gamma$$

From Bragg's law,

$$\lambda=2d_{hkl}\sin\theta_{hkl}$$

$$\sin^2\theta_{hkl}=\lambda^2/4d_{hkl}^2$$

Substituting the triclinic interplanar spacing equation,

$$\sin^2\theta_{hkl}=\frac{\lambda^2}{4E}(h^2(1-\cos^2\alpha)/a^2-hk\cos\gamma/ab+hl\cos\alpha\cos\gamma/ac+hk\cos\alpha\cos\beta/ab-hl\cos\beta/ac+k^2/b^2-kl\cos\alpha/bc-hk\cos\gamma/ab+hk\cos\alpha\cos\beta/ab+kl\cos\beta\cos\gamma/bc-k^2\cos^2\beta/b^2$$

$$+l^2/c^2-klcos\alpha/bc-l^2cos^2\gamma/c^2+klcos\beta$$
$$cos\gamma/bc+hlcos\alpha cos\beta/ac-hlcos\beta/ac)$$
$$=\frac{\lambda^2}{4E}(h^2sin^2\alpha/a^2+k^2sin^2\beta/b^2+l^2sin^2\gamma/c^2$$
$$+2hk(cos\alpha cos\beta-cos\gamma)/ab+2kl(cos\beta$$
$$cos\gamma-cos\alpha)/bc+2hl(cos\alpha cos\gamma-cos\beta)/ac)$$
$$=\frac{1}{4a^2b^2c^2E}(h^2(\lambda^2b^2c^2sin^2\alpha)+k^2(\lambda^2a^2c^2sin^2\beta)$$
$$+l^2(\lambda^2a^2b^2sin^2\gamma)+hl(2\lambda^2ab^2c(cos\alpha cos\gamma$$
$$-cos\beta))+hk(2\lambda^2abc^2(cos\alpha cos\beta-cos\gamma))$$
$$+kl((2\lambda^2a^2bc(cos\beta cos\gamma-cos\alpha)))$$

By definition,

$$D=4a^2b^2c^2(1-cos^2\alpha-cos^2\beta-cos^2\gamma+2cos\alpha cos\beta cos\gamma)$$
$$=4a^2b^2c^2E$$

Thus, $sin^2\theta_{hkl}=1/D(h^2(\lambda^2b^2c^2sin^2\alpha)+k^2(\lambda^2a^2c^2sin^2\beta)$
$$+l^2(\lambda^2a^2b^2sin^2\gamma)+hl(2\lambda^2ab^2c(cos\alpha cos\gamma$$
$$-cos\beta))+hk(2\lambda^2abc^2(cos\alpha cos\beta-cos\gamma))$$
$$+kl(2\lambda^2a^2bc(cos\beta cos\gamma-cos\alpha)))$$

When the above equation is compared with the following equation,

$$sin^2\theta_{hkl}=h^2s_{11}+k^2s_{22}+l^2s_{33}+hks_{12}+hls_{13}+kls_{23}$$

It is evident that

$$s_{11}=\lambda^2b^2c^2sin^2\alpha/D$$
$$s_{22}=\lambda^2a^2c^2sin^2\beta/D$$
$$s_{33}=\lambda^2a^2b^2sin^2\gamma/D$$
$$s_{12}=2\lambda^2abc^2(cos\alpha cos\beta-cos\gamma)/D$$
$$s_{13}=2\lambda^2ab^2c(cos\alpha cos\gamma-cos\beta)/D$$

$$s_{23}=2\lambda^2a^2bc(\cos\beta\cos\gamma-\cos\alpha)/D$$

2. Derivation of the triclinic interplanar spacing equation

This equation is given in standard references without derivation. Since I was unable to find derivation, this derivation is also included here. See (6,32).

The triclinic interplanar spacing equation is

$$d_{hkl}=\frac{1}{\sqrt{\begin{vmatrix} h/a & \cos\gamma & \cos\beta \\ k/b & 1 & \cos\alpha \\ l/c & \cos\alpha & 1 \end{vmatrix} h/a + \begin{vmatrix} 1 & h/a & \cos\beta \\ \cos\gamma & k/b & \cos\alpha \\ \cos\beta & l/c & 1 \end{vmatrix} k/b + \begin{vmatrix} 1 & \cos\gamma & h/a \\ \cos\gamma & 1 & k/b \\ \cos\beta & \cos\alpha & l/c \end{vmatrix} l/c}{\begin{vmatrix} 1 & \cos\gamma & \cos\beta \\ \cos\gamma & 1 & \cos\alpha \\ \cos\beta & \cos\alpha & 1 \end{vmatrix}}}}$$

The following two mathematical formulas will be used for this derivation.

a. The normal vector $\vec{N}$ to a general plane $px+ry+sz=t$, where x, y, z are rectangular coordinates, i.e., an orthogonal system is

$$\vec{N}=p\vec{i}+r\vec{j}+s\vec{k}$$

where i, j, k are the unit vector along x, y, z.

b. The vertical distance from any point $x_1$, $y_1$, $z_1$ to the plane $px+ry+sz=t$ is

$$d=(px_1+ry_1+sz_1-t)/\pm(p^2+r^2+s^2)^{1/2}$$

A derivation of the above two mathematical formulas can be found in many standard reference books (31,34).

In Fig. 13, the solid lines A, B, C represent the oblique coordin-

ates, i.e., a non-orthogonal system along the three axes of the triclinic system, while the dotted lines x, y, z are the rectangular coordinates. From the definition of the Miller index h, k, l, the intercepts of the hkl plane on the oblique coordinate A, B, C are a/h, b/k, c/l where a, b, c are the axial lengths of the triclinic system. The equation of the hkl plane, when put into its intercept form, is

$$A/(a/h)+B/(b/k)+C/(c/l)=1$$

or $$hA/a+kB/b+lC/c=1$$

Let the normal vector $\vec{N}$ to the hkl plane be $\vec{N}=u\vec{A}+v\vec{B}+w\vec{C}$ where $\vec{A}$, $\vec{B}$, $\vec{C}$ represent the unit vector along A, B, C axes of the triclinic system.

Suppose the hkl plane intercepts the rectangular coordinates x, y, z at l/p, l/r, l/s then the hkl plane equation in its intercept form can be represented in terms of x, y, z coordinate as below.

$$x/(l/p)+y/(l/r)+z/(l/s)=1$$

or $$px+ry+sz=1 \quad \ldots\ldots\ldots\ldots\ldots\ldots \quad (15)$$

As stated previously, the normal vector $\vec{N}$ to the hkl plane of $px+ry+sz=1$ is $\vec{N}=p\vec{i}+r\vec{j}+s\vec{k}$

Although two different coordinate systems are used, they represent the same hkl plane and the same normal vector, thus they should be equal.

$$hA/a+kB/b+lC/c=px+ry+sz=1$$

$$\vec{N}=u\vec{A}+v\vec{B}+w\vec{C}=p\vec{i}+r\vec{j}+s\vec{k}$$

The orthogonal system x, y, z is introduced for the ease in finding the interplanar spacing $d_{hkl}$. The vertical distance $d_{hkl}$ from the origin

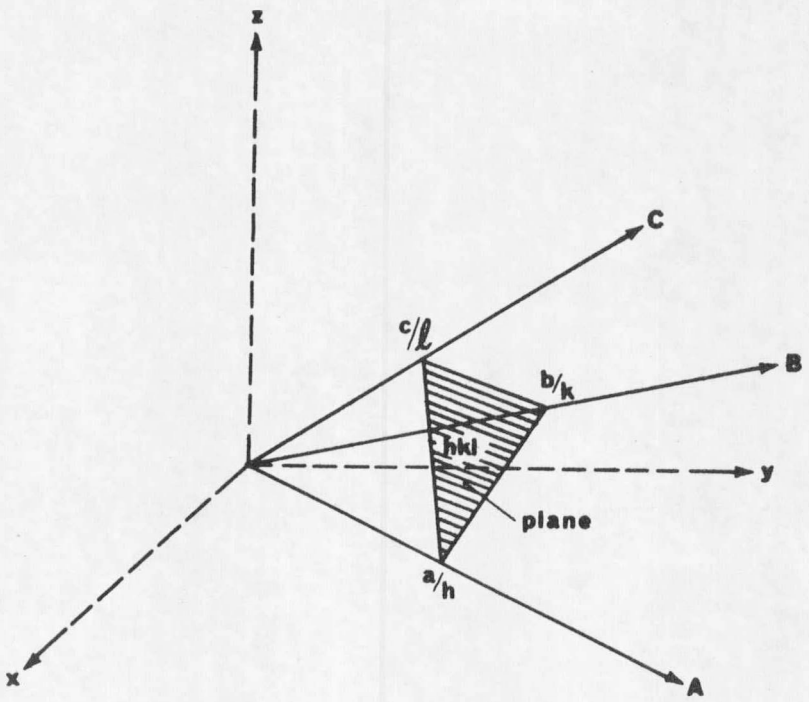



Figure 13 The hkl plane in both the rectangular and oblique coordinates

(0,0, 0) to the hkl plane px+ry+sz=1 is

$$d_{hkl}=(p(0)+r(0)+s(0)-1)/\pm(p^2+r^2+s^2)^{1/2}=1/(p^2+r^2+s^2)^{1/2}$$

To find the p, r, s proceed as follows:

Let Q(A, B, C) and $Q_1(A_1, B_1, C_1)$ by any two points on the hkl plane of hA/a+kB/b+lC/c=1

Since $\vec{N}=u\vec{A}+y\vec{B}+w\vec{C}$ is normal to the hkl plane of hA/a+kB/b+lC/c=1, $\vec{N}$ is normal to any vector $\vec{Q_1Q}$ on the plane.

Then, $\vec{N}\cdot\vec{Q_1Q}=0$

or $(u\vec{A}+v\vec{B}+w\vec{C})\cdot((A-A_1)\vec{A}+(B-B_1)\vec{B}+(C-C_1)\vec{C})=0$ . . . . . .(14)

It is noted that $\vec{A}\cdot\vec{A}=1$, $\vec{B}\cdot\vec{B}=1$, $\vec{C}\cdot\vec{C}=1$

$$\vec{A}\cdot\vec{B}=\cos\gamma\,,\qquad \vec{A}\cdot\vec{C}=\cos\beta\,,\qquad \vec{B}\cdot\vec{C}=\cos\alpha$$

Using these relationships, the expansion of equation (14) becomes as below.

$$u(A-A_1)+v(A-A_1)\cos\gamma+w(A-A_1)\cos\beta+u(B-B_1)\cos\gamma$$
$$+v(B-B_1)+w(B-B_1)\cos\alpha+u(C-C_1)\cos\beta+v(C-C_1)\cos\alpha$$
$$+w(C-C_1)=0$$

Collecting the common terms,

$$A(u+v\cos\gamma+w\cos\beta)+B(u\cos\gamma+v+w\cos\alpha)+C(u\cos\beta+$$
$$v\cos\alpha+w)$$
$$=A_1(u+v\cos\gamma+w\cos\beta)+B_1(u\cos\gamma+v+w\cos\alpha)+C_1(u\cos\beta$$
$$+v\cos\alpha+w)$$

This must be identical to the following hkl plane equation (15), since they represent the same plane.

$$hA/a+kB/b+lC/c=1 \quad . . . . . .(16)$$

From comparison, we have

$$u+v\cos\gamma+w\cos\beta=h/a \quad \ldots\ldots\ldots\ldots\ldots (17)$$

$$u\cos\gamma+v+w\cos\alpha=k/b \quad \ldots\ldots\ldots\ldots\ldots (18)$$

$$u\cos\beta+v\cos\alpha+w=l/c \quad \ldots\ldots\ldots\ldots\ldots (19)$$

and also $A_1(u+v\cos\gamma+w\cos\beta)+B_1(u\cos\gamma+v+w\cos\alpha)+C_1$

$$(u\cos\beta+v\cos\alpha+w)=1 \quad \ldots\ldots\ldots\ldots\ldots (20)$$

To show equation (20) is valid, first substitute equation (17), (18), (19) into equation (20), giving $hA_1/a+kB_1/b+lC_1/c=1$, and then remember that $Q_1(A_1, B_1, C_1)$ must satisfy the hkl plane equation of $hA/a+kB/b+lC/c=1$. Thus $hA_1/a+kB_1/b+lC_1/c=1$.

Solving equations (17), (18), (19) simultaneously for u, v, w by the determinant method,

$$u=\frac{\begin{vmatrix} h/a & \cos\gamma & \cos\beta \\ k/b & 1 & \cos\alpha \\ l/c & \cos\alpha & 1 \end{vmatrix}}{\begin{vmatrix} 1 & \cos\gamma & \cos\beta \\ \cos\gamma & 1 & \cos\alpha \\ \cos\beta & \cos\alpha & 1 \end{vmatrix}} \quad v=\frac{\begin{vmatrix} 1 & h/a & \cos\beta \\ \cos\gamma & k/b & \cos\alpha \\ \cos\beta & l/c & 1 \end{vmatrix}}{\begin{vmatrix} 1 & \cos\gamma & \cos\beta \\ \cos\gamma & 1 & \cos\alpha \\ \cos\beta & \cos\alpha & 1 \end{vmatrix}} \quad w=\frac{\begin{vmatrix} 1 & \cos\gamma & h/a \\ \cos\gamma & 1 & k/b \\ \cos\beta & \cos\alpha & l/c \end{vmatrix}}{\begin{vmatrix} 1 & \cos\gamma & \cos\beta \\ \cos\gamma & 1 & \cos\alpha \\ \cos\beta & \cos\alpha & 1 \end{vmatrix}}$$

Let $\vec{A}=a_x\vec{i}+a_y\vec{j}+a_z\vec{k}$

$\vec{B}=b_x\vec{i}+b_y\vec{j}+b_z\vec{k}$

$\vec{C}=c_x\vec{i}+c_y\vec{j}+c_z\vec{k}$

Then $\vec{N}=u\vec{A}+v\vec{B}+w\vec{C}$

$=u(a_x\vec{i}+a_y\vec{j}+a_z\vec{k})+v(b_x\vec{i}+b_y\vec{j}+b_z\vec{k})+w(c_x\vec{i}+c_y\vec{j}+c_z\vec{k})$

Collecting the common terms of $\vec{i}$, $\vec{j}$, $\vec{k}$,

$$\vec{N}=\vec{i}(ua_x+vb_x+wc_x)+\vec{j}(ua_y+vb_y+wc_y)+\vec{k}(ua_z+vb_z+wc_z)$$

Also $\vec{N}=p\vec{i}+r\vec{j}+s\vec{k}$

Hence $p=ua_x+vb_x+wc_x$

$r=ua_y+vb_y+wc_y$

$s=ua_z+vb_z+wc_z$

$$p^2+r^2+s^2=(ua_x+vb_x+wc_x)^2+(ua_y+vb_y+wc_y)^2+(ua_z+vb_z+wc_z)^2$$
$$=u^2(a_x^2+a_y^2+a_z^2)+v^2(b_x^2+b_y^2+b_z^2)+w^2(c_x^2$$
$$+c_y^2+c_z^2)+2uv(a_xb_x+a_yb_y+a_zb_z)+2uw(a_xc_x+$$
$$a_yc_y+a_zc_z)+2vw(b_xc_x+b_yc_y+b_zc_z).$$

It should be noted that

$$\vec{A}\cdot\vec{A}=1=(a_x\vec{i}+a_y\vec{j}+a_z\vec{k})\cdot(a_x\vec{i}+a_y\vec{j}+a_z\vec{k})=a_x^2+a_y^2+a_z^2$$

$$\vec{B}\cdot\vec{B}=1=(b_x\vec{i}+b_y\vec{j}+b_z\vec{k})\cdot(b_x\vec{i}+b_y\vec{j}+b_z\vec{k})=b_x^2+b_y^2+b_z^2$$

$$\vec{C}\cdot\vec{C}=1=(c_x\vec{i}+c_y\vec{j}+c_z\vec{k})\cdot(c_x\vec{i}+c_y\vec{j}+c_z\vec{k})=c_x^2+c_y^2+c_z^2$$

$$\vec{A}\cdot\vec{B}=\cos\gamma=(a_x\vec{i}+a_y\vec{j}+a_z\vec{k})\cdot(b_x\vec{i}+b_y\vec{j}+b_z\vec{k})$$
$$=a_xb_x+a_yb_y+a_zb_z$$

$$\vec{A}\cdot\vec{C}=\cos\beta=(a_x\vec{i}+a_y\vec{j}+a_z\vec{k})\cdot(c_x\vec{i}+c_y\vec{j}+c_z\vec{k})$$
$$=a_xc_x+a_yc_y+a_zc_z$$

$$\vec{B}\cdot\vec{C}=\cos\alpha=(b_x\vec{i}+b_y\vec{j}+b_z\vec{k})\cdot(c_x\vec{i}+c_y\vec{j}+c_z\vec{k})$$
$$=b_xc_x+b_yc_y+b_zc_z$$

Using these relationships,

$$p^2+r^2+s^2=u^2+v^2+w^2+2uv\cos\gamma+2uw\cos\beta+2vw\cos\alpha)$$

Rearranging the equation,

$$p^2+r^2+s^2=(u^2+uv\cos\gamma+uw\cos\beta)+(uv\cos\gamma+v^2+vw\cos\alpha)$$
$$+(uw\cos\beta+vw\cos\alpha+w^2)$$
$$=u(u+v\cos\gamma+w\cos\beta)+v(u\cos\gamma+v+w\cos\alpha)$$
$$+w(u\cos\beta+v\cos\alpha+w)$$

From equations (17), (18), (19)

$$p^2+r^2+s^2=hu/a+kv/b+lw/c$$

Hence $$d_{hkl}=1/(p^2+r^2+s^2)^{1/2}$$

$$=1/(hu/a+kv/b+lw/c)^{1/2}$$

Substituting the u,v, w (in the determinant form),

$$d_{hkl}=\frac{1}{\sqrt{\begin{vmatrix} h/a & \cos\gamma & \cos\beta \\ k/b & 1 & \cos\alpha \\ l/c & \cos\alpha & 1 \end{vmatrix} h/a + \begin{vmatrix} 1 & h/a & \cos\beta \\ \cos\gamma & k/b & \cos\alpha \\ \cos\beta & l/c & 1 \end{vmatrix} k/b + \begin{vmatrix} 1 & \cos\gamma & h/a \\ \cos\gamma & 1 & k/b \\ \cos\beta & \cos\alpha & l/c \end{vmatrix} l/c \Big/ \begin{vmatrix} 1 & \cos\gamma & \cos\beta \\ \cos\gamma & 1 & \cos\alpha \\ \cos\beta & \cos\alpha & 1 \end{vmatrix}}}$$

D. Absorption correction for rectangular cross section

1. Basic principle of absorption correction

$$I_o=I/A$$

Where $I_o$ is the intensity free from the absorption correction.

I is the intensity to be corrected by the absorption factor.

A is the absorption factor.

For Weissenberg photographs, the absorption factor A may be calculated as follows.

a. For zero level Weissenberg photograph (21)

$$A^o=\int_v e^{-\mu x}dx/v=\int_s e^{-\mu x}1ds/1ds=\int_s e^{-\mu x}ds/ds$$

$$\doteqdot\sum_i e^{-\mu x_i}\Delta s/n\Delta s\doteqdot\sum_i e^{-\mu x_i}/n$$

Where $\mu$ is the linear absorption coefficient

v is the volume of crystal

s is the cross section of crystal

l is the length of crystal

x is the path length

n is the total number of the element area $\Delta s$ in the cross section. The smaller the element area $\Delta s$, the better the A will be.

b. For upper equi-inclination Weissenberg photograph (17).

$$A^{up}=\cos\nu\, A^{o}(\mu x\sec\nu\,,\Upsilon/2)$$
$$\doteq(\Sigma_i e^{-\mu x_i\sec\nu})/n\sec\nu$$
$$=\cos\nu(\Sigma_i e^{-\mu x_i\sec\nu})/n \quad \ldots\ldots\ldots (21)$$

Where $\nu$ is the equi-inclination angle

$\Upsilon$ is the reflection angle

The other symbols have the same meaning as mentioned in section a.

This is a general equation for all equi-inclination Weissenberg levels including the zero level. This is because $\sin\Upsilon/2=\sec\nu\,(\sin^2\Theta-\sin^2\nu)^{1/2}$. For zero level, $\nu=o$, then $\sin\Upsilon/2=\sin\Theta$

2. Computation of the path length for the constant rectangular cross section

The computation of the path length is difficult, because it is a function of the diffraction angle, crystal shape and the x-ray method. For the constant rectangular cross section, the path length may be calculated as follows. Let a, b, be the two sides of the constant rectangular cross section. To calculate the path

length for any particular reflection, the x-ray beam is assumed to pass through this cross section as many incident parallel and many reflected parallel rays. The total length of the incident and the reflected ray is the path length of an element area. Absorption corrections must be made for each element area. The summation of all the element area absorption corrections divided by the total number of elements is the average A for that reflection. Consider the case shown in Fig. 14 for illustration. In Fig. 14, the incident x-ray is assumed to be parallel to the side b. Three of such parallel incident x-ray at a spacing of e has been entered at the cross section. The x-ray is assumed to reflect at such an angle that the reflected x-rays are parallel to the side a. Five of the reflected x-rays are recorded. The rectangular cross section is thus divided into fifteen diamond-shape elements of which each side has a length of $x=e/\sin\gamma$, where e is the interline spacing. The fifteen elements have the following path lengths as counted from element no. 1 to element no 15: 2x, 3x, 4x, 5x, and 6x or $(n_b+1)x$; 3x, 4x, 5x, 6x, & 7x or $(n_b+2)x$; 4x, 5x, 6x, 7x, & 8x or $(n_a+n_b)x$. The average absorption factor is

$$A^{up}=(\cos\nu/n_a n_b)(e^{-2x\mu\sec\nu}+2e^{-3x\mu\sec\nu}+3e^{-4x\mu\sec\nu}$$
$$+3e^{-5x\mu\sec\nu}+3e^{-6x\mu\sec\nu}+2e^{-7x\mu\sec\nu}+e^{-8x\mu\sec\nu}).$$

If side b is greater than side a, the general absorption factor is

$$A^{up}=(\cos\nu/n_a n_b)(e^{-2x\mu\sec\nu}+2e^{-3x\mu\sec\nu}+3e^{-4x\mu\sec\nu}$$
$$+\ \ldots\ +n_a e^{-(n_a+1)x\mu\sec\nu}+n_a e^{-(n_a+2)x\mu\sec\nu}+$$

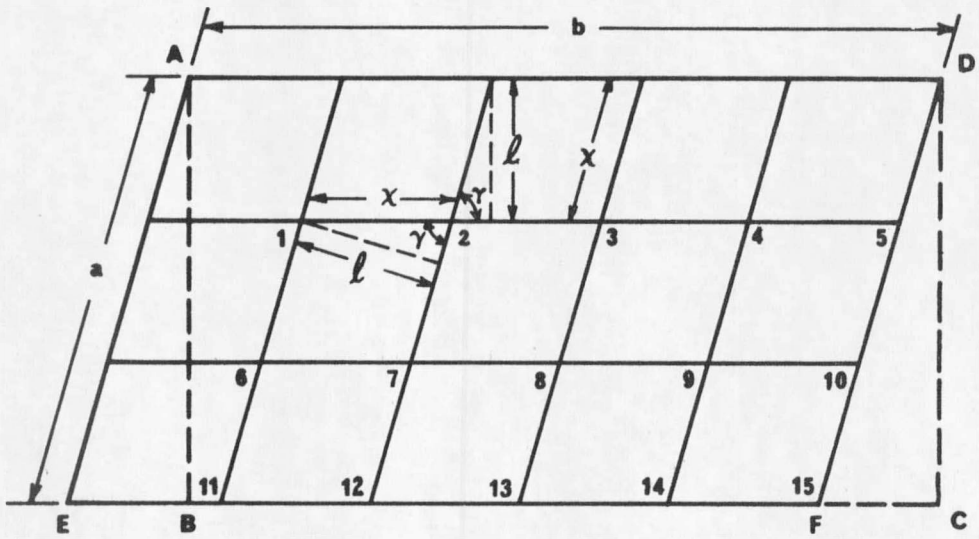



Figure 14 Computation of the path length for the constant rectangular cross section in the absorption correction

$$\ldots + n_a e^{-(n_b+1)x\mu\sec\nu} + (n_a-1)e^{-(n_b+2)x\mu\sec\nu}$$
$$+ (n_a-2)e^{-(n_b+3)x\mu\sec\nu} + \ldots + e^{-(n_a+n_b)x\mu\sec\nu} \quad (22)$$

It is not necessary for the reflected x-ray to be parallel to the side a. This is only used for the ease of illustration. If the crystal has a cross section of ABCD instead of AEFD as shown in Fig. 14, the reflected x-ray is not parallel to the side a. Yet $n_a$ ($n_a$=a/e, i.e., no. of division of a) is still three, and since the area of ABCD is equal to the area of AEFD, the total path length for each element is approximately the same, giving the same absorption factor. By the same reasoning, the incident x-ray need not be parallel to the side b. Thus, equation (22) as the general absorption factor is justified. To calculate equation (22), several terms must be computed before corrections are made.

a. A proper interline spacing e. The smaller the e, the smaller the element area and the more correct the absorption correction will be, but the longer the calculation will take, because of greater number of terms in the absorption equation (22).

b. $n_a = a/e$

c. $\sin\Upsilon = 2(1-\sin^2(\Upsilon/2))^{1/2}\sin(\Upsilon/2)$

$\sin(\Upsilon/2) = (\sin^2\Theta - \sin^2\nu)^{1/2}/(1-\sin^2\nu)^{1/2}$

d. $x = e/\sin\Upsilon$

e. $n_b = b/x$

For calcium 1-naphthyl phosphate

a. Crystal dimension

Crystal is a parallelopiped of 1.3 mm long having an approximate constant cross section of 0.216 mm by 0.125 mm.

b. Linear-absorption coefficient

The linear-absorption coefficient, $\mu$, for calcium 1-naphthyl phosphate was calculated by the following equation (9).

$$\mu = G(P_A(\mu/\rho)_A + P_B(\mu/\rho)_B + P(\mu/\rho)_C + \ldots)$$

Where, G is the density of crystal

$\mu/\rho$ is the mass absorption coefficient of the element atom (22).

$P_A$ is the weight fraction of element A in compound ABC . . . A, B, C representing the different elements in crystal.

For Cu K$\alpha$ radiation, calculation of the linear-absorption coefficient for calcium 1-naphthyl phosphate is shown in the following table.

Table IX. Linear-absorption coefficient calculation for calcium 1-naphthyl phosphate

| Atom | Atomic wt. | Total wt. of atom in compound | Fraction of total wt. P | Mass-absorp. coefficient $\mu/\rho$ ($cm^2/g$) | $P(\mu/\rho)$ ($cm^2/g$) |
|---|---|---|---|---|---|
| Ca | 40.80 | 40.08 | 7.42% | 162 | 12.20 |
| 2P | 30.975 | 61.95 | 11.46% | 74.1 | 8.49 |

| Atom | Atomic wt. | Total wt. of atom in compound | Fraction of total wt. P | Mass-absorp. coefficient $\mu/\rho$ ($cm^2/g$) | $P(\mu/\rho)$ ($cm^2/g$) |
|---|---|---|---|---|---|
| 11O | 16.0 | 176.0 | 32.57% | 11.5 | 3.75 |
| 20C | 12.011 | 240.22 | 44.45% | 4.60 | 2.05 |
| 22H | 1.008 | 22.176 | 4.10% | 0.435 | 0.02 |
| | | 540.426 | 100.00% | | 26.33 |

Linear-absorption coefficient $G\sum P(\mu/\rho)=(1.5031)(26.33)$

$=39.58\ cm^{-1}$

E. Wilson plot for calcium 1-naphthyl phosphate

1. General description

The Wilson plot is prepared according to the following equation.

$$\ln\left(\sum_r |F_{rel}|^2 / r\left(\sum_i q_i f_i^2\right)_{mean}\right)=(-2B)\left(\sin^2\theta/\lambda^2\right)_{mean}+\ln K$$

$$y=mx+c$$

Where $\sum_r F_{rel}^2/r$ is the average value of the squares of the relative F's for the r reflections that fall within the group.

$\left(\sum_i q_i f_i^2\right)_{mean}$ is the set of the square of the atomic scattering factors, weighted for the various atom types at the mean value of $\sin\theta/\lambda$ for the group.

-2B is the slope of the straight line and B is the temperature factor.

lnK is the intercept of the straight line and K is the absolute scale constant for scaling the absolute $F^{o2}$ to $F_{obs}^2$. This scale constant usually is different from the one used in the

structure factor program calcualtion where the scale constant k is used to scale the $F_o$ to $F_c$. $k=(1/K)^{1/2}$.

A good Wilson plot will result only when all the possible independent reflections (observed, unobserved, and extinct) are included.

2. Results

The Wilson plot, besides giving the temperature factor and the scale constant, may indicate the reliability of the intensity data after being corrected by the different factors.

Data for the different Wilson plots for calcium 1-naphthyl phosphate are recorded in Table X, XI, and the plots are shown in the Fig. 15. It is evident that the Wilson plot which is corrected by the Lorentz and polarization and the absorption factors is the best straight line.

Table X. Wilson plot with no correction for calcium 1-naphthyl phosphate

| Group no. | no. reflections in each group | $(\sin^2\theta/\lambda^2)_m$ | $\ln \frac{\sum_r F_{rel}^2}{r(\sum_i q_i f_i^2)_m}$ |
|---|---|---|---|
| 1 | 213 | 0.0262920 | -1.14570 |
| 2 | 400 | 0.0788760 | -1.93102 |
| 3 | 421 | 0.1314600 | -2.64508 |
| 4 | 421 | 0.1840440 | -2.95651 |
| 5 | 402 | 0.2366280 | -3.47377 |

| Group no. | no. reflections in each group | $(\sin^2\theta/\lambda^2)_m$ | $\ln \frac{\sum_r F^2_{rel}}{r(\sum_i q_i f_i^2)_m}$ |
|---|---|---|---|
| 6 | 370 | 0.2892120 | -3.72970 |
| 7 | 327 | 0.3417960 | -3.81671 |
| 8 | 225 | 0.3943800 | -3.61192 |

Table XI. Wilson plot for calcium 1-naphthyl phosphate

| Group no. | no. of reflections | $(\sin^2\theta/\lambda^2)_m$ | $\ln(\sum_r F^2_{rel} / r(\sum_i q_i f_i^2)_m)$ | |
|---|---|---|---|---|
| | | | Lp correction | Lp, A correction |
| 1 | 213 | 0.0262920 | -2.13707 | -0.69115 |
| 2 | 400 | 0.0788760 | -2.15417 | -1.07587 |
| 3 | 421 | 0.1314600 | -2.44185 | -1.44392 |
| 4 | 421 | 0.8140440 | -2.51331 | -1.55117 |
| 5 | 402 | 0.2366280 | -2.97593 | -2.04794 |
| 6 | 370 | 0.2893130 | -3.38139 | -2.47694 |
| 7 | 327 | 0.3417960 | -3.81671 | -2.81341 |
| 8 | 225 | 0.3943800 | -4.19971 | -2.95651 |

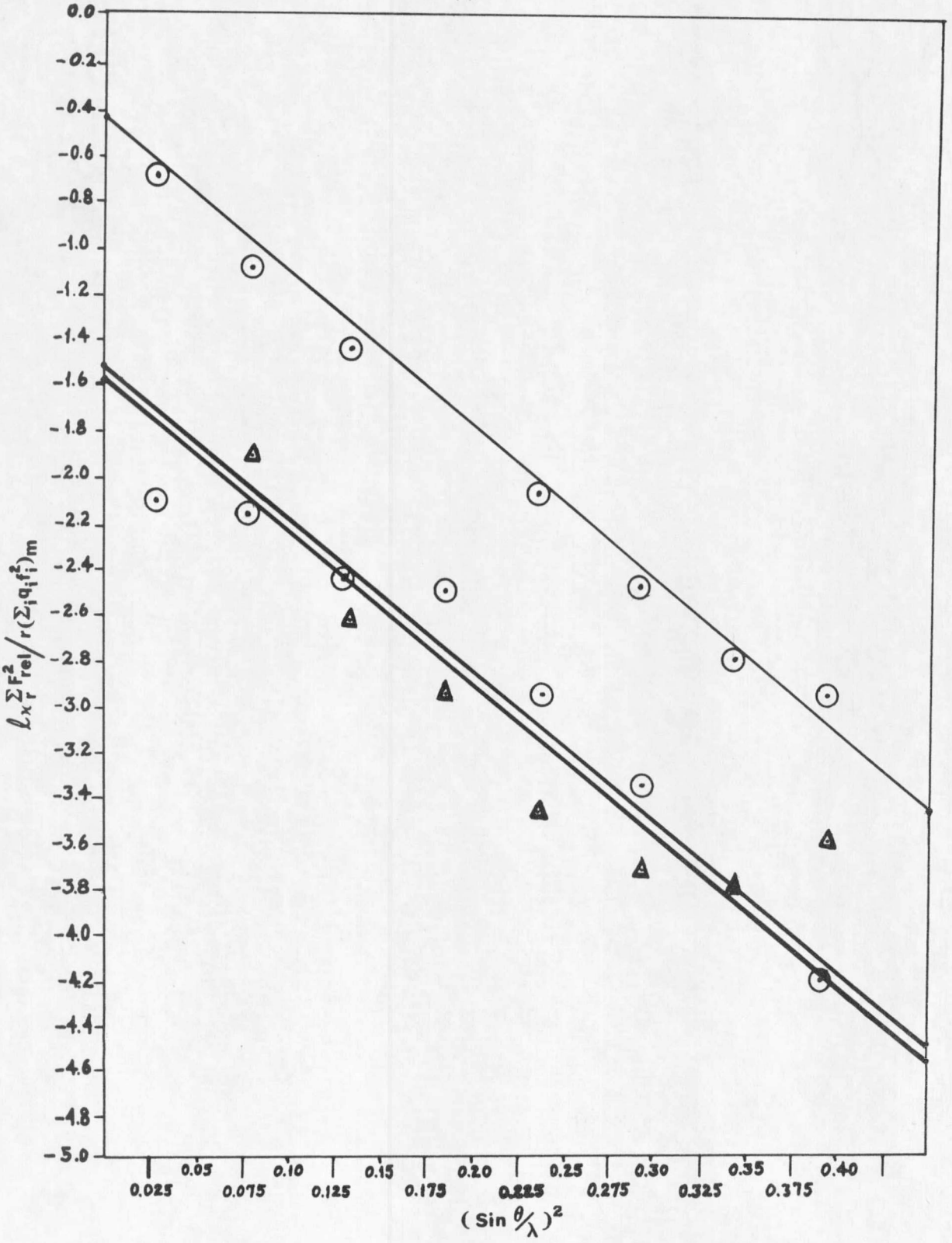



Figure 15 Wilson plot for calcium 1-naphthyl phosphate

## SECTION VI

## STRUCTURE DETERMINATION

### A. Intensity statistics

#### 1. General description

Howells, Phillips and Rogers (17) devised a method to distinguish centro-symmetrical crystal from non-centrosymmetrical crystals by using the statistics distribution of reflection intensities. They showed that the fractions N(z) of reflections whose intensities are equal to or less than a fraction z of the local average are given

a. for non-centrosymmetrical crystal, by

$$N(z)=1-\exp(-z)$$

b. for centro-symmetrical crystal, by

$$N(z)=\mathrm{erf}(z/2)^{1/2}$$

Where erf is the error function.

The method can be described briefly as follows. The reflections and their intensities are tabulated in order of increasing $\sin\theta$ (This should be done after correcting for the Lorentz and polarization factors, and the absorption factor). The list is then divided into several proper groups. Since the temperature factor and the scattering factors do not vary rapidly at low values of $\theta$, larger range may be taken for such values. Lipson and Cochran (26) suggested the using of the following groups (in terms of $\sin\theta$): 0.2-0.6, 0.6-0.8, 0.8-1.0, the 0-0.2 group is discarded. For each group, intensities or $F^2$ is calculated

and the values of N(z) for z=10, 20, . . . . up to 100% are determined. Finally, for each z, the mean of N(z) over all sinθ groups is compared graphically with the theoretical values and the centrosymmetry or not is determined.

The reliablility of this method depends upon two things. First, that no atom heavy enough to dominate the intensity distribution is present and most of the atoms occupy the general positions. Second, a sufficiently large number of intensities including both unobserved and extinct reflections are used.

According to Howells, Phillips and Rogers, this method can be applied satisfactory to zones of reflections. The tedious calculations for three dimensional data can thus be avoided. It was found that for this crystal the method was applied satisfactorily even to one quadrant of a two dimensional zone. In this quadrant, a weight of ½ is applied to all reflections on the border lines. The method of calculation is illustrated as follows. For group 1 of hol zone (see Table XII), the total $F^2$ is obtained by summing the $F^2$ of each reflection in the group except taking ½ of $F^2$ of those reflections on the border lines. The total $F^2$ is found to be 31,552.3. The total reflections are 72, but 14 of them are on the border lines. Thus, the true number of reflections is 58 plus 14/2 or 65. The mean value of $F^2$ for group 1 is 31,552.3/65 or 485.4. The value of N(0.1) is obtained as follows: First, count the number of reflections with $F^2$ equal to or less than 48.5(0.1 times 485.4); there are 22 plus 4/2 or

24 of them. Thus, the value of N(0.1) is 24/65 or 36.8%. To calculate N(0.2), it is found that the number of reflections with $F^2$ greater than 48.5 but equal to or less than 97.1(0.2 times 485.4) is 9. Thus, the total number of reflections with $F^2$ equal to or less than 97.1 is 24 plus 9 or 33. Therefore, N(0.2) is 33/65 or 50.7%. The calculation of N(0.3) up to N(1.0) can be done in the same manner.

2. Data and results

Both hol and okl zones have been tested by this method. The hol zone has almost all the reflections for one quadrant while the okl has most of the reflections. The data are included in the following tables. The theoretical and the experimental curves are plotted in Fig. 16. From Fig. 16, it appears that calcium 1-naphthyl phosphate is centrosymmetrical, because both hol and okl curves are close to or higher than the theoretical centrosymmetrical curve.

Table XII. Values of $F^2$ for hol reflections of $Ca(C_{10}H_7HOP_4)_2 \cdot 3H_2O$

| | $F^2$ (Sin$\theta$) | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| $1^h$ | 0 | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 |
| 0 | | 6756.8 (.107) | 2088.5 (.215) | 772.8 (.322) | 475.2 (.430) | 6.3 (.536) | 7.7 (.644) | 190.4 (.752) | 75.7 (.860) | 28.0 (.966) |
| 1 | | 6806.3 (.107) | 5610.0 (.211) | 533.6 (.317) | 121.0 (.423) | 6.3 (.530) | 231.0 (.638) | 96.0 (.745) | 112.4 (.852) | 3.4 (.958) |
| 2 | 2143.6 (.084) | 954.8 (.122) | 2016.0 (.214) | 533.6 (.316) | 4.8 (.421) | 5.8 (.527) | 645.2 (.633) | 7.7 (.738) | 11.9 (.846) | 3.4 (.954) |
| 3 | 1608.0 (.125) | 1062.8 (.148) | 7.0 (.226) | 723.6 (.322) | 121.0 (.423) | 5.8 (.527) | 712.9 (.632) | 30.5 (.736) | 6.3 (.843) | 9.0 (.950) |
| 4 | 2601.0 (.167) | 4692.3 (.180) | 1857.6 (.244) | 519.8 (.332) | 542.9 (.429) | 6.3 (.528) | 702.3 (.633) | 25.6 (.735) | 6.3 (.842) | 14.4 (.946) |
| 5 | 1632.2 (.209) | 2652.3 (.215) | 4006.9 (.268) | 15.3 (.346) | 228.0 (.439) | 8.3 (.535) | 198.8 (.636) | 7.7 (.738) | 6.3 (.842) | 11.9 (.945) |
| 6 | 789.6 (.251) | 823.7 (.252) | 26.0 (.296) | 56.3 (.367) | 1149.2 (.452) | 166.4 (.545) | 7.7 (.643) | 96.0 (.743) | 6.3 (.845) | 9.6 (.948) |
| 7 | 3.4 (.293) | 136.9 (.291) | 640.1 (.326) | 141.6 (.389) | 190.4 (.469) | 6.3 (.557) | 29.4 (.651) | 116.6 (.750) | 75.7 (.851) | 3.8 (.952) |
| 8 | 404.0 (.335) | 17.1 (.330) | 41.0 (.360) | 182.3 (.415) | 29.1 (.488) | 91.3 (.572) | 104.0 (.664) | 466.6 (.759) | 75.7 (.857) | 3.4 (.957) |
| 9 | 2580.6 (.376) | 4.4 (.370) | 50.4 (.394) | 237.2 (.444) | 7.7 (.511) | 88.8 (.590) | 9.6 (.678) | 320.4 (.770) | 22.2 (.865) | 3.4 (.963) |
| 10 | 1592.0 (.418) | 190.4 (.410) | 15.3 (.436) | 338.6 (.474) | 20.1 (.535) | 610.1 (.611) | 108.2 (.694) | 7.7 (.784) | 5.3 (.875) | 23.4 (.972) |
| 11 | 1069.3 (.460) | 5.3 (.450) | 68.9 (.467) | 11.1 (.505) | 8.3 (.562) | 571.2 (.633) | 566.4 (.713) | 9.0 (.798) | 5.3 (.888) | |
| 12 | 43.6 (.502) | 75.7 (.492) | 57.6 (.504) | 52.4 (.537) | 161.3 (.592) | 196.0 (.657) | 506.3 (.733) | 22.2 (.815) | 4.8 (.904) | |
| 13 | 285.6 (.544) | 24.5 (.532) | 77.4 (.543) | 44.4 (.574) | 7.7 (.621) | 15.3 (.682) | 96.0 (.755) | 8.3 (.834) | 4.4 (.919) | |
| 14 | 43.6 (.585) | 285.6 (.574) | 610.1 (.582) | 7.5 (.608) | 96.0 (.653) | 30.4 (.710) | 7.7 (.778) | 11.1 (.855) | 7.7 (.936) | |
| 15 | 9.7 (.626) | 38.6 (.614) | 37.2 (.620) | 292.4 (.645) | 466.6 (.685) | 100.0 (.739) | 7.7 (.802) | 67.2 (.855) | 9.0 (.956) | |
| 16 | 882.1 (.669) | 67.2 (.656) | 11.9 (.660) | 50.9 (.680) | 306.3 (.719) | 29.4 (.767) | 6.3 (.830) | 72.3 (.901) | 37.2 (.975) | |
| 17 | 285.6 (.711) | 7.7 (.695) | 320.4 (.700) | 40.0 (.718) | 49.2 (.746) | 16.3 (.800) | 6.3 (.858) | 96.0 (.925) | | |
| 18 | 219.0 (.753) | 30.6 (.738) | 15.3 (.740) | 14.4 (.756) | 52.5 (.788) | 6.4 (.830) | 5.3 (.885) | 44.9 (.951) | | |
| 19 | 11.9 (.795) | 7.7 (.780) | 14.4 (.780) | 7.5 (.795) | 7.0 (.821) | 19.1 (.865) | 7.0 (.915) | 11.1 (.975) | | |

| $1^h$ | 0 | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 |
|---|---|---|---|---|---|---|---|---|---|---|
| 20 | 17.2 | 10.4 | 7.0 | 6.3 | 5.8 | 41.5 | 47.6 | | | |
| | (.835) | (.820) | (.820) | (.833) | (.860) | (.896) | (.946) | | | |
| 21 | 5.3 | 11.1 | 29.2 | 5.8 | 5.3 | 62.9 | 112.3 | | | |
| | (.879) | (.862) | (.860) | (.872) | (.895) | (.932) | (.978) | | | |
| 22 | 4.8 | 15.3 | 15.3 | | 3.8 | 8.3 | | | | |
| | (.918) | (.904) | (.900) | | (.934) | (.966) | | | | |
| 23 | 9.7 | 16.3 | 37.3 | | 3.8 | | | | | |
| | (.960) | (.945) | (.942) | | (.970) | | | | | |

Table XIII. Values of $F^2$ for $0kl$ reflections of $Ca(C_{10}H_7HOP_4)_2 \cdot 3H_2O$

| | $F^2$ (Sin$\theta$) | | | | | |
|---|---|---|---|---|---|---|
| k / l | 0 | -1 | -2 | -3 | -4 | -5 |
| 0 | | | | | | |
| 1 | | | | 1.7 | 1584.0 | 3.6 |
| | | | | (.263) | (.347) | (.431) |
| 2 | 2143.7 | 1.7 | 7225.0 | 1.4 | 2097.6 | 2.9 |
| | (.084) | (.125) | (.197) | (.276) | (.358) | (.441) |
| 3 | 1608.0 | 1.7 | 5821.7 | 2.0 | 686.4 | 3.2 |
| | (.125) | (.158) | (.221) | (.295) | (.374) | (.455) |
| 4 | 2601.0 | 1.7 | 5270.7 | 2.0 | 331.2 | 3.6 |
| | (.167) | (.195) | (.250) | (.319) | (.394) | (.472) |
| 5 | 1632.2 | 2.0 | 1376.4 | 2.0 | 259.2 | 4.0 |
| | (.209) | (.233) | (.282) | (.346) | (.417) | (.492) |
| 6 | 789.6 | 2.3 | 1436.4 | 2.3 | 900.0 | 4.4 |
| | (.251) | (.273) | (.317) | (.375) | (.442) | (.515) |
| 7 | 3.4 | 2.6 | 492.8 | 2.6 | 1024.0 | 5.3 |
| | (.292) | (.313) | (.353) | (.407) | (.470) | (.540) |
| 8 | 404.0 | 2.9 | 2480.0 | 2.9 | 571.2 | 5.8 |
| | (.335) | (.353) | (.390) | (.440) | (.500) | (.567) |
| 9 | 2580.6 | 2.9 | 118.8 | 3.2 | 65.6 | 6.3 |
| | (.376) | (.394) | (.428) | (.475) | (.532) | (.595) |
| 10 | 1592.0 | 3.2 | 65.6 | 3.2 | 342.3 | 6.3 |
| | (.418) | (.435) | (.467) | (.511) | (.565) | (.625) |
| 11 | 1069.3 | 3.6 | 767.3 | 4.0 | 292.4 | 6.8 |
| | (.460) | (.476) | (.506) | (.548) | (.599) | (.657) |
| 12 | 43.6 | 4.0 | 1892.3 | 4.4 | 49.0 | 7.3 |
| | (.502) | (.517) | (.546) | (.585) | (.634) | (.689) |
| 13 | 285.6 | 4.4 | 1246.1 | 4.8 | 5.1 | 7.3 |
| | (.544) | (.559) | (.586) | (.623) | (.668) | (.723) |
| 14 | 43.6 | 5.3 | 316.8 | 4.8 | 364.8 | 7.3 |
| | (.585) | (.599) | (.626) | (.662) | (.706) | (.757) |
| 15 | 9.6 | 5.3 | 16.5 | 4.8 | 615.0 | 6.8 |
| | (.626) | (.641) | (.666) | (.700) | (.743) | (.792) |
| 16 | 882.1 | 5.8 | 45.5 | 4.8 | 282.2 | 6.3 |
| | (.669) | (.683) | (.706) | (.740) | (.780) | (.828) |
| 17 | 285.6 | 5.8 | 6.7 | 4.8 | 272.2 | 5.8 |
| | (.711) | (.724) | (.746) | (.779) | (.818) | (.864) |
| 18 | 219.0 | 5.3 | 5.2 | 4.4 | 79.2 | 4.4 |
| | (.753) | (.766) | (.788) | (.819) | (.856) | (.901) |
| 19 | 11.9 | 4.8 | 6.2 | 3.6 | 4.2 | 3.6 |
| | (.795) | (.808) | (.829) | (.858) | (.895) | (.938) |
| 20 | 17.2 | 4.0 | 5.2 | 2.9 | 9.6 | 2.6 |

$F^2$
(Sin$\theta$)

| $l_0$ \ k | 0 | -1 | -2 | -3 | -4 | -5 |
|---|---|---|---|---|---|---|
| | (.836) | (.849) | (.870) | (.898) | (.934) | (.975) |
| 21 | 5.3 | 3.6 | 51.0 | 2.3 | 8.4 | |
| | (.877) | (.891) | (.911) | (.939) | (.973) | |
| 22 | 4.2 | 2.6 | 74.3 | 1.7 | | |
| | (.920) | (.932) | (.952) | (.979) | | |
| 23 | 9.6 | | | | | |
| | (.960) | | | | | |

Table XIV. Values of N(z), in percentages, for hol reflections of

$Ca(C_{10}H_7HPO_4)_2.3H_2O$

| Group no. | N(z) 0.1 | 0.2 | 0.3 | 0.4 | 0.5 | 0.6 | 0.7 | 0.8 | 0.9 | 1.0 |
|---|---|---|---|---|---|---|---|---|---|---|
| 1 | 36.8 | 50.7 | 57.6 | 65.3 | 70.0 | 71.5 | 73.0 | 73.7 | 74.5 | 74.5 |
| 2 | 32.2 | 42.6 | 47.8 | 53.0 | 54.8 | 62.5 | 68.6 | 70.4 | 71.3 | 71.3 |
| 3 | 0 | 12.3 | 37.6 | 49.2 | 55.4 | 63.0 | 65.3 | 71.5 | 73.0 | 73.0 |
| Mean | 23.0 | 35.2 | 47.7 | 55.8 | 60.1 | 65.7 | 68.9 | 71.9 | 72.9 | 72.9 |

Table XV. Values of N(z), in percentages, for okl reflections of

$Ca(C_{10}H_7HPO_4)_2.3H_2O$

| Group no. | N(z) 0.1 | 0.2 | 0.3 | 0.4 | 0.5 | 0.6 | 0.7 | 0.8 | 0.9 | 1.0 |
|---|---|---|---|---|---|---|---|---|---|---|
| 1 | 56.0 | 59.4 | 62.0 | 62.8 | 64.5 | 69.8 | 70.6 | 70.6 | 72.4 | 75.0 |
| 2 | 69.0 | 72.6 | 72.6 | 72.6 | 76.3 | 80.0 | 80.0 | 80.0 | 80.0 | 80.0 |
| 3 | 6.0 | 48.0 | 78.0 | 82.0 | 88.0 | 88.0 | 88.0 | 88.0 | 88.0 | 88.0 |
| Mean | 43.7 | 60.0 | 70.8 | 72.4 | 76.3 | 79.3 | 79.6 | 79.6 | 80.4 | 81.2 |

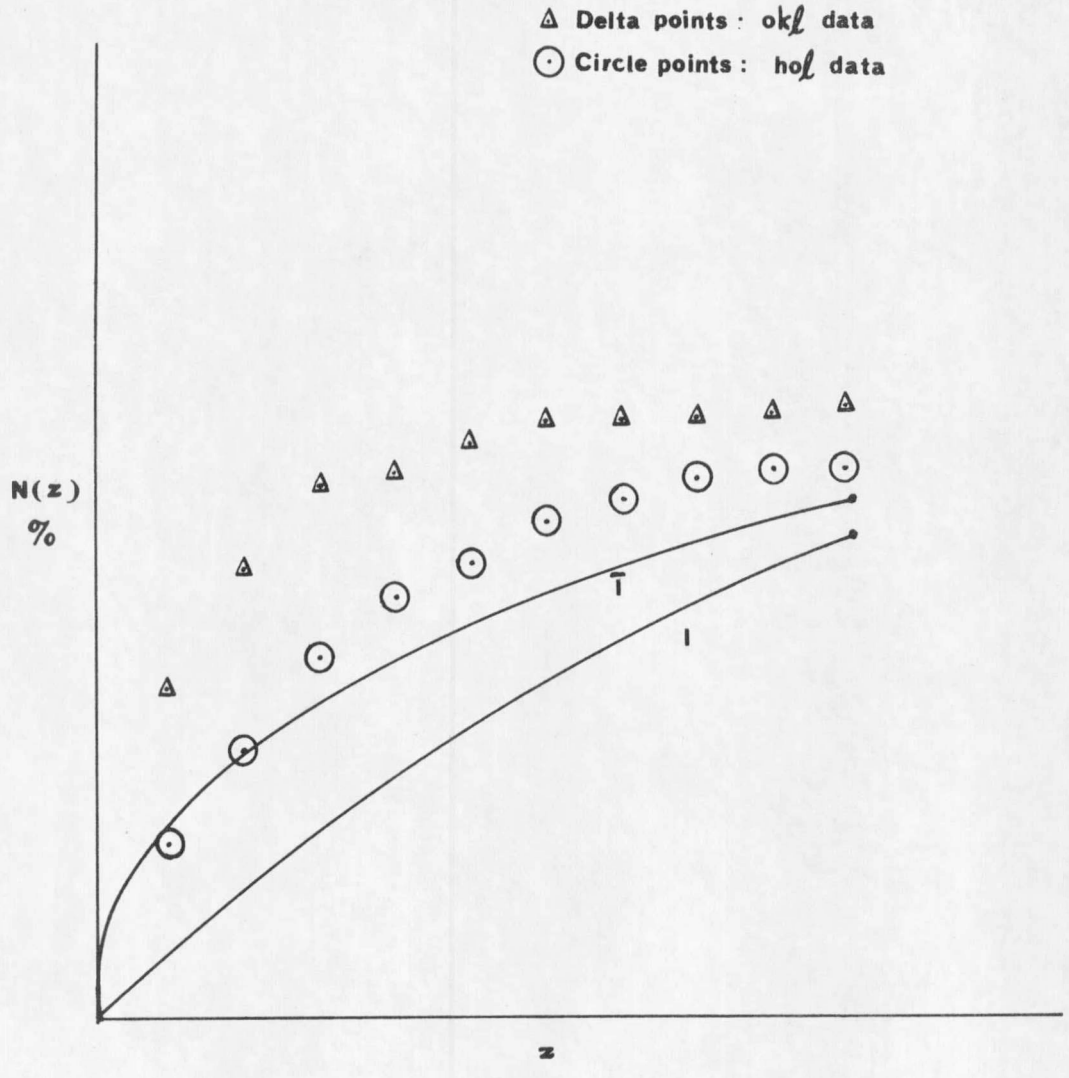



Figure 16 Intensity distribution for calcium 1-naphthyl phosphate

B. Patterson function

1. General description

The Patterson function has the following Fourier form.

$$P(uvw)=1/v\sum_{\bar{h}_3}^{h_3}\sum_{\bar{h}_2}^{h_2}\sum_{\bar{h}_1}^{h_1}\left|F_{h_1h_2h_3}\right|^2\exp(-2\pi i(h_1u+h_2v+h_3w))$$

It is similar to the electron density Fourier equation as below.

$$\rho(x_1x_2x_3)=1/v\sum_{\bar{h}_3}^{h_3}\sum_{\bar{h}_2}^{h_2}\sum_{\bar{h}_1}^{h_1}F_{h_1h_2h_3}\exp(-2\pi i(h_1x_1+h_2x_2+h_3x_3))$$

The important properties of the Patterson function will be described briefly as follows.

a. The Patterson synthesis is the vector set of the electron density. The vector interpretation can, then be used for the Patterson map.

For the electron density

$$F_{h_1h_2h_3}=\sum_i f_i\exp(2\pi i(h_1x_1+h_2x_2+h_3x_3))$$

There is a peak in the electron density map for any atom of location $x_1x_2x_3$.

For the Patterson function

$$\left|F_{h_1h_2h_3}\right|^2=F_{h_1h_2h_3}\bar{F}_{h_1h_2h_3}=\sum_i\sum_j f_if_j\exp(2\pi ih(x_{1i}-x_{1j})+h_2(x_{2i}-x_{2j})+h_3(x_{3i}-x_{3j}))$$

A Patterson peak will be found for every pair of atoms i and j at their interatomic distance or the vectorial dif-

ference.

b. The Patterson function is centrosymmetrical

$$P(uvw)=1/v\sum_{\bar{h}_3}^{h_3}\sum_{\bar{h}_2}^{h_2}\sum_{\bar{h}_1}^{h_1}\left|F_{h_1h_2h_3}\right|^2\cos 2\pi(h_1u+h_2v+h_3w)$$

This is due to Friedel's law.

c. The Patterson peak usually is broader and harder to resolve than that of the electron density.

d. The Patterson peaks are a continuously variable function rather than a set of discrete points. (So are electron density peaks).

$$P_{12}=\int_o^v \rho_1\ \rho_2 dv$$

2. Application

a. Predication of the peak height

Before an attempt is made to interpret any Patterson whatever, it is very desirable to tabulate the peak heights for all pairs of atoms. The volume of a Patterson peak due to a pair of atoms i and j in the crystal is $Z_iZ_j$, (8), where Z is the number of electrons in an atom.

$$V_{ij}=Z_iZ_j$$

Since $V_{origin}=\sum_i Z_i^2$

Then $V_{ij}=\dfrac{Z_iZ_j}{\sum_i Z_i^2}V_{origin}$

Since the peak height is approximately proportional to its volume

$$H\doteq KV$$

Thus $H_{ij} \fallingdotseq \frac{Z_i Z_j}{\sum_i Z_i^2} H$ origin

There are two molecules of $Ca(C_{10}H_7HPO_4)_2 \cdot 3H_2O$ or $Ca_2P_4O_{22}C_{40}H_{44}$ in the unit cell, which corresponds to $\sum_i Z_i^2 = 4,440$. Since the origin peak is always adjusted to be 999, the peak height $H_{ij}$ for each pair of atoms i and j is calculated and listed in the following table.

$H_{ij}$

| | Ca | P | O | C | H |
|---|---|---|---|---|---|
| Ca | 72.9 | 60.8 | 32.4 | 24.3 | 4.1 |
| P | 60.8 | 50.6 | 27.0 | 20.3 | 3.4 |
| O | 32.4 | 27.0 | 14.4 | 10.8 | 1.8 |
| C | 24.3 | 20.3 | 10.8 | 8.1 | 1.4 |
| H | 4.1 | 3.4 | 1.8 | 1.4 | 0.2 |

b. The locating of heavy atoms

The locating of all the heavy atoms is based on the following method.

For the ease of illustration, suppose there are three independent heavy atoms occupying the general positions, which is the case for our crystal of $Ca(C_{10}H_7HPO_4)_2 \cdot 3H_2O$. (Independent atom means atom not related by symmetry). The method stated below will also work for four or more independ-

ent heavy atoms occupying the general positions. It will be discussed later for some of the independent heavy atoms occupying the special positions. Take one dimension for illustration (The two and three dimensional cases can be done in an analogous manner). Let the general positions which the three independent heavy atoms occupy be $x_1$, $x_2$ and $x_3$. Take the centrosymmetrical case for example (The noncentrosymmetrical case will be discussed later). From the vector set nature of the Patterson function, the Patterson peaks of a centrosymmetrical crystal are expected to include the following: $x_1-x_2$ (the vector point from $x_2$ to $x_1$), $x_1-x_3$, $x_2-x_3$ and $x_1+x_2$ (the vector point from $-x_2$ to $x_1$), $x_1+x_3$, $x_2+x_3$, plus $2x_1$, $2x_2$, $2x_3$. For the centrosymmetrical case, those vector points like $x_1-x_2$, $x_1+x_2$, etc., which are formed from two different atoms of the same or different kinds are double weight or more, depending on the symmetry of the particular crystal, while the vector points forming between the atom itself, e.g. $2x_1$, $2x_2$ etc. are single weight or more, depending also upon the symmetry of the particular crystal. Let $x_1+x_2$ and $2x_1$ have the double weight and single weight respectively (This is done mainly for the ease of illustration). The double weight peaks like $x_1+x_2$, $x_1-x_2$ etc. can be recognized in the following way.

From twice the calculated peak height, the double weight peaks which we are after can be narrowed down to a very small number which is always greater than six due to the ease of

superimposing of the Patterson peaks. Suppose the six big peaks of double weight in the following order $x_1+x_2$, $x_1+x_3$, $x_2+x_3$, $x_1-x_2$, $x_1-x_3$ and $x_2-x_3$ are known. In the method stated here, these big peaks do not have to be known. The fact that they are assumed to be known is only for the ease of illustration. Take the first peak $x_1+x_2$ and add to it all the peaks which follow it and the corresponding inverse peaks as below.

| | | | | |
|---|---|---|---|---|
| $x_1+x_2$ | $x_1+x_2$ | $x_1+x_2$ | $x_1+x_2$ | $x_1+x_2$ |
| $x_1+x_3$ | $-x_1-x_3$ | $x_2+x_3$ | $-x_2-x_3$ | $x_1-x_2$ |
| $2x_1+x_2+x_3$ | $x_2-x_3$ | $x_1+2x_2+x_3$ | $x-x_3$ | $2x_1$ |
| $x_1+x_2$ | $x_1+x_2$ | $x_1+x_2$ | $x_1+x_2$ | $x_1+x_2$ |
| $-x_1+x_2$ | $x_1-x_3$ | $-x_1+x_3$ | $x_2-x_3$ | $-x_2+x_3$ |
| $2x_2$ | $2x_1+x_2-x_3$ | $x_2+x_3$ | $x_1+2x_2-x_3$ | $x_1+x_3$ |

Upon examining the above results, we find that all the big peaks have been come back except the first peak $x_1+x_2$ used and its sister peak $x_1-x_2$ which is formed by the same pair of atoms but in a different direction. Next, the second peak $x_1+x_3$ is taken and is added to it all the peaks which follow it and the corresponding inverse peaks as follows.

| | | | |
|---|---|---|---|
| $x_1+x_3$ | $x_1+x_3$ | $x_1+x_3$ | $x_1+x_3$ |
| $x_2+x_3$ | $-x_2-x_3$ | $x_1-x_2$ | $-x_1+x_2$ |
| $x_1+x_2+2x_3$ | $x_1-x_2$ | $2x_1-x_2+x_3$ | $x_2+x_3$ |

$$\begin{array}{cccc} x_1+x_3 & x_1+x_3 & x_1+x_3 & x_1+x_3 \\ \underline{x_1-x_3} & \underline{-x_1+x_3} & \underline{x_2-x_3} & \underline{-x_2+x_3} \\ 2x_1 & 2x_3 & x_1+x_2 & x_1-x_2+2x_3 \end{array}$$

If we continue in this manner, we shall end up with the following four independent relationships which compose only the six double weight peaks with each peak occurring twice.

$$\begin{array}{cccc} x_1+x_3 & x_1-x_3 & x_1-x_3 & x_1+x_3 \\ \underline{x_2-x_3} & \underline{x_2+x_3} & \underline{-x_2+x_3} & \underline{-x_2-x_3} \\ x_1+x_2 & x_1+x_2 & x_1-x_2 & x_1-x_2 \end{array}$$

It is noted that each one of the above four independent relationships may have three different forms according to how they are arranged. One example is given in the following.

$$\begin{array}{ccc} x_1+x_3 & x_1+x_3 & x_1-x_2 \\ \underline{-x_2-x_3} & \underline{-x_1+x_2} & \underline{x_2+x_3} \\ x_1-x_2 & x_2+x_3 & x_1+x_3 \end{array}$$

All three of them represent the same relationship. As we mentioned earlier, these six big peaks of double weight do not have to be known. For these unknown big peaks, we do know that from the structural formula there exist three independent heavy atoms which correspond to six big peaks of double weight for the centrosymmetrical case. There are always more than six big peaks showing up even in the three

dimensional Patterson maps. Follow the adding procedures described above for all the possible big peaks found. Pick up all the independent relationships we can have. Those six big peaks composing the four independent relationships are the peaks we are after. Sometimes due to the symmetry of the particular crystal, the single weight peak like $2x_1$, $2x_2$ or $2x_3$ may show up as big as the double weight peak. This single weight peak can be distinguished from the double weight peaks by the close packing and the symmetry consideration. This is the case for the crystal $Ca(C_{10}H_7HPO_4)_2 \cdot 3H_2O$. More detail will be discussed later. The assignment of $x_1+x_2$, $x_1-x_2$, $x_1+x_3$, $x_1-x_3$, $x_2+x_3$, and $x_2-x_3$ to these six big peaks can be done, besides the calculated peak heights, by the close packing consideration, i. e., from the known bond distances. The six big peaks will be labelled temporarily by the calculated peak heights. Then, by a simple computation like $(x_1+x_2)+(x_1-x_2)=2x_1$, $x_1=(2x_1)/2$, all the three independent heavy atoms locations $x_1$, $x_2$, $x_3$ can be determined. A scale model is set up and from the known bond distances, and close packing consideration, the $x_1$, $x_2$, $x_3$ can be readjusted to the correct values.

Now consider the case where some independent heavy atoms occupy special positions, space group $P\bar{1}$, for example. The number of heavy atoms occupying the special positions must be even or in pairs. Suppose one pair or one independent

atom of the three independent heavy atoms occupy the special positions of ½, ½, 0 and 0, 0, 0 (Independent meaning not related by symmetry). Let the other two independent atoms occupy the locations of $x_1y_1z_1$ and $x_2y_2z_2$. These heavy atoms will produce the following Patterson peaks (a) Seven single weight peaks, namely $x_1$, $y_1$, $z_1$; $x_2$, $y_2$, $z_2$; $x_1-½$, $y_1-½$ $z_1-½$; $x_2-½$, $y_2-½$, $z_2-½$; ½, ½, 0; $2x_1$, $2y_1$, $2z_1$; $2x_2$, $2y_2$, $2z_2$ (b) two double weight peaks i. e., $x_1+x_2$, $y_1+y_2$, $z_1+z_2$; $x_1-x_2$, $y_1-y_2$, $z_1-z_2$. It is advisable to test for whether a heavy atom occupys a special position before using the method described above for general positions. The possibility of the heavy atoms occupying the special positions may be considered in the following way (a) If any atom occupies a special position, the surrounding atoms must be related by the symmetry of that special position. For $Ca(C_{10}H_7HPO_4)_2 \cdot 3H_2O$, the heavy atoms are calcium and phosphorus. Since the phosphate group is approximately a tetrahedral configuration with the phosphorus atom at the center, phosphorus is unlikely to sit on a center of symmetry and only calcium could be in a special position. (b) If there are some Patterson peaks of single weight or more occupying the special locations of the Patterson space, there may be some heavy atoms occupying special positions in crystal space. If there is a heavy atom at the origin, a Patterson peak of single weight or more will show up both at $x_iy_iz_i$ and $2x_i2y_i2z_i$ of the Patterson space where i is the

heavy atom identification number occupying the general positions. After the heavy atoms at the special positions have been located, the other atoms occupying the general position may be found by the addition method.

If the crystal is noncentrosymmetrical, the above method can also be used except the number of the possible peaks to be tested is much greater since most of the peaks are single-weight.

The method just described is illustrated by the locating of the independent heavy atoms of one calcium and two phosphorus for the crystal of $Ca(C_{10}H_7HPO_4)_2 \cdot 3H_2O$ as below.

From the three dimensional un-sharpened and sharpened (the temperature factor being 1.5) Patterson maps, those Patterson peaks having approximate magnitude equal to or greater than 100 (which corresponds to twice the P-P interaction) are listed in the following table. The Patterson coordinate is in 1/40th of unit cell.

Table XVI. Three dimensional Patterson Peaks Equal to or Greater Than 100

| Patterson Coordinates | | | Patterson Peak | |
|---|---|---|---|---|
| x | y | z | Un-sharpened | Sharpened(B 1.5) |
| 0 | 9 | 0 | 42 | 114 |
| 6 | 20 | 0 | 192 | 225 |
| 20 | 20 | 0 | 215 | 176 |
| 1 | 16 | 0 | 118 | 93 |
| 12 | 20 | 0 | 93 | 80 |
| 4 | 5 | 1 | 78 | 92 |
| 18 | 11 | 3 | 134 | 144 |
| 38 | 31 | 3 | 125 | 90 |
| 12 | 7 | 4 | 146 | 200 |
| 24 | 7 | 4 | 161 | 215 |
| 5 | 27 | 4 | 114 | 189 |
| 30 | 27 | 4 | 101 | 187 |
| 36 | 15 | 9 | 165 | 171 |
| 36 | 31 | 9 | 154 | 85 |
| 10 | 39 | 19 | 137 | 54 |

Calcium 1-naphthyl phosphate was assumed to be in space group $P\bar{1}$, and the number of molecules per unit cell was found to be two. Before the adding method was used, the Patterson was examined to see whether any heavy atoms occupy special positions. Since neither

phosphorus nor oxygen can be expected to have a centrosymmetric environment, the only heavy atom which might occupy the special position, is the calcium. To see if the two calcium atoms occupy the special location, proceed as follows. For $P\bar{1}$, centers of symmetry occur at 000, ½00, 0½0, 00½, ½½0, ½0½, 0½½ and ½½½. The Patterson peaks at these special locations are listed in the following table (in terms of the Patterson space).

Table XVII. Patterson Peaks at Special Locations

| | 000 | ½00 | 0½0 | 00½ | ½½0 | ½0½ | 0½½ | ½½½ |
|---|---|---|---|---|---|---|---|---|
| Unsharpened Patterson | 999 | (9) | 0 | 0 | 215 | 0 | 63 | 81 |
| Sharpened Patterson | 999 | (34) | 0 | 0 | 176 | (3) | 37 | 51 |

Note: The values in parentheses indicate that there is not a peak at these locations.

If the two calcium atoms occupy the special positions, the only possible locations are (000, ½½0), (000, 0½½), (000, ½½½). These were tested and none of them gave a reasonable R-factor and a Ca-Ca distance as reported in the literature. Therefore it appears that no heavy atom will occupy the special position.

Next the fifteen big peaks obtained from both the unsharpened and the sharpened Patterson maps were tested by the adding method. It was found that only seven of the

fifteen peaks had the proper "cyclic" properties. These seven peaks were those at 6, 20, 0; 20, 20, 0; 12, 7, 4; 24, 7, 4; 5, 27, 4; 30, 27, 4; 36, 15, 9. Six independent relationships were found among them as below.

| | | |
|---|---|---|
| 24, 7, 4 | 30, 27, 4 | 30, 27, 4 |
| 12, 7, 4 | 5, 27, 4 | 16, 33,36 |
| 36, 14,8 | 35, 14, 8 | 6, 20, 0 |
| 35, 13, 36 | 5, 27, 4 | 30, 27, 4 |
| 12, 7, 4 | 16, 33,36 | 28, 33,36 |
| 7, 20, 0 | 21, 20, 0 | 18, 20, 0 |

Note that each coordinate remains the same when 40 (the fraction 1.0 is equal to 40) is added to or subtracted from it.

Three independent heavy atoms should produce six big peaks of double weight and three smaller peaks of single weight, and there are four independent relationships existing among these six double weight peaks. The three independent heavy atoms produce seven "cyclic" big peaks and there are six independent relationships among them. As discussed earlier, this is due to some smaller peak of single weight or more becoming as big as those double weight peaks because of the symmetry. Since this crystal has a pseudo b-glide plane, either the peak of 6, 20, 0 or the peak of 20, 20, 0 are not the double weight peak, i. e., the single weight which grows bigger due to the pseudo b-glide plane. The way to determine which of the two peaks

6,20,0 and 20,20,0 is the real double-weight peak is to take each one in turn and assign it as the single weight peak and then determine the locations for the heavy atoms (For detail, see the following illustration). Finally the bond distance between calcium and phosphorus was calculated and compared with approximate known value from the literature. Those which agree with the known bond distances are most probably the correct ones. By this method, the peak of 6,20,0 were found to be the real double weight peak. Let 1, 2, 3 represent the independent calcium, first and second independent phosphorus respectively. The assignment of 1, 2, and 3 to each of the peaks in the six independent relationships follows the method discussed previously i. e., first assign temporarily by the calculated peak height, then re-adjusted these from the close packing consideration. The correct labelling is as below.

| | | | | | |
|---|---|---|---|---|---|
| 24, 7, 4 | $-x_3+x_1$ | 30, 27, 4 | $x_2+x_1$ | 30, 27, 4 | $x_2+x_1$ |
| 12, 7, 4 | $x_2-x_1$ | 5, 27, 4 | $-x_3-x_1$ | 16, 33,36 | $x_3-x_1$ |
| 36,14, 8 | $x_2-x_3$ | 35, 14, 8 | $x_2-x_3$ | 6, 20, 0 | $x_2+x_3$ |
| 35,13,36 | $x_3+x_1$ | 5, 27, 4 | $-x_3-x_1$ | 30, 27, 4 | $x_2+x_1$ |
| 12, 7, 4 | $x_2-x_1$ | 16, 33,36 | $x_3-x_1$ | 28, 33,36 | $-x_2+x_1$ |
| 7,20, 0 | $x_2+x_3$ | 21, 20, 0 | $-2x_1$ | 18, 20, 0 | $2x_1$ |

The three heavy atoms locations were obtained by the very simple calculations as follow.

| | |
|---|---|
| 36, 15, 9 | $x_2-x_3$ |
| 6, 20, 0 | $x_2+x_3$ |
| 42, 35, 9 | $2x_2$ |

Thus $x_2$, $y_2$, $z_2$ of $P_1$ are 21, 17.5, 4.5

$x_3$, $y_3$, $z_3$ of $P_2$ are -15, 2.5, -4.5

From these, $x_1$, $y_1$, $z_1$ of Ca were 9, 10, 0

or in summary:

Ca: 9, 10, 0

$P_1$: 21, 17.5, 4.5

$P_2$: -15, 2.5, -4.5

When only these heavy atoms (one calcium and two phosphorus and those from the centers of symmetry) were included, the R-factor was 38.65% for hol projections, 46.96% for the okl projection and 57.35% for the hko projection. The closest Ca-P distance is 3.66Å which is quite close to the value of 3.63Å as determined by Trueblood (28).

c. The locating of the oxygen atoms

Most of the oxygen atoms were located from the Patterson maps by the two following methods.

(1) From the phosphorus location and the known P-O bond distance

To find the four oxygens around each phosphorus, first locate each P-P vector point which is represented by $2x_p$. Let the P-O vector point be represented by $x_{p+o}$. The vector from origin to the P-P vector point

is $\vec{2x_p}$ and the vector from origin to the P-O vector point is $\vec{x}_{p+o}$. Then the vector from $x_{p+o}$ to $2x_p$ will be $\vec{x}_{p-o}$ whose distance is approximately equal to the P-O bond of 1.5Å. Therefore, to locate the P-O vector point, i. e., $x_{p+o}$ in the Patterson map, take the P-P vector point, $2x_p$ as center and draw a sphere of 1.5Å radius in the scaled Patterson maps. All the peaks near the surface of this sphere may be the P-O vector points. Since it is not easy to draw a sphere in the three dimensional Patterson map, which consisted of many sections, this was carried out on each section. The P-P vector point $2x_p$ was used as a center and a circle of 1.5Å radius drawn on the section on which the phosphorus lies. For the other sections, the $2x_p$ projection was taken as a center and smaller circles drawn. The size of the circle depended upon the spacing between sections, the farther a particular section was from the phosphorus atom, the smaller the circle radius. All the peaks at about $\pm$0.2Å from these circles are the possible P-O vector points, i. e., $x_{p+o}$. Then these possible oxygen locations were tested by (a) the distance of an oxygen to any other oxygens of the same phosphate group, which should be around 2.5Å and (b) for correct oxygen positions, the R-factor should be reasonably lower.

All the eight oxygens except one were located by

the above method.

Table XVIII. The Oxygens Found Around the First Phosphorus $x_p$ equals 21,17.5,4.5. (in 1/40 of unit cell) by Patterson Method I

| P-O peak | P-O Coordinates ($x_{p+o}$) | Oxygen Location $x_o$ This Method | Location used |
|---|---|---|---|
| 77 | 36,39,10 | 15,21.5,5.5 | 14,21.5,5.5 |
| 154 | 36,31, 9 | 15,13.5,4.5 | 17,12.5,3.5 |
| 34 | 4,32,12 | 23,14.5,7.5 | 23,15.5,7.5 |

Table XIX. The Oxygens Found Around the Second Phosphorus $x_p$ Equals -15,2.5,-4.5 by Patterson Method I

| P-O peak | P-O Coordinates ($x_{p+o}$) | Oxygen Location $x_o$ This Method | Location used |
|---|---|---|---|
| 26 | 16,2,33 | 31,39.5,37.5 | 30.5,39.5,37 |
| 77 | 4,1,33 | 19,38.5,34.5 | 20.5,37.5,34.5 |
| 154 | 4,9,31 | 19, 6.5,35.5 | 19.5, 7.0,36.5 |
| 44 | 16,9,38 | 31, 6.5,32.5 | 29.0, 5.5,32.5 |

(2) From the superimposed big peaks

On the Table XVI, there are fifteen big peaks of magnitude around or greater than 100. Only seven of them were found due to the heavy atoms interactions. The other eight big peaks must be due to the superimposing of many small peaks, of which the Ca-O and the P-O peaks are the largest and the second largest ones. Thus, it is quite

possible that the Ca-O and the P-O peaks may superimpose on many of the eight remaining big peaks. This was found to be the case and many oxygens were located in this way. The detailed procedure for locating the oxygens is given below. For each remaining big peak, six possible peaks due to Ca-O and P-O interactions may superimpose on it. These six possible peaks are Ca+O, Ca-O, $P_1$+O, $P_1$-O, $P_2$+O, $P_2$-O. The possible oxygen locations are obtained when the calcium and phosphorus positions are subtracted from them. Take the remaining big peak of 1,16,0 as an example. Since the Ca, $P_1$, $P_2$ have the following locations of 9,10,0; 21,17.5,4.5; 15,-2.5,4.5 respectively, the six possible oxygen locations are 20,1.5,4.5; 22,-6.5,4.5; 16,13.5,4.5; 14,21.5,4.5; 32,6,0; 10,4,0. Any of these possible oxygens may be a real one if the following tests are passed. (a) It has the proper bond distance, e.g., P-O bond around 1.5Å, Ca-O distance from 2.2 to 2.6Å, O-O 2.5Å. (b) When it is included, R-factor becomes smaller. Six of the eight phosphate oxygens were located by this method, and their locations are compared with the ones finally used.

Table XX. Oxygens found around the first phosphorus of 21,17.5, 4.5 by Patterson Method II

| Big peaks involved | Oxygen locations This method | Location used |
|---|---|---|
| 1,16,0 | 14,21.5,4.5 | 14,21.5,5.5 |
| 1,16,0;36,31,9;4,5,1 | 17,12.5,3.5 | 17,12.5,3.5 |
| 18,11,3; 38,31,3 | 29.21.0,3.0 | 27,21.0,3.0 |

Table XXI. Oxygen Found Around the Second Phosphorus of 15,-2.5, 4.5 by Patterson Method II

| Big peaks involved | Oxygen Location This method | Location used |
|---|---|---|
| 18,11,3; 38,31,3 | 9, 1,2.5 | 9.5, 0.5,3 |
| 1,16,0; 4, 5,1 | 21, 2,5.5 | 19.5, 2.5,5 |
| 1,16,0; 36,31,9 | 21,34,4.5 | 20.5,33,3.5 |

D. Minimum function

1. General description

Up to the present time, the minimum function is the best image-seeking function which is a general approach to the solution of the Patterson synthesis. A detailed discussion about the minimum function was made by Buerger (8). However, one question needs considering here. When a line image is found by a roving search vector over the

Patterson maps, what place on line image should be used to record the minimum function? Buerger suggests the midpoint of the line. The advantage for using the midpoint is that the $M_2$ has the same origin as the Patterson function. For the ease of writing the computer program, the minimum function is recorded at the lower end of the line image. This $M_2$ has a different origin from the Patterson function. The interpretation listed in the next paragraph will help to make the best use of this.

2. Interpretation of the minimum function

a. Search vectors

Whether the Patterson synthesis can be solved by the minimum function depends upon the proper selection of the search vectors. This minimum function program can handle search vectors up to five. The key point of selecting these search vectors is that they should have a common intersection point (no two parallel vectors can be used) and at least the crystal space coordinates of the common intersection point must be known.Otherwise, each search vector produced a solution with a different origin in crystal space. Proper search vectors can be obtained in the following two ways. (a) The vectors corresponding to the known atoms which are located by some other method like the Patterson method, will be the proper search vectors

to be used. (b) For the centrosymmetrical case, the inversion vector (2x, 2y, 2z) can be used for the one search vector case.

It is immaterial whether the search vectors used are single or double weight, as long as the crystal space coordinate of the common intersection point of these vectors are known. Even though the inverse solution may be produced by the using of the double weight vectors, this can usually be eliminated.

b. Origin transformation

If a search vector is chosen from $x_2y_2z_2$ to $x_1y_1z_1$, point $x_1y_1z_1$ becomes 0,0,0 in the minimum function map. Thus a transformation is required to reproduce the crystal space. To make the proper transformation, the $x_1y_1z_1$ is simply added to each point in the minimum function map. The minimum function origin is thus transformed to $x_1y_1z_1$ and other points in the minimum function space converted to the proper crystal space coordinates.

Since we are dealing with only half of the whole Patterson function, it is quite possible that certain critical parts crystal space will not be obtained. In order to obtain as much as possible, it is recommended to run another minimum function with the same search vectors but in exactly the reverse directions.

For the centrosymmetrical case, the common point for these reverse vector is $-x_1-y_1-z_1$ to each point in the Patterson space.

C. Sharpened Patterson function

It was found that the sharpened Patterson function produced a better minimum function than the un-sharpened one. This is because the peaks in the sharpened Patterson maps have better resolution. This is illustrated in the following example. The temperature factor used to sharpen the Patterson function was 1.5, which was selected from the temperature factors 0.5, 1.0, 1.5 2.0, 2.5, and 3.0 giving the best resolved Patterson projection. A second rank minimum function was obtained from both the un-sharpened and sharpened Patterson functions by the using of first the search vector 4,-15,-9, then its reverse vector -4,15,9. All the oxygen and carbon atoms found in these minimum functions are listed in the following tables. Oxygen atoms thus found are compared with the best oxygen locations used; best oxygen locations were selected by the best bond distance and the lowest R-factor , while carbon atoms found are compared with those located by the three dimensional electron density maps.

Table XXII. Carbon Positions located by Both Minimum Function and Three Dimensional Electron Density Maps

| Atom | Un-sharpened $M_2$ | | Sharpened $M_2$ | | Location from 3-d Fourier map |
|---|---|---|---|---|---|
| | Peak height | Location | Peak height | Location | |
| 1 | 32 | 27,20.5, 9.5 | 18 | 31,25, 9.5 | 28,23, 9 |
| 2 | 32 | 31,22, 12.5 | 23 | 25,26.5,12.5 | 28,25, 12 |
| 3 | | | 17 | 27,20.5,14.5 | 27,24, 14 |
| 4 | | | | | 24,17, 15 |
| 5 | 34 | 21,10.5,18.5 | 27 | 23,12, 18.5 | 23,13, 18 |
| 6 | 32 | 23,12.5,18.5 | 23 | 21, 9.5,18.5 | 20, 9, 18 |
| 7 | 65 | 15, 4.5,15.5 | 26 | 17, 3.5,16.5 | 18, 4, 16 |
| 8 | 61 | 17, 8.5,13.5 | 18 | 21,10.5,13.5 | 20, 8, 13 |
| 9 | 39 | 21,12.5,12.5 | 17 | 23,15.5,12.5 | 22,14, 12 |
| 10 | | | 21 | 23,18.5, 9.5 | 24,17, 10 |
| 11 | | | 19 | 3, 1.5, 9.5 | 4, 3, 9 |
| 12 | 21 | -1, 6, 11.5 | 14 | -3, 4.5,12.5 | 0, 5, 12 |
| 13 | | | 22 | 37, 1.5,14.5 | 37, 3, 14 |
| 14 | | | 19 | -1, 0.5,15.5 | 1,-3, 15 |
| 15 | 29 | -1,31.5,18.5 | 18 | -1,31.5,18.5 | -,32, 18 |
| 16 | 37 | 1,30.5,18.5 | 17 | 3,28.5,18.5 | 2,28, 18 |
| 17 | 65 | 9,24.5,15.5 | 13 | 5,24.5,15.5 | 6,25, 16 |
| 18 | 20 | 7,26.5,11.5 | 28 | 7,27.5,12.5 | 8,28, 13 |
| 19 | 28 | 5,33.5,12.5 | 32 | 5,33.5,12.5 | 5,33.5,12 |
| 20 | 31 | 9,35.5,10.5 | 38 | 7,38.5, 9.5 | 6,37, 10 |

Table XXIII. Oxygen Positions Located by Minimum Function

| Atom | Un-sharpened $M_2$ | | Sharpened $M_2$ | | |
|---|---|---|---|---|---|
| | Peak height | Location | Peak height | Location | Location used |
| $PO_4$ Oxy 1 | 77 | 15,21.5,5.5 | 61 | 15,21.5,5.5 | 14,21.5,5.5 |
| : 2 | 111 | 15,13.5,4.5 | 85 | 15,13.5,4.5 | 17,12.5,3.5 |
| : 3 | 20 | 29,21.5,2.5 | 39 | 27,20.5,2.5 | 27,21, 3 |
| : 4 | 77 | 21,14.5,7.5 | 39 | 21,14.5,7.5 | 23,15.5,7.5 |
| : 5 | 29 | 9, 0.5,4.5 | 22 | 9, 0.5,2.5 | 9.5, 0.5,3 |
| : 6 | 77 | 21, 1.5,5.5 | 54 | 19, 1.5,5.5 | 19.5, 2.5,5.5 |
| : 7 | 111 | 21,33.5,4.5 | 85 | 21,33.5,4.5 | 20.5,33, 3.5 |
| : 8 | 78 | 11,34.5,7.5 | 42 | 11,34.5,7.5 | 11,34.5,7.5 |
| $H_2O$ Oxy 1 | 23 | 33,35.5,3.5 | 48 | 34,35.5,4 | 33,35.5,3.5 |
| 2 | 30 | 3,15.5,3.5 | 35 | 3,16.0,3.5 | 3,15.5,3.5 |
| 3 | 54 | 37,10.0,0 | 156 | 37,10.5,0.5 | 36,11.0,0 |

3. Application

The search vectors used for obtaining the minimum functions were taken from the vectors corresponding to the heavy atoms found by the Patterson method. Since the heavy atom locations found by the Patterson method were very crude, most minimum functions were calculated by only one search vector with both positive and negative directions. The second rank minimum functions $M_2$ thus found have the following advantages. (a) All the $M_2$ show up the heavy atoms, all the oxygen atoms and most of the carbon atoms, but there were four oxygens disappearing in the $M_4$ which was calculated mainly

for the comparison purpose. (b) It is much faster to calculate the $M_2$ than the $M_4$. The only disadvantage of the $M_2$ over the $M_4$ was that many false peaks showed. The way we recognize these oxygen atoms is as below.

a. From approximate bond distances of P-O and Ca-O

The bond distances of P-O and O-O in the phosphate group are about 1.5Å and 2.5Å respectively, while the Ca-O (the calcium and its coordination oxygen) bond distance is from 2.2 to 2.6Å. With phosphorus as a center, draw two circles of the radius 1.7Å and 1.3Å on the section containing the phosphorus and two smaller circles on each of the other sections. All the peaks between these two circles are the possible oxygen peaks. Positions of actual oxygen atoms were identified from the proper bond distances and the lower R-factor. The hydration water oxygens can be located in a similar manner.

b. From the pseudo glide plane

The existence of a pseudo b-glide plane in this triclinic crystal of calcium 1-naphthyl phosphate was indicated by,(1) The okl reflections on all the x-ray photographs were too weak to be seen for $k \neq 2n$. (2) There was a strong Harker line at u,½,0 of the Patterson maps. (3) In the okl Patterson projection, all peaks were repeated every b/2.

Since calcium and phosphorus atoms were found to be related by this pseudo b-glide, it was reasonable to assume that all the oxygens and carbons might be related by this pseudo

glide plane also. This was found to be the case. Since it is a pseudo b-glide plane, each pair of atoms related by it have the same z coordinate and differ in y coordinate by ½ fraction unit. By the help of this pseudo b-glide plane, the oxygens were located by pairs except for one hydration water oxygen which was located by the three dimensional electron density maps.

All the atoms located by the minimum functions are listed in the following table where the first number represents the peak height and the next three numbers separated by the commas represent the x, y, z coordinates in 1/40th of a unit cell.

Table XXIV. Comparison of the Positions of All Calcium, Phosphorus, and Oxygen Atoms Located by Different Minimum Functions

| Atom | $M_4$ Peak | x, y, z | Peak | $M_2$ x, y, z | Peak | $M_2$ x, y, z |
|---|---|---|---|---|---|---|
| Ca | 82: | 9,10.0,0.5 | 108: | 9,10.0,0 | 138: | 9,10.0,0.5 |
| $P_1$ | 65: | 19,16,5,4.5 | 192: | 21,17.5,4.5 | 165: | 21,17,5,4.5 |
| $P_2$ | 67: | 15,38, 4.5 | 192: | 15,37.5,4.5 | 165: | 15,37.5,4.5 |
| $O_1$ | 29: | 15,21, 4.5 | 74: | 17,22.5,5.5 | 77: | 15,21.5,5.5 |
| $O_2$ | 48: | 17,14, 3.5 | 101: | 16,13.5,4.5 | 111: | 15,13.5,4.5 |
| $O_3$ | | | 55: | 27,20.5,4.5 | 20: | 29,21.5,2.5 |
| $O_4$ | 31: | 23,15, 7.5 | 45: | 23,17.5,7.5 | 77: | 21,14.5,7.5 |
| $O_5$ | 10: | 9,-1 3.5 | 39: | 9, 0.5,4.5 | 29: | 9, 0.5,4.5 |
| $O_6$ | 16: | 23, 2, 3.5 | 101: | 19, 1.5,4.5 | 77: | 21, 1.5,5.5 |
| $O_7$ | 39: | 19,-7, 3.5 | 74: | 19,-7.5,3.5 | 111: | 21,-6.5,4.5 |

| Atom | Peak | $M_4$ x, y, z | Peak | $M_2$ x, y, z | Peak | $M_2$ x, y, z |
|---|---|---|---|---|---|---|
| $O_8$ | 31: | 14,-4, 7.5 | 43: | 11,-4.5,8.5 | 78: | 11,-5.5,7.5 |
| $O_9$ | | | 23: | 33,35.5,3.5 | 23: | 33,35.5,3.5 |
| $O_{10}$ | | | 30: | 3,15.5,3.5 | 30: | 3,15.5,3.5 |

Vectors for calculating minimum functions:

$M_4$: (-6,-20,0; 30,-6,9; 36,14.5,9; and reverse vectors)

$M_2$: (6,20,0 and -6,-20,0)

$M_2$: (4,-15,-9 and -4,15,9)

E. Electron density maps

The diffracting power of each type of atom as contributing to the intensity can be predicated approximately as the square of the atomic number.

Table XXV. The Estimated Diffracting Power for Calcium Naphthyl Phosphate.

| Atoms | $z^2$ | % |
|---|---|---|
| 2Ca | $2 \times 18^2 = 648$ | 14.6 |
| 4P | $4 \times 15^2 = 900$ | 20.3 |
| 22O | $22 \times 8^2 = 1408$ | 31.7 |
| 40C | $40 \times 6^2 = 1440$ | 32.4 |
| 44H | $44 \times 1^2 = 44$ | 1.0 |
| | $\sum_j z_j^2$ 4440 | 100.0 |

From the above table, the diffracting power of both calcium and

phosphorus atoms only amounts to 34.9%, which is not sufficient to control enough of the phases to show the rest of the structure. When all the oxygen atom positions were added to the calcium and phosphorus positions, their total diffracting power was 66.6%, which controlled enough of the phases to determine the complete structure. All the carbon atoms showed up in the three dimensional electron density maps thus calculated. See Table XXII for the carbon locations thus found.

F. Determination of the correct structural formulas for the calcium 1-naphthyl phosphate from the structural-analysis.

At the beginning of the structural determination, the calcium 1-naphthyl phosphate was erroneously taken to be $CaC_{10}H_7PO_4 \cdot H_2O$, since it was purchased as this compound. After considerable effort to solve the Patterson, it became evident that the compound was $Ca(C_{10}H_7HPO_4)_2 \cdot 3H_2O$. The problems encountered are summarized below.

If the $CaC_{10}H_7PO_4 \cdot H_2O$ were the correct structural formulas, the number of molecules per unit cell would be four, calculated according to the cell constants and density. There would be four independent heavy atoms (two calcium and two phosphorus) in the unit cell. The following evidence shows that the $CaC_{10}H_7PO_4 \cdot H_2O$ was the incorrect structural formula.

1. The inconsistent Patterson maps

From the theories discussed earlier, four independent heavy atoms should produce at least twelve big peaks of double weight and there would be eight independent relationships among them. The Patterson synthesis did show up fifteen fairly big peaks, yet only seven

of them had the proper "cyclic" properties which produced six independent relationships among them. For the sake of safety, these theories were checked as follows. If two independent heavy atoms $x_1$ and $x_2$ existed, two big double weight peaks are expected, i.e., $x_1+x_2$ and $x_1-x_2$. From these, $x_1$ and $x_2$ can be determinated. To locate the two heavy atoms $x_1$ and $x_2$, two big peaks out of the total fifteen are taken out one pair at a time, for testing. If any pair of these big peaks happen to be the $x_1+x_2$ and $x_1-x_2$, the $x_1$ and $x_2$ determinated from them should give a lower R-factor. To locate the third heavy atom $x_3$, the big peaks other than the $x_1+x_2$ and $x_1-x_2$ are assumed to be $x_1+x_3$, $x_1-x_3$, $x_2+x_3$ or $x_2-x_3$. Each big peak will thus produce four different possible $x_3$. The third heavy atom $x_3$ was located as below. (a) At least four different big peaks would produce the same $x_3$. (b) The $x_3$ should have proper distances with $x_1$ and $x_2$. (c) The R-factor should be lower when the $x_3$ is included. Following the same manner, the $x_4$ (the four heavy atom) was determinated. The same three heavy atoms were always found by this method as determinated by the adding method. This indicated that there were only three heavy atoms instead of four.

2. The close packing consideration

The three heavy atoms located by the Patterson method were identified as one calcium and two phosphorus by the close packing consideration. If the "missing" calcium were present, it should be in a position as good as the one already located. In other words, the distances of the two phosphorus atoms from the "missing" calcium should be more or less the same as those from the calcium already located. From this consideration, an approximate location for this "missing" calcium was

determined. Yet when this additional calcium at the predicated location was included, the R-factor increased too much to be accepted..

3. The minimum function

All the minimum functions calculated showed approximately acceptable locations for all the oxygen atoms and all the heavy atoms but this calcium atom could not be found.

Based on the above evidence and chemical analysis, the correct formula was taken as $Ca(C_{10}H_7HPO_4)_2 \cdot 3H_2O$.

## SECTION VII

## REFINEMENT AND DISCUSSION OF THE STRUCTURE

### A. Refinement of the structure

Refinement of the structure was carried out on the IBM 1620 data processing machine, using a least-squares refinement program which is a modification (from tape to card) of the one written by van der Helm (35). The number of observed reflections used for this refinement was 1750. The overall temperature factor and scale constant used at the start were

$$B=3.478 \qquad k=1.2461$$

The weighting scheme of Hughes (18) was used. After seven cycles, R-factor (Residue, discrepancy or reliability factor) dropped from 33.80% to 19.8%. At this point, it appeared likely that some of the reflections were effected by the primary extinction. The primary extinction (9,21) is

tanhsq/sq

Where s is the number of planes in sequence

$$q=N2d^2e^2p^{1/2}F/nmc^2$$

N is the number of pattern units in a unit volume

d is the interplanar spacing

e is electron charge

p is polarization factor

F is structure factor

n is order of reflection

m is mass of electron

c is light velocity

The extinction correction is greater for large structure factor, F, large spacing, d, and small order, n. Lonsdale (27) determined the primary extinction correction for sodium chloride. Part of her results are listed in the following table for illustration.

Table XXVI. Primary Extinction Correction for Nacl as Calculated by Lonsdale

| Reflection | d | Primary Extinct Correction (Depth of Block Being $10^{-3}$cm) |
|---|---|---|
| 200 | 2.814A | 0.14 |
| 400 | 1.407 | 0.46 |
| 600 | 0.938 | 0.81 |

Accordingly the following reflections were removed from the calculation. These are reflections for which d is greater than 1.41Å and for which F is greater than 500.

Table XXVII. Reflections Removed Due to Primary Extinction

| hkl | $d_{hkl}$ | $F_o$ | $F_c$ |
|---|---|---|---|
| 009 | 2.05Å | 589 | 706 |
| $\bar{1}11$ | 5.24 | 852 | 1343 |
| 112 | 5.35 | 976 | -1337 |
| $\bar{2}11$ | 3.20 | 882 | -1091 |
| 213 | 3.25 | 873 | 1133 |
| 211 | 3.42 | 791 | -924 |
| $\bar{2}1\bar{1}$ | 3.37 | 824 | 953 |
| $\bar{3}14$ | 1.94 | 534 | -634 |
| 317 | 1.97 | 510 | 630 |
| $02\bar{2}$ | 3.92 | 985 | -1390 |
| $02\bar{3}$ | 3.49 | 885 | -1066 |
| $22\bar{6}$ | 1.88 | 660 | 817 |
| $02\bar{8}$ | 1.98 | 577 | 689 |
| $\bar{2}2\bar{8}$ | 1.87 | 637 | 814 |
| $\bar{1}37$ | 1.93 | 592 | -776 |
| 138 | 1.95 | 628 | 801 |

The isotropic refinement (7 hours for each cycle) was then continued. When the R-factor reached 17.47%, a careful examination of the structure factors was made and some of the intensities were re-checked. There were ten reflections for which the $F_o$ seemed in error due to either an apparent reading error or because the spots were close to the

edges of the films. These were discarded. The isotropic refinement stopped at 14.01%. A calculation of the bond distances at this time showed some of the carbon-carbon distances as short as 1.15 and 1.20Å. A three dimensional electron density map was calculated and some of the carbon locations were adjusted to positions observed on this. One more isotropic temperature refinement gave a R-factor of 13.63%. Next, anisotropic temperature factors were included in the refinement. The coefficients for the anisotropic equation were calculated to give the correct isotropic B in the following manner:

$$B(\sin\theta/\lambda)^2=b_{11}h^2+b_{12}hk+b_{13}hl+b_{22}k^2+b_{23}kl+b_{33}l^2$$

Thus $b_{11}$, $b_{12}$ etc. were calculated to give same isotropic effect as B. To determine the anisotropic temperature factors, Cruickshank (12) recommended the using of the high-order reflections only, for which the major part of the x-ray scattering are from the inner electrons. For the ease of calculation, the following six high-order reflections were used.

| Reflection | sinθ |
|---|---|
| 800 | 0.8595 |
| 0010 | 0.4182 |
| 506 | 0.5453 |
| 810 | 0.8637 |
| $\bar{5}10$ | 0.5439 |
| 026 | 0.2886 |

The first cycle of the anisotropic temperature factor refinement (each cycle takes 14 hours) gave a slightly higher R-factor of 13.72%, but

after 14 cycles R-factor dropped to 10.30%. The progress of least-squares refinement is listed in the following table. An examination of this table showed the slow convergence in the process of refinement. This is because the off-diagonal terms in the refinement matrix are neglected.

Table XXVIII. The Progress of Least-Squares Refinement

| Cycle no. | R-factor Isotropic | R-factor Anisotropic Temp. Factor |
|---|---|---|
| 1 | 33.80% | 13.72% |
| 2 | 28.80 | 13.12 |
| 3 | 25.53 | 12.58 |
| 4 | 22.98 | 12.13 |
| 5 | 21.16 | 11.75 |
| 6 | 20.41 | 11.42 |
| 7 | 19.86 | 11.18 |
| 8 | 19.43 | 10.95 |
| 9 | 18.92 | 10.78 |
| 10 | 18.25 | 10.64 |
| 11 | 17.47 | 10.53 |
| 12 | 16.56 | 10.44 |
| 13 | 16.04 | 10.33 |
| 14 | 15.59 | 10.30 |
| 15 | 14.95 | |
| 16 | 14.78 | |
| 17 | 14.64 | |
| 18 | 14.42 | |
| 19 | 14.07 | |
| 20 | 14.01 | |
| 21 | 13.93 | |
| 22 | 13.63 | |

The final atomic positions and the corresponding standard deviations are listed in the next table.

Table XXIX. Positional Parameters of Non-hydrogen Atoms in Fractional Coordinates and Their Estimated Standard Derivations

| Atom No. | Atom | Location x | Location y | Location z | Estimated Standard Deviation (Å) x | Estimated Standard Deviation (Å) y | Estimated Standard Deviation (Å) z |
|---|---|---|---|---|---|---|---|
| 1 | Ca | .2309 | .2503 | .0001 | .010 | .015 | .011 |
| 2 | P | .5261 | .4341 | .0199 | .014 | .022 | .015 |
| 3 | P | .3649 | -.0658 | .1098 | .014 | .022 | .015 |
| 4 | O | .3610 | .5444 | .1311 | .041 | .054 | .045 |
| 5 | O | .4545 | .3081 | .0772 | .036 | .050 | .041 |
| 6 | O | .6965 | .5136 | .0661 | .038 | .055 | .043 |
| 7 | O | .5627 | .3600 | .1866 | .046 | .058 | .045 |
| 8 | O | .2365 | .0139 | .0670 | .039 | .054 | .047 |
| 9 | O | .5072 | .0437 | .1312 | .039 | .051 | .041 |
| 10 | O | .4683 | -.1921 | .0770 | .938 | .051 | .041 |
| 11 | O | .2495 | -.1409 | .1855 | .044 | .058 | .045 |
| 12 | O | .1539 | .1132 | -.0959 | .045 | .069 | .054 |
| 13 | O | .0598 | .3879 | .0964 | .046 | .068 | .054 |
| 14 | O | -.1057 | .2500 | .0006 | .051 | .077 | .064 |
| 15 | C | .6804 | .5785 | .2338 | .083 | .117 | .086 |
| 16 | C | .7223 | .6320 | .2949 | .100 | .128 | .103 |
| 17 | C | .6818 | .5598 | .3631 | .123 | .135 | .101 |
| 18 | C | .6045 | .4164 | .3718 | .092 | .115 | .088 |
| 19 | C | .5645 | .3373 | .4425 | .094 | .121 | .086 |
| 20 | C | .4842 | .2059 | .4513 | .102 | .125 | .090 |

| Atom No. | Atom | Location x | y | z | Estimated Standard Deviation (Å) x | y | z |
|---|---|---|---|---|---|---|---|
| 21 | C | .4419 | .1318 | .3931 | .105 | .142 | .095 |
| 22 | C | .4792 | .2111 | .3244 | .079 | .104 | .077 |
| 23 | C | .5638 | .3545 | .3121 | .072 | .098 | .069 |
| 24 | C | .6054 | .4366 | .2438 | .066 | .092 | .069 |
| 25 | C | .0878 | .0725 | .2328 | .080 | .105 | .084 |
| 26 | C | -.0172 | .1361 | .2947 | .0906 | .129 | .101 |
| 27 | C | -.0445 | .0660 | .3607 | .104 | .133 | .106 |
| 28 | C | .0224 | -.0790 | .3722 | .093 | .126 | .094 |
| 29 | C | -.0060 | -.1664 | .4447 | .102 | .126 | .094 |
| 30 | C | .0642 | -.2990 | .4530 | .115 | .126 | .090 |
| 31 | C | .1604 | -.3666 | .3921 | .104 | .136 | .099 |
| 32 | C | .1939 | -.2922 | .3242 | .080 | .103 | .079 |
| 33 | C | .1251 | -.1498 | .3115 | .072 | .099 | .073 |
| 34 | C | .1531 | -.0634 | .2431 | .063 | .090 | .069 |

B. Description and discussion of the structure

The bond distances and bond angles for calcium 1-naphthyl phosphate were calculated and are listed in the following tables. Most of these and the packing of the crystal are shown in Figs. 17, 18, 19, which represent the three two-dimensional projections okl, hko and hol respectively. Atom identification numbers in the tables refer to those assigned in Fig. 17.

Table XXX. Bond Distances for Calcium 1-naphthyl phosphate

| | | | |
|---|---|---|---|
| $P_2-O_4$ | 1.554 | $P_3-O_9$ | 1.573 |
| $P_2-O_5$ | 1.488 | $P_3-O_8$ | 1.476 |
| $P_2-O_6$ | 1.491 | $P_3-O_{10}$ | 1.466 |
| $P_2-O_7$ | 1.591 | $P_3-O_{11}$ | 1.589 |
| $O_4-O_5$ | 2.468 | $O_8-O_9$ | 2.527 |
| $O_4-O_6$ | 2.516 | $O_9-O_{10}$ | 2.484 |
| $O_4-O_7$ | 2.476 | $O_9-O_{11}$ | 2.512 |
| $O_5-O_6$ | 2.538 | $O_8-O_{10}$ | 2.494 |
| $O_5-O_7$ | 2.423 | $O_8-O_{11}$ | 2.517 |
| $O_6-O_7$ | 2.551 | $O_{10}-O_{11}$ | 2.393 |

| | |
|---|---|
| $Ca_1-O_5$ | 2.468 |
| $Ca_1-O_8$ | 2.362 |
| $Ca_1-O_{6'}$ | 2.363 |
| $Ca_1-O_{10'}$ | 2.441 |
| $Ca_1-O_{12}$ | 2.435 |
| $Ca_1-O_{13}$ | 2.411 |
| $Ca_1-O_{14}$ | 2.437 |

| | | | |
|---|---|---|---|
| $O_7-C_{24}$ | 1.400 | $O_{11}-C_{34}$ | 1.402 |
| $C_{15}-C_{16}$ | 1.373 | $C_{25}-C_{26}$ | 1.419 |
| $C_{16}-C_{17}$ | 1.354 | $C_{26}-C_{27}$ | 1.310 |
| $C_{17}-C_{18}$ | 1.398 | $C_{27}-C_{28}$ | 1.394 |
| $C_{18}-C_{19}$ | 1.418 | $C_{28}-C_{29}$ | 1.479 |

| | | | |
|---|---|---|---|
| $C_{18}-C_{23}$ | 1.381 | $C_{28}-C_{33}$ | 1.428 |
| $C_{19}-C_{20}$ | 1.309 | $C_{29}-C_{30}$ | 1.295 |
| $C_{20}-C_{21}$ | 1.418 | $C_{30}-C_{31}$ | 1.400 |
| $C_{21}-C_{22}$ | 1.387 | $C_{31}-C_{32}$ | 1.356 |
| $C_{22}-C_{23}$ | 1.417 | $C_{32}-C_{33}$ | 1.381 |
| $C_{23}-C_{24}$ | 1.408 | $C_{33}-C_{34}$ | 1.411 |

| | |
|---|---|
| $O_{12}-O_{14}$ | 2.704 |
| $O_{13}-O_{14}$ | 2.747 |
| $O_5-O_9$ | 2.543 |
| $O_4-O_{10}$ | 2.556 |

Table XXXI. Bond Angles for Calcium 1-naphthyl Phosphate

| | | | |
|---|---|---|---|
| $O_4-P_2-O_5$ | 108.4° | $O_9-P_3-O_8$ | 111.9° |
| $O_4-P_2-O_6$ | 111.4 | $O_9-P_3-O_{10}$ | 109.6 |
| $O_4-P_2-O_7$ | 103.9 | $O_9-P_3-O_{11}$ | 105.2 |
| $O_5-P_2-O_6$ | 116.8 | $O_8-P_3-O_{10}$ | 115.9 |
| $O_5-P_2-O_7$ | 103.7 | $O_8-P_3-O_{11}$ | 110.4 |
| $O_6-P_2-O_7$ | 111.6 | $O_{10}-P_3-O_{11}$ | 103.0 |
| $P_2-O_7-C_{24}$ | 125.9 | $P_3-O_{11}-O_{34}$ | 125.3 |
| $C_{16}-C_{15}-C_{24}$ | 116.6 | $C_{26}-C_{25}-C_{34}$ | 117. |
| $C_{15}-C_{16}-C_{17}$ | 124.4 | $C_{25}-C_{26}-C_{27}$ | 12 .9 |
| $C_{16}-C_{17}-C_{18}$ | 118.4 | $C_{26}-C_{27}-C_{28}$ | 120.6 |
| $C_{17}-C_{18}-C_{23}$ | 119.9 | $C_{27}-C_{28}-C_{33}$ | 119.4 |
| $C_{17}-C_{18}-C_{19}$ | 119.4 | $C_{27}-C_{28}-C_{29}$ | 123.8 |
| $C_{19}-C_{18}-C_{23}$ | 120.6 | $C_{29}-C_{28}-C_{33}$ | 116.9 |

| | | | |
|---|---|---|---|
| $C_{18}-C_{19}-C_{20}$ | 119.5 | $C_{28}-C_{29}-C_{30}$ | 121.5 |
| $C_{19}-C_{20}-C_{21}$ | 123.8 | $C_{29}-C_{30}-C_{31}$ | 120.2 |
| $C_{20}-C_{21}-C_{22}$ | 116.0 | $C_{30}-C_{31}-C_{32}$ | 121.4 |
| $C_{21}-C_{22}-C_{23}$ | 122.2 | $C_{31}-C_{32}-C_{33}$ | 121.4 |
| $C_{22}-C_{23}-C_{18}$ | 117.7 | $C_{23}-C_{33}-C_{28}$ | 118.6 |
| $C_{22}-C_{23}-C_{24}$ | 123.4 | $C_{32}-C_{33}-C_{34}$ | 125.5 |
| $C_{18}-C_{23}-C_{24}$ | 119.0 | $C_{28}-C_{33}-C_{34}$ | 115.9 |
| $C_{23}-C_{24}-C_{15}$ | 121.5 | $C_{33}-C_{34}-C_{25}$ | 124.2 |
| | $O_5-Ca_1-O_6$ | 87.7 | |
| | $O_5-Ca_1-O_8$ | 81.4 | |
| | $O_5-Ca_1-O_{10}$ | 78.6 | |
| | $O_5-Ca_1-O_{12}$ | 149.8 | |
| | $O_5-Ca_1-O_{13}$ | 72.8 | |
| | $O_5-Ca_1-O_{14}$ | 140.8 | |
| | $O_6-Ca_1-O_8$ | 166.2 | |
| | $O_6-Ca_1-O_{10}$ | 80.2 | |
| | $O_6-Ca_1-O_{12}$ | 100.0 | |
| | $O_6-Ca_1-O_{13}$ | 85.7 | |
| | $O_6-Ca_1-O_{14}$ | 98.0 | |
| | $O_8-Ca_1-O_{10}$ | 89.3 | |
| | $O_8-Ca_1-O_{12}$ | 85.6 | |
| | $O_8-Ca_1-O_{13}$ | 99.0 | |
| | $O_8-Ca_1-O_{14}$ | 95.9 | |
| | $O_{10}-Ca_1-O_{12}$ | 74.1 | |
| | $O_{10}-Ca_1-O_{13}$ | 148.5 | |

| | |
|---|---|
| $O_{10}$-$Ca_1$-$O_{14}$ | 140.6 |
| $O_{12}$-$Ca_1$-$O_{13}$ | 136.5 |
| $O_{12}$-$Ca_1$-$O_{14}$ | 67.4 |
| $O_{14}$-$Ca_1$-$O_{13}$ | 69.0 |

The two independent phosphate groups are quite similar. One group consists of $P_2$, $O_4$, $O_5$, $O_6$ and $O_7$. The corresponding atoms in the other phosphate group are $P_3$, $O_8$, $O_9$, $O_{10}$, and $O_{11}$. A comparison was made in the above bond distances and angles tables. The four phosphate oxygens are bonded in the following manner. One oxygen is bonded to the naphthyl group, another oxygen is bonded to a H, and the other two oxygens are coordinated to two calcium atoms which are related to each other by an inversion center. A careful examination of the bond distances and the bond angles indicated: (1) the P-O ($C_{10}H_7$) ester bond is the longest and the P-O (H) bond is the next longest, while the bond distances between phosphorus and the two oxygens coordinated with calcium atoms are shorter. This agrees with other organic phosphates structures (15,34,24,25). (2) The maximum O-P-O angle corresponds to the angle subtended by the two very short P-O distances. This is quite reasonable, because the shorter the P-O bond distances, the greater the mutual repulsion between oxygens will be. By the same reasoning, the angle subtended by the two longest P-O distances should be, at least, one of the minimum angles and this was found to be the case. (3) The minimum distance from the oxygen (the ester bond oxygen) to the oxygens other than those on the same phosphate group is 3.18Å. This indicates that there is no hydrogen bonding from these two ester bond

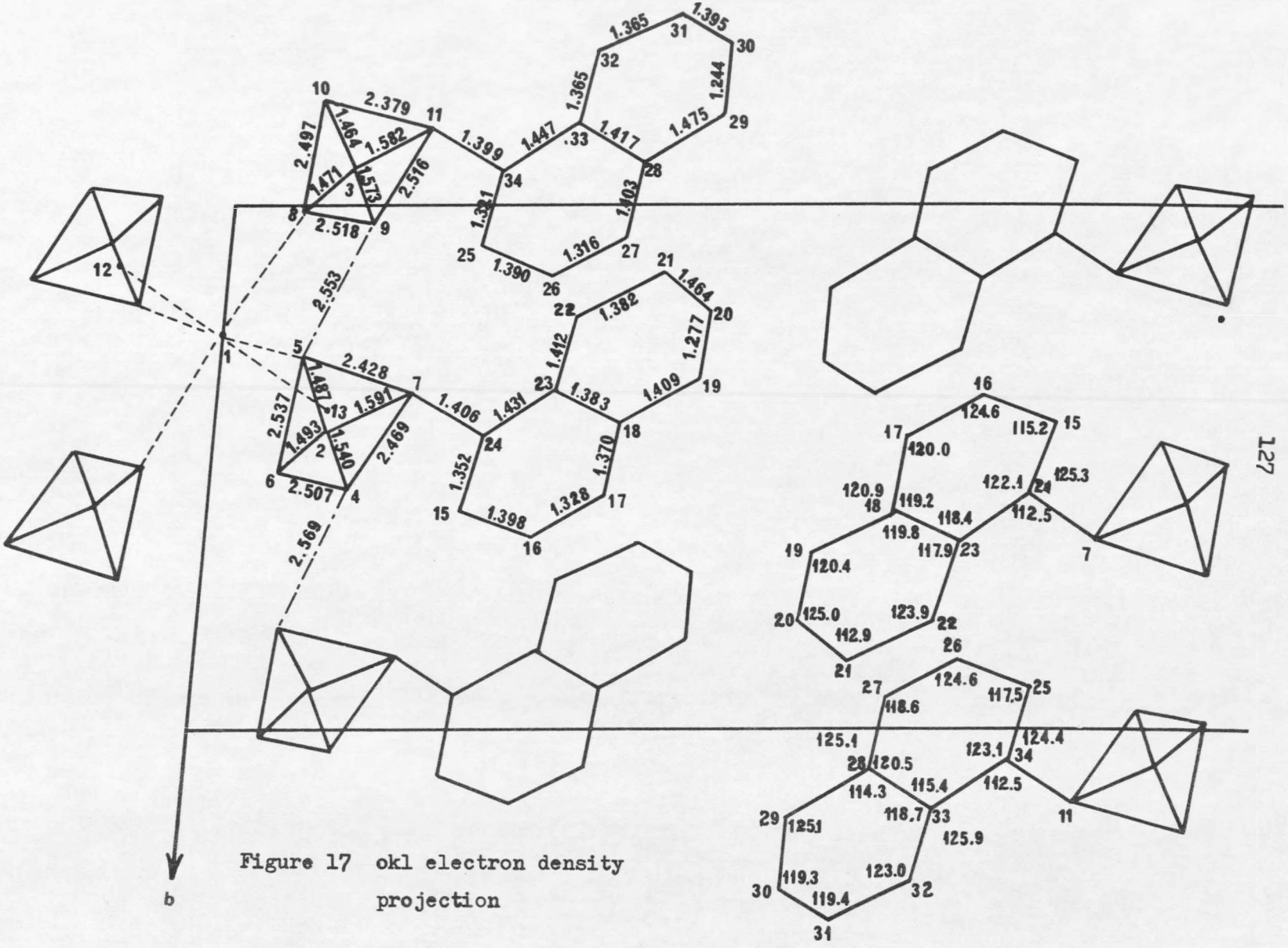



Figure 17 okl electron density projection

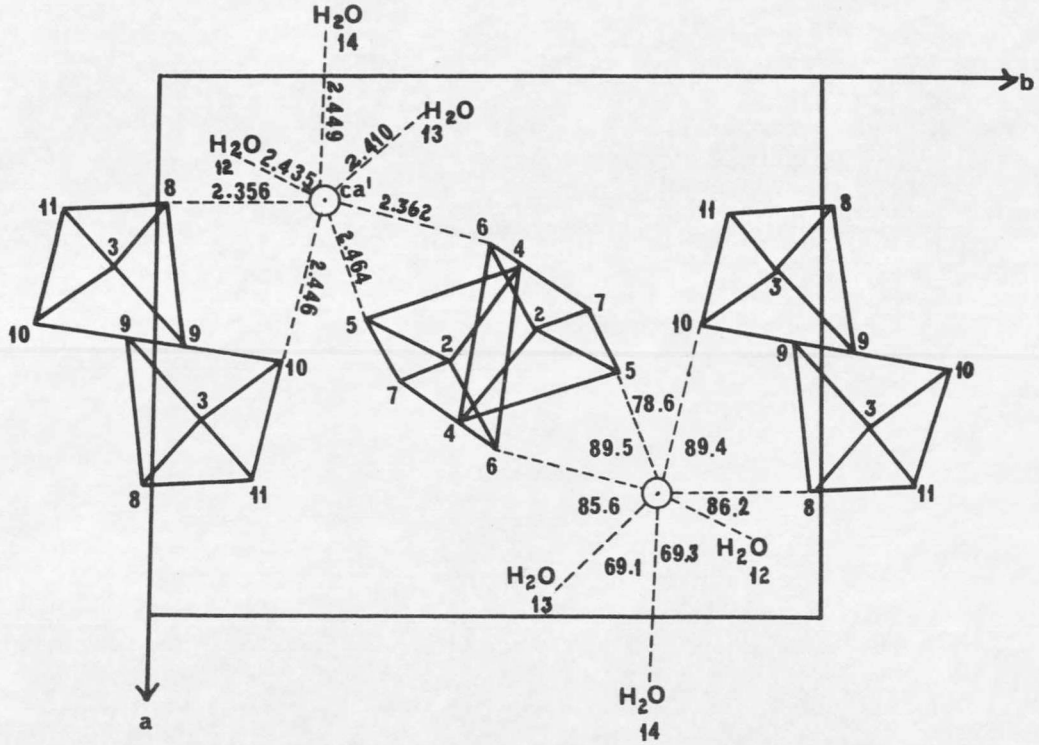



Figure 18 hko electron density projection

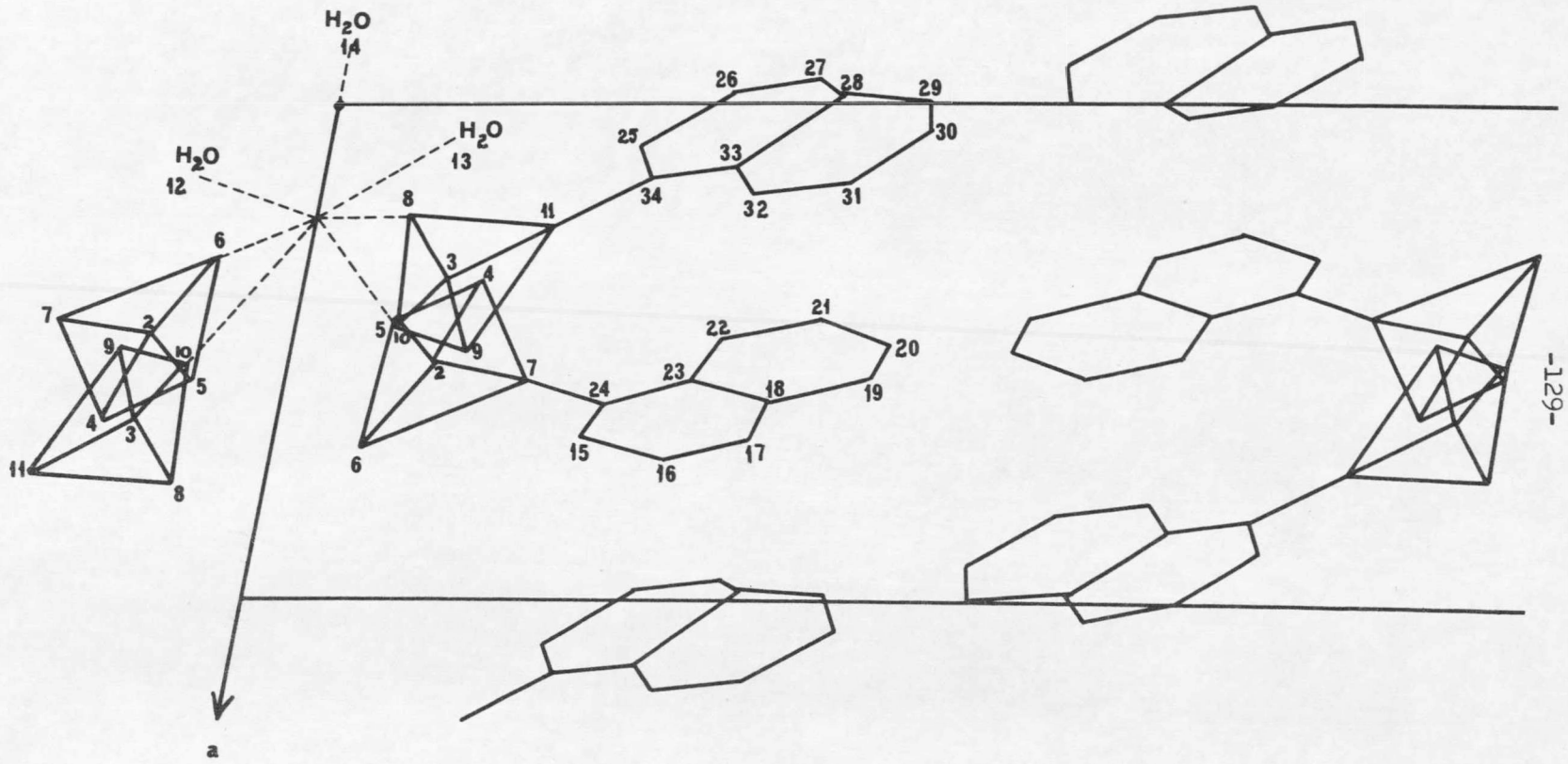



Figure 19 hol electron density projection

oxygens to other hydrogens. Kraut and Jensen (25) reported the same thing in the structure of adenosine-5'-phosphate.

The general features of the phosphate group agree well with other organic phosphate structures which have been reported. This can be seen from a comparison of this data with those reported in the literature in the following table.

Table XXXII. Comparison of Calcium 1-Naphthyl Phosphate with Other Organic Phosphates Reported

| | Our Data $PO_4 1$ | $PO_4 2$ | Adenosine-5'-$PO_4$ | 2-amino ethanol-$PO_4$ | Ca-Thymidylate | Dibenzyl Phosphoric Acid |
|---|---|---|---|---|---|---|
| P-O | | | | | | |
| Range | 1.488 to 1.591 | 1.466 to 1.589 | 1.514 to 1.610 | 1.493 to 1.591 | 1.474 to 1.587 | 1.469 to 1.566 |
| Average | 1.531 | 1.526 | 1.546 | 1.536 | 1.515 | 1.531 |
| P-OR | 1.591 | 1.589 | 1.610 | 1.591 | 1.587 | 1.566 & 1.545 |
| P-OH | 1.554 | 1.573 | 1.566 | 1.557 | -- | 1.545 |
| O-P-O | | | | | | |
| Range | 103.7 to 116.8 | 103.0 to 115.9 | 105.7 to 118.2 | 103.9 to 117.4 | 102.1 to 11 .4 | 103.8 to 117.2 |
| Average | 109.3 | 109.3 | 109.4 | 109.4 | 109.3 | 109.3 |
| Angle bet. 2 long P-O | 103.9 (103.7) | 105.2 (103.0) | 106.5 (105.7) | 106.2 (103.9) | 107.6 (102.1) | 104.2 (103.8) |
| Angle bet. 2 short P-O | 116.8 (max.) | 115.9 (max.) | 118.2 (max.) | 117.4 (max.) | 118.4 (max.) | 117.2 (max.) |
| Angle bet. Longest & Shortest P-O | 103.7 (min.) | 103.0 (min.) | 105.7 (min.) | 103.9 (min.) | 102.1 (min.) | 103.8 (min.) |
| C-O ($PO_4$) | 1.400 | 1.402 | 1.475 | 1.429 | 1.472 | 1.464 & 1.465 |
| P-O-C | 125.9 | 125.3 | 114.7 | 118.7 | 118.8 | 118.8 & 122.3 |

From Table XXXII, it is seen that calcium 1-naphthyl phosphate has the shortest C-O bond and largest P-O-C angle. Trueblood et al. (34) noted that for a given phosphate group, the shorter of the two shortest P-O bonds has a larger Ca-O distance. This is also the case for calcium 1-naphthyl phosphate. For P-O bond lengths 1.488 and 1.491Å, Ca-O lengths are 2.468 and 2.363Å. For P-O bond lengths 1.466 and 1.476Å, Ca-O are 2.441 and 2.362Å. Thus, more or less the same distances are maintained between phosphorus and the two calciums related by an inversion center.

Each calcium ion was found to be coordinated to seven oxygens, four of which are from four different phosphate groups and three from water molecules. The seven oxygens are arranged in a distorted pentagonal bipyramid. The calcium, $O_5$, $O_{10'}$, (two phosphate oxygens) $O_{12}$, $O_{13}$, $O_{14}$ (three water oxygens) occupy the distorted pentagonal plane; the other two phosphate oxygens are on a line through the calcium nearly perpendicular to this plane. The pentagonal angles are 78.6°, 72.8°, 74.1°, 67.4°, and 69.0° with the average of 72.4°. The seven Ca-O distances range from 2.362 to 2.468, with an average of 2.418Å. The range of the seven Ca-O distances in calcium thymidylate is from 2.29 to 2.65Å which is considerably more variation than in calcium 1-naphthyl phosphate, but gives the same average. The small variation of Ca-O distances is probably because all oxygens are from different groups.

Naphthalene has been shown to be planar (1), with the C-C distance from 1.354 to 1.421Å and an average of 1.39Å. The large P-O-C angle in calcium naphthyl phosphate is probably due to close packing of the

large planar naphthalene group. A distorted naphthyl ring might thus be expected. This was found to be the case, as can be seen from the following data. The C-C distance has a range from 1.309 to 1.418Å and an average of 1.386Å for the first naphthyl group, while for the second one, the range is from 1.295 to 1.479 with an average of 1.380Å. The range of C-C-C angles is from 116.0° to 124.4° in the first group and from 115.9° to 125.5° in the second group, while the average is 120.2° in the first and 120.7° in the second group. The minimum C-C bond distance in a naphthyl group occurs between two carbons which are closest to the nearby naphthyl groups. Minimum non-bonded carbon distances are 3.620, 3.719Å indicating van der Waals forces.

Hydrogen bonding plays an important role in holding groups together in the crystal of calcium 1-naphthyl phosphate. The closest distances between oxygen and oxygen (one of these two oxygens has a hydrogen on it) from two neighboring phosphate groups are 2.543 and 2.556Å. Other oxygen distances suggesting hydrogen bonding are $O_4$ to $O_{13}$: 2.834, $O_5$ to $O_{13}$: 2.895, $O_{12}$ to $O_{14}$: 2.704, $O_{13}$ to $O_{14}$: 2.747Å.

# APPENDIX

# APPENDIX A

## Calcium and phosphorus analysis for calcium 1-naphthyl phosphate

### Calcium determination

About 0.2 gm is weighed very accurately in a 50 ml florence flask. Add about 4 ml concentrated nitric acid (69.4%, Baker analyzed reagent). Then add about 6 ml concentrated perchloric acid (71.1%, Baker analyzed reagent). Digest the sample on a hot plate till almost dry (Evaporation to dryness makes it difficult to re-dissolve). After cooling, dilute it with a little water. Transfer to a 500 ml volumetric flask. Rinse well and save every drop. Make to volume with water. Shake well and let settle. The calcium concentration of this solution is determined with Beckman Flame Quartz Spectrophotometer (model DU) by comparing with a standard calcium solution prepared in the following manner: $CaCo_3$ is digested with some concentrated nitric to dryness. Several different calcium concentration solutions (from zero to 50 ppm) are made from this. Each solution is so adjusted that it contains 15 ppm of phosphorus ($H_3PO_4$ is added before diluting to volume with water). The addition of phosphorus suppresses the standard solutions about the same as the unknown.

The standard curve for determining calcium by this method is shown in Fig. 20.

The data corresponding to this standard calcium curve are as follows.

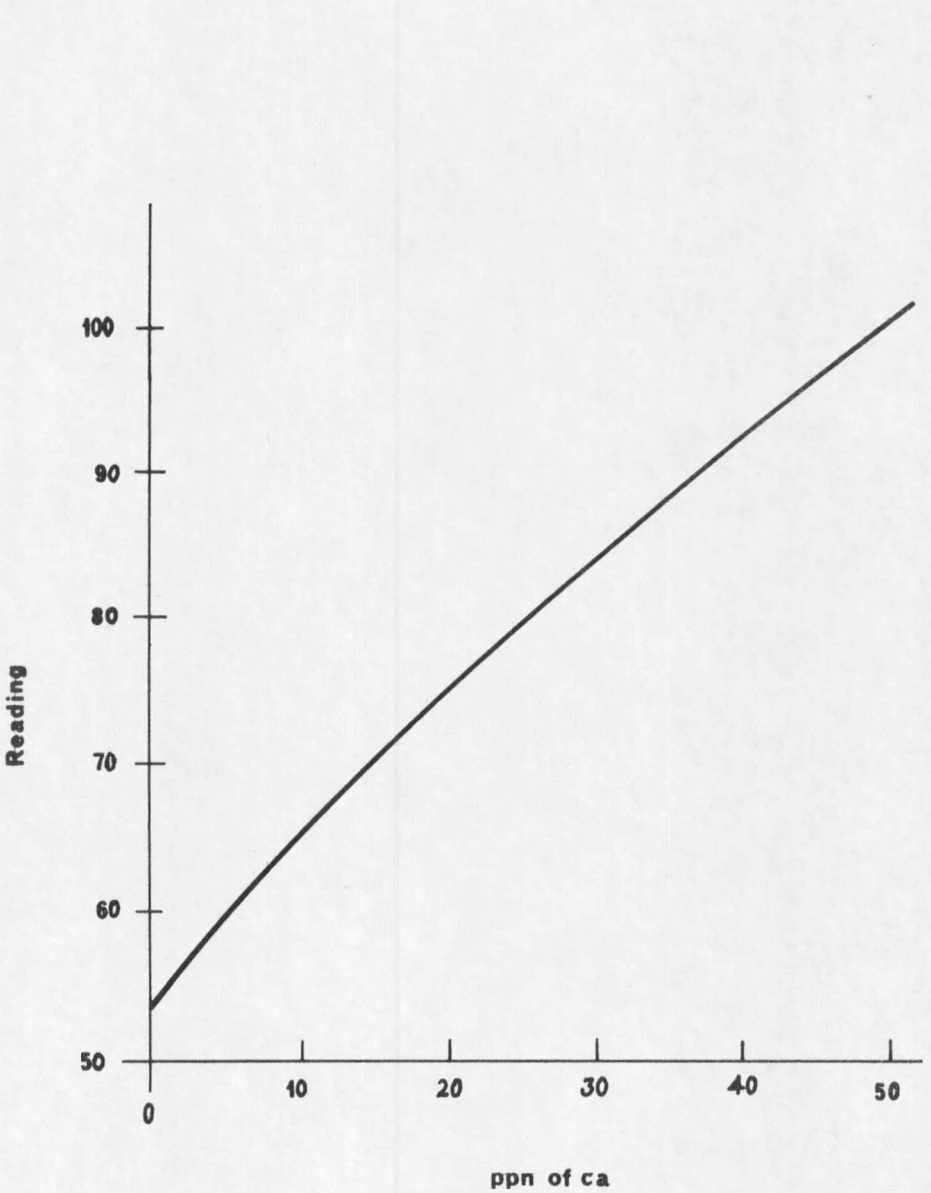



Figure 20 The standard calcium calibration curve for the Beckman flame quartz spectrophotometer

Table XXXIII. Calcium Calibration Data for Beckman Flame Quartz Spectrophotometer

| ppm of Ca | Reading |
|---|---|
| 50 | 100 |
| 40 | 92 |
| 30 | 84 |
| 20 | 75 |
| 10 | 65 |
| 0 | 53 |

The unknown (sample weight being 0.1955 gm) has a reading of 85, which corresponds to 31.3 ppm.

Phosphorus determination

The preparation of the sample follows exactly the same procedure as that for calcium determination. In fact, part of the same solution prepared for calcium is used for the phosphorus determination.

With a pipette, transfer 1 ml of the prepared solution into a 25 ml graduated test tube; add 2 ml of 10 N sulphuric acid, then add 2 ml of amidol, and finally 1 ml of molybdate. Dilute to 25 ml with water. Transfer to a matched test tube. Mix the solution by pouring back and forth several times between the 25 ml graduate test tube and the matched test tube. Let it stand for 30 minutes. Read the percentage transmittance on a Beckman Model B Spectrophotometer at wave length 650 against a blank solution which is prepared exactly the same way as

the testing sample except no sample in it. The concentration of the sample is determined by comparing the percentage transmittance with that of a known standard phosphorus compound.

Three tests were done. Each contained one ml of the prepared solution. The results are compared with the curve (Fig. 21) of known standard solutions using $K_2HPO_4$. The results are given below.

Table XXXIV. Phosphorus Analysis Results by the Colorimetric Method

| Test no. | Transmittance | g/ml or ppm |
|---|---|---|
| 1 | 46.3 | 43.8 |
| 2 | 46.1 | 43.9 |
| 3 | 46.0 | 44.0 |

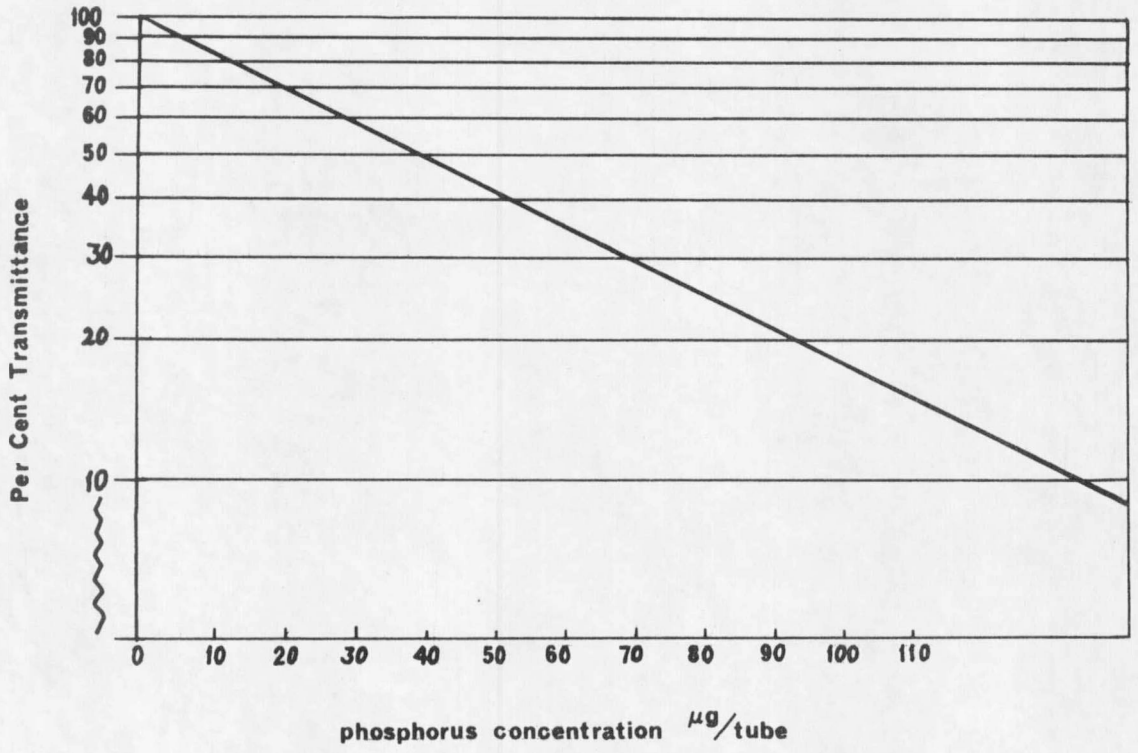



Figure 21 The standard phosphorus calibration curve for the Beckman Model B spectrophotometer at wave length 650

# APPENDIX B

## Film Processing

To process the films, the following materials were used.

1. Developing solution

   Kodax rapid x-ray developer (1 lb. and 1 oz. powder will make up one gallon solution).

2. Fixing solution

   Kodak rapid fixer with hardner.

3. Acid stop bath

   Very dilute acetic acid (6 oz. or 180 ml of 28% acetic acid in a gallon of water).

The integrated pictures were processed in the following manner. They are first developing for 7 minutes in a fresh Kodak rapid x-ray developer which is maintaining at a constant temperature of 20° C. Then they are washed in the acid stop bath for 30 seconds. They are fixing for 15 minutes in a fresh Kodak rapid fixer which is also kept at a constant temperature of 20° c. Wash them in running water for half an hour. After rinsing with distilled water, we hung them up for drying.

APPENDIX C

Table XXXV. Equi-inclination Weissenberg index-checking results for Ca 1-naphthyl phosphate

| h | k | l | $x_o$ | $x_c$ | error% | h | k | l | $x_o$ | $x_c$ | error% |
|---|---|---|---|---|---|---|---|---|---|---|---|
| -1 | | | 6.1 | 6.2 | 2.20 | 2 | | 4 | 14.3 | 14.3 | .12 |
| 2 | | | 12.7 | 12.5 | -1.22 | 3 | | 4 | 19.8 | 19.6 | -.85 |
| 3 | | | 19.1 | 19.0 | -.45 | -3 | | 4 | 22.8 | 23.2 | 2.17 |
| 4 | | | 25.9 | 25.7 | -.59 | 6 | | 4 | 40.0 | 39.7 | -.53 |
| 7 | | | 49.1 | 49.4 | .77 | -6 | | 4 | 44.0 | 44.8 | 1.82 |
| 8 | | | 59.8 | 60.3 | .86 | | | -4 | 10.0 | 9.7 | -2.80 |
| 1 | | 1 | 6.4 | 6.2 | -2.72 | 1 | | -4 | 12.8 | 12.5 | -1.60 |
| 2 | | 1 | 12.3 | 12.2 | -.06 | -1 | | -4 | 10.4 | 10.4 | .69 |
| 3 | | 1 | 19.0 | 18.6 | -1.73 | -1 | | -4 | 10.2 | 10.4 | 2.66 |
| 4 | | 1 | 25.2 | 25.3 | .56 | 2 | | -4 | 17.7 | 17.4 | -1.26 |
| 6 | | 1 | 40.2 | 40.1 | -.17 | -2 | | -4 | 14.1 | 14.3 | 1.54 |
| 7 | | 1 | 48.2 | 48.8 | 1.34 | 3 | | -4 | 23.4 | 23.2 | -.44 |
| 1 | | -1 | 7.2 | 7.1 | -1.02 | -3 | | -4 | 19.3 | 19.6 | 1.71 |
| 3 | | -1 | 19.9 | 19.6 | -1.12 | 4 | | -4 | 29.6 | 29.7 | .50 |
| 4 | | -1 | 26.5 | 26.4 | -.37 | -4 | | -4 | 25.7 | 25.7 | .02 |
| 5 | | -1 | 33.6 | 33.5 | -.10 | 6 | | -4 | 44.8 | 44.8 | .01 |
| 7 | | -1 | 50.0 | 50.3 | .64 | 1 | | 5 | 12.4 | 12.5 | 1.24 |
| -8 | | -1 | 58.9 | 59.4 | .97 | 2 | | 5 | 15.7 | 15.7 | .23 |
| | | 2 | 4.7 | 4.8 | 3.02 | 6 | | 5 | 40.1 | 40.0 | -.03 |
| 3 | | 2 | 18.9 | 18.6 | -1.26 | | | -5 | 12.2 | 12.1 | -.14 |
| 6 | | 2 | 39.8 | 39.8 | .02 | 1 | | -5 | 14.8 | 14.8 | .11 |
| -7 | | 2 | 50.9 | 51.3 | .93 | 2 | | -5 | 19.5 | 19.3 | -.73 |
| 1 | | 2 | 8.9 | 8.6 | -2.96 | 3 | | -5 | 24.7 | 24.9 | .99 |
| -1 | | -2 | 7.1 | 7.1 | .03 | -3 | | -5 | 20.6 | 20.5 | -.14 |
| 2 | | -2 | 14.5 | 14.3 | -.92 | -3 | | -5 | 20.4 | 20.5 | .83 |
| -2 | | -2 | 12.2 | 12.5 | 2.67 | -4 | | -5 | 26.3 | 26.3 | .16 |
| 3 | | -2 | 20.5 | 20.6 | .63 | 5 | | -5 | 38.2 | 38.3 | .35 |
| 4 | | -2 | 27.4 | 27.2 | -.37 | 6 | | -5 | 46.2 | 46.3 | .31 |
| 6 | | -2 | 42.2 | 42.3 | .30 | 1 | | 6 | 14.6 | 14.7 | 1.19 |
| | | 3 | 7.1 | 7.2 | 2.45 | 3 | | 6 | 21.7 | 21.7 | .34 |
| 3 | | 3 | 19.2 | 18.9 | -1.11 | 4 | | 6 | 27.2 | 27.2 | .08 |
| 4 | | 3 | 25.3 | 25.3 | .09 | 7 | | 6 | 48.5 | 48.7 | .57 |
| 6 | | 3 | 39.8 | 39.6 | -.26 | | | -6 | 14.6 | 14.6 | .47 |
| 1 | | -3 | 10.8 | 10.5 | -2.69 | 1 | | -6 | 17.2 | 17.1 | -.37 |
| -1 | | -3 | 8.7 | 8.6 | -1.10 | 2 | | -6 | 21.4 | 21.3 | -.02 |
| -1 | | -3 | 8.2 | 8.6 | 4.92 | -2 | | -6 | 17.0 | 17.4 | 2.41 |
| 2 | | -3 | 16.0 | 15.7 | -1.28 | 3 | | -6 | 26.9 | 26.7 | -.46 |
| -2 | | -3 | 13.0 | 13.2 | 1.70 | 4 | | -6 | 32.8 | 32.9 | .55 |
| 3 | | -3 | 21.8 | 21.8 | .22 | 5 | | -6 | 39.9 | 40.0 | .28 |
| 4 | | -3 | 28.5 | 28.4 | -.28 | -5 | | -6 | 33.4 | 33.4 | .27 |
| 5 | | -3 | 35.2 | 35.5 | .99 | 6 | | -6 | 48.0 | 48.0 | .20 |

| h | k | l | $x_o$ | $x_c$ | error% |
|---|---|---|---|---|---|
| 1 | | 7 | 16.8 | 17.0 | 1.73 |
| 2 | | 7 | 19.2 | 19.2 | .43 |
| -2 | | 7 | 23.0 | 23.5 | 2.46 |
| 3 | | 7 | 23.2 | 23.2 | .04 |
| 1 | | -7 | 19.7 | 19.5 | -.85 |
| 2 | | -7 | 23.6 | 23.5 | -.14 |
| 3 | | -7 | 28.8 | 28.7 | -.13 |
| -4 | | -7 | 28.3 | 28.3 | .09 |
| 5 | | -7 | 41.8 | 41.8 | .18 |
| 6 | | -7 | 49.9 | 50.0 | .34 |
| -7 | | -7 | 49.0 | 49.3 | .78 |
| -8 | | -7 | 58.9 | 59.3 | .79 |
| 2 | | 8 | 21.0 | 21.3 | 1.50 |
| -2 | | 8 | 25.3 | 25.8 | 2.20 |
| | | -8 | 19.7 | 19.7 | .16 |
| -1 | | -8 | 19.2 | 19.4 | 1.49 |
| -2 | | -8 | 21.1 | 21.3 | 1.02 |
| -3 | | -8 | 24.8 | 24.8 | .19 |
| 4 | | -8 | 36.8 | 36.9 | .31 |
| -4 | | -8 | 29.8 | 29.6 | -.52 |
| 5 | | -8 | 43.6 | 43.9 | .76 |
| -6 | | -8 | 42.0 | 42.2 | .50 |
| 7 | | -8 | 62.2 | 62.9 | 1.23 |
| -7 | | -8 | 49.9 | 50.1 | .59 |
| -8 | | -8 | 59.5 | 60.1 | 1.13 |
| | | -9 | 22.3 | 22.3 | .10 |
| 1 | | -9 | 24.2 | 24.5 | 1.37 |
| 2 | | -9 | 28.2 | 28.2 | .19 |
| -2 | | -9 | 23.2 | 23.4 | 1.22 |
| 3 | | -9 | 33.0 | 33.1 | .52 |
| -3 | | -9 | 26.8 | 26.6 | -.49 |
| 5 | | -9 | 45.8 | 46.1 | .85 |
| -5 | | -9 | 36.8 | 36.7 | -.22 |
| 7 | | -9 | 65.5 | 66.1 | .98 |
| -7 | | -9 | 51.0 | 51.2 | .44 |
| | | -10 | 24.9 | 24.9 | .25 |
| -1 | | -10 | 24.2 | 24.4 | 1.17 |
| 2 | | -10 | 30.6 | 30.7 | .52 |
| -2 | | -10 | 25.6 | 25.7 | .66 |
| 3 | | -10 | 35.5 | 35.5 | .82 |
| -3 | | -10 | 28.7 | 28.6 | -.18 |
| 4 | | -10 | 41.5 | 41.5 | .04 |
| -4 | | -10 | 32.9 | 32.8 | -.15 |
| 5 | | -10 | 48.2 | 48.6 | .94 |
| -5 | | -10 | 38.1 | 38.1 | .23 |
| -6 | | -10 | 44.4 | 44.6 | .55 |
| 7 | | -10 | 69.1 | 69.9 | 1.29 |
| -9 | | -10 | 79.0 | 80.0 | 1.30 |
| | | -11 | 27.8 | 27.6 | -.49 |
| 1 | | -11 | 29.8 | 29.8 | .06 |
| 2 | | -11 | 33.2 | 33.3 | .52 |
| -2 | | -11 | 27.9 | 28.1 | .94 |
| -3 | | -11 | 30.7 | 30.7 | .24 |
| 4 | | -11 | 43.9 | 44.0 | .42 |
| 5 | | -11 | 50.9 | 51.3 | .90 |
| -5 | | -11 | 39.8 | 39.8 | .12 |
| -6 | | -11 | 46.0 | 46.1 | .35 |
| 7 | | -11 | 73.8 | 75.0 | 1.63 |
| 1 | | 12 | 29.4 | 29.7 | 1.25 |
| 2 | | 12 | 30.4 | 30.6 | .87 |
| | | -12 | 30.4 | 30.4 | .09 |
| 1 | | -12 | 32.4 | 32.5 | .57 |
| 2 | | -12 | 36.0 | 36.1 | .28 |
| 3 | | -12 | 40.8 | 40.8 | .14 |
| -3 | | -12 | 33.0 | 33.0 | .13 |
| 4 | | -12 | 46.6 | 46.8 | .53 |
| -4 | | -12 | 36.8 | 36.7 | -.11 |
| -5 | | -12 | 41.5 | 41.6 | .47 |
| -6 | | -12 | 47.8 | 47.8 | .19 |
| -7 | | -12 | 55.1 | 55.6 | 1.03 |
| 2 | | 13 | 33.1 | 33.2 | .52 |
| | | -13 | 33.2 | 33.2 | .22 |
| 1 | | -13 | 35.3 | 35.4 | .42 |
| -1 | | -13 | 32.1 | 32.5 | 1.35 |
| 2 | | -13 | 38.8 | 38.9 | .41 |
| 3 | | -13 | 43.5 | 43.7 | .54 |
| -3 | | -13 | 35.4 | 35.4 | .14 |
| 4 | | -13 | 49.5 | 49.8 | .68 |
| -6 | | -13 | 49.8 | 49.8 | .07 |
| -7 | | -13 | 58.2 | 57.6 | -.93 |
| -2 | | 14 | 41.1 | 41.9 | 2.10 |
| | | -14 | 36.1 | 36.2 | .32 |
| 1 | | -14 | 38.4 | 38.4 | .07 |
| -1 | | -14 | 35.2 | 35.3 | .55 |
| -2 | | -14 | 35.9 | 36.0 | .27 |
| 3 | | -14 | 46.5 | 46.8 | .65 |

| h | k | l | $x_o$ | $x_c$ | error% |
|---|---|---|---|---|---|
| 4 | | -14 | 52.8 | 53.0 | .55 |
| -4 | | -14 | 41.2 | 41.3 | .32 |
| 6 | | -14 | 73.0 | 74.2 | 1.67 |
| 1 | | -15 | 41.4 | 41.5 | .34 |
| -1 | | -15 | 37.9 | 38.3 | 1.24 |
| 2 | | -15 | 44.8 | 45.1 | .75 |
| -2 | | -15 | 38.8 | 38.8 | .13 |
| -3 | | -15 | 40.8 | 40.7 | -.23 |
| -4 | | -15 | 43.9 | 43.8 | -.02 |
| 5 | | -15 | 65.1 | 65.7 | 1.04 |
| -5 | | -15 | 48.4 | 48.4 | .03 |
| -7 | | -15 | 62.5 | 62.5 | .14 |
| | | 16 | 42.0 | 42.4 | 1.13 |
| -1 | | -16 | 41.1 | 41.4 | .93 |
| -2 | | -16 | 41.8 | 41.8 | .11 |
| -3 | | -16 | 43.5 | 43.5 | .16 |
| -4 | | -16 | 46.5 | 46.6 | .29 |
| 5 | | -16 | 70.5 | 71.1 | .97 |
| -7 | | -16 | 65.3 | 65.6 | .61 |
| | | -17 | 45.8 | 45.8 | .10 |
| 1 | | -17 | 48.0 | 48.2 | .61 |
| -2 | | -17 | 44.8 | 45.0 | .48 |
| -3 | | -17 | 46.5 | 46.6 | .27 |
| -4 | | -17 | 49.5 | 49.6 | .21 |
| -7 | | -17 | 69.2 | 69.4 | .35 |
| | | -18 | 49.0 | 49.4 | .89 |
| -1 | | -18 | 47.8 | 48.2 | .90 |
| -2 | | -18 | 48.0 | 48.3 | .80 |
| -4 | | -18 | 52.9 | 52.8 | -.10 |
| -7 | | -18 | 73.7 | 74.2 | .75 |
| 2 | | -19 | 60.2 | 60.6 | .68 |
| -2 | | -19 | 51.9 | 52.0 | .22 |
| 2 | | -20 | 65.1 | 65.8 | 1.10 |
| -6 | | -20 | 73.2 | 73.4 | .40 |
| 1 | | -21 | 65.6 | 66.0 | .71 |
| 2 | | -21 | 71.3 | 72.4 | 1.59 |
| -2 | | -21 | 60.0 | 60.4 | .72 |
| -5 | | -21 | 70.1 | 70.6 | .73 |
| 1 | | -22 | 72.3 | 72.9 | .87 |
| -2 | | -22 | 64.9 | 65.6 | 1.09 |
| -1 | | -23 | 72.1 | 72.7 | .94 |
| -2 | | -23 | 71.5 | 72.1 | .90 |
| 1 | 1 | | 6.6 | 6.3 | -4.10 |
| -2 | 1 | | 12.1 | 12.6 | 4.35 |
| 3 | 1 | | 19.2 | 19.1 | -.47 |
| -3 | 1 | | 18.6 | 19.1 | 2.73 |
| -5 | 1 | | 32.3 | 33.0 | 2.28 |
| -6 | 1 | | 40.0 | 40.8 | 2.13 |
| -7 | 1 | | 48.8 | 49.7 | 1.91 |
| 8 | 1 | | 60.2 | 60.6 | .82 |
| -8 | 1 | | 60.2 | 60.6 | .82 |
| 2 | 1 | 1 | 12.7 | 12.2 | -3.33 |
| -2 | 1 | 1 | 12.9 | 13.2 | 2.70 |
| 3 | 1 | 1 | 19.0 | 18.6 | -1.58 |
| -3 | 1 | 1 | 19.1 | 19.7 | 3.19 |
| 4 | 1 | 1 | 25.4 | 25.4 | .03 |
| -4 | 1 | 1 | 25.8 | 26.4 | 2.60 |
| 5 | 1 | 1 | 32.2 | 32.5 | 1.02 |
| -5 | 1 | 1 | 33.0 | 33.6 | 2.04 |
| -6 | 1 | 1 | 40.8 | 41.5 | 1.83 |
| -7 | 1 | 1 | 50.0 | 50.5 | 1.08 |
| 8 | 1 | 1 | 59.5 | 59.7 | .49 |
| -8 | 1 | 1 | 61.2 | 61.7 | .91 |
| 2 | 1 | -1 | 13.8 | 13.4 | -2.68 |
| 3 | 1 | -1 | 20.0 | 19.8 | -.81 |
| -3 | 1 | -1 | 18.3 | 18.8 | 2.09 |
| -5 | 1 | -1 | 32.0 | 32.6 | 1.93 |
| 6 | 1 | -1 | 41.8 | 41.6 | -.40 |
| -6 | 1 | -1 | 40.1 | 40.3 | .65 |
| -7 | 1 | -1 | 48.8 | 49.1 | .69 |
| 1 | 1 | 2 | 7.1 | 6.8 | -3.42 |
| 2 | 1 | 2 | 12.8 | 12.4 | -2.99 |
| -2 | 1 | 2 | 13.8 | 14.2 | 3.48 |
| 3 | 1 | 2 | 18.9 | 18.6 | -1.47 |
| -3 | 1 | 2 | 20.0 | 20.6 | 3.04 |
| 4 | 1 | 2 | 25.2 | 25.2 | .04 |
| -4 | 1 | 2 | 26.7 | 27.3 | 2.33 |
| 5 | 1 | 2 | 32.1 | 32.2 | .45 |
| -5 | 1 | 2 | 33.8 | 34.5 | 2.14 |
| 6 | 1 | 2 | 39.9 | 39.9 | .03 |
| -6 | 1 | 2 | 41.3 | 42.4 | 2.78 |
| 8 | 1 | 2 | 59.1 | 59.1 | .07 |
| -8 | 1 | 2 | 62.3 | 63.1 | 1.30 |
| 1 | 1 | -2 | 9.1 | 8.9 | -1.23 |
| -1 | 1 | -2 | 7.4 | 7.5 | 1.52 |
| 2 | 1 | -2 | 14.8 | 14.6 | -1.23 |

| h | k | l | $x_o$ | $x_c$ | error% | h | k | l | $x_o$ | $x_c$ | error% |
|---|---|---|---|---|---|---|---|---|---|---|---|
| 3 | 1 | -2 | 21.0 | 20.8 | -.69 | -6 | 1 | 4 | 44.0 | 44.8 | 1.95 |
| -3 | 1 | -2 | 18.3 | 18.8 | 3.12 | 7 | 1 | 4 | 48.0 | 48.2 | .56 |
| 4 | 1 | -2 | 27.6 | 27.5 | -.28 | 8 | 1 | 4 | 58.6 | 58.5 | -.07 |
| -4 | 1 | -2 | 24.9 | 25.4 | 2.10 | -8 | 1 | 4 | 66.0 | 66.7 | 1.21 |
| -5 | 1 | -2 | 31.9 | 32.4 | 1.65 | 1 | 1 | -4 | 13.2 | 13.0 | -1.11 |
| 6 | 1 | -2 | 42.7 | 42.6 | -.20 | -1 | 1 | -4 | 11.0 | 10.9 | -.02 |
| -6 | 1 | -2 | 39.9 | 40.0 | .44 | 2 | 1 | -4 | 18.0 | 17.8 | -.83 |
| 7 | 1 | -2 | 51.0 | 51.7 | 1.44 | -2 | 1 | -4 | 14.8 | 14.7 | -.42 |
| -7 | 1 | -2 | 48.3 | 48.7 | .93 | 3 | 1 | -4 | 23.7 | 23.6 | -.29 |
| 1 | 1 | 3 | 8.1 | 8.2 | 2.08 | -3 | 1 | -4 | 20.0 | 19.9 | -.08 |
| -1 | 1 | 3 | 9.8 | 10.2 | 4.56 | 4 | 1 | -4 | 30.0 | 30.0 | .24 |
| 2 | 1 | 3 | 13.3 | 13.0 | -2.02 | 5 | 1 | -4 | 37.1 | 37.1 | .23 |
| -2 | 1 | 3 | 15.1 | 15.6 | 3.63 | -5 | 1 | -4 | 32.7 | 32.7 | .06 |
| 3 | 1 | 3 | 19.2 | 18.8 | -1.65 | 6 | 1 | -4 | 44.9 | 45.1 | .64 |
| -3 | 1 | 3 | 21.2 | 21.7 | 2.72 | -6 | 1 | -4 | 39.9 | 40.1 | .59 |
| -4 | 1 | 3 | 27.8 | 28.4 | 2.16 | -8 | 1 | -4 | 58.7 | 58.9 | .37 |
| 5 | 1 | 3 | 32.2 | 32.1 | -.02 | -9 | 1 | -4 | 73.4 | 74.4 | 1.43 |
| -5 | 1 | 3 | 35.0 | 35.5 | 1.67 | 1 | 1 | 5 | 12.0 | 12.1 | 1.26 |
| -6 | 1 | 3 | 42.8 | 43.5 | 1.76 | -1 | 1 | 5 | 14.1 | 14.4 | 2.75 |
| 8 | 1 | 3 | 58.8 | 58.7 | -.11 | 2 | 1 | 5 | 15.9 | 15.4 | -2.94 |
| -8 | 1 | 3 | 64.1 | 64.7 | 1.04 | -2 | 1 | 5 | 18.6 | 19.1 | 2.83 |
| 1 | 1 | -3 | 11.1 | 10.9 | -1.58 | 3 | 1 | 5 | 20.9 | 20.3 | -2.57 |
| -1 | 1 | -3 | 9.1 | 9.0 | -.13 | -3 | 1 | 5 | 24.2 | 24.7 | 2.46 |
| 2 | 1 | -3 | 16.3 | 16.1 | -1.14 | 4 | 1 | 5 | 26.5 | 26.2 | -1.09 |
| -2 | 1 | -3 | 13.6 | 13.5 | -.17 | -4 | 1 | 5 | 30.7 | 31.1 | 1.59 |
| 3 | 1 | -3 | 22.2 | 22.1 | -.31 | 5 | 1 | 5 | 32.9 | 32.7 | -.42 |
| -3 | 1 | -3 | 19.1 | 19.2 | .93 | -5 | 1 | 5 | 37.3 | 38.3 | 2.69 |
| 4 | 1 | -3 | 28.7 | 28.6 | -.02 | 6 | 1 | 5 | 40.0 | 40.0 | .17 |
| -4 | 1 | -3 | 25.5 | 25.5 | .38 | -6 | 1 | 5 | 45.3 | 46.3 | 2.37 |
| 5 | 1 | -3 | 35.8 | 35.8 | .12 | 7 | 1 | 5 | 48.1 | 48.4 | .67 |
| -5 | 1 | -3 | 32.3 | 32.4 | .50 | -8 | 1 | 5 | 68.2 | 69.2 | 1.58 |
| 6 | 1 | -3 | 43.7 | 43.7 | .22 | 1 | 1 | -5 | 15.5 | 15.3 | -1.24 |
| 7 | 1 | -3 | 52.7 | 53.0 | .69 | -1 | 1 | -5 | 13.0 | 13.1 | .81 |
| -7 | 1 | -3 | 47.8 | 48.5 | 1.61 | 2 | 1 | -5 | 19.9 | 19.7 | -.62 |
| 1 | 1 | 4 | 9.8 | 10.0 | 2.98 | -2 | 1 | -5 | 16.2 | 16.2 | .05 |
| -1 | 1 | 4 | 11.9 | 12.2 | 3.29 | 3 | 1 | -5 | 25.3 | 25.3 | .10 |
| 2 | 1 | 4 | 14.3 | 14.0 | -1.66 | -3 | 1 | -5 | 21.0 | 20.9 | -.10 |
| -2 | 1 | 4 | 16.8 | 17.2 | 2.87 | 4 | 1 | -5 | 31.7 | 31.6 | -.17 |
| 3 | 1 | 4 | 19.7 | 19.4 | -1.16 | 5 | 1 | -5 | 38.8 | 38.7 | -.20 |
| -3 | 1 | 4 | 22.6 | 23.1 | 2.57 | 6 | 1 | -5 | 46.7 | 46.7 | .17 |
| -4 | 1 | 4 | 29.0 | 29.6 | 2.40 | 8 | 1 | -5 | 69.0 | 69.9 | 1.13 |
| 5 | 1 | 4 | 32.4 | 32.3 | -.11 | -8 | 1 | -5 | 58.8 | 59.0 | .45 |
| 6 | 1 | 4 | 39.8 | 39.8 | .02 | -9 | 1 | -5 | 73.8 | 74.4 | .94 |

| h | k | l | $x_o$ | $x_c$ | error% |
|---|---|---|---|---|---|
| 1 | 1 | 6 | 14.1 | 14.3 | 1.84 |
| -1 | 1 | 6 | 16.3 | 16.7 | 3.00 |
| -2 | 1 | 6 | 20.7 | 21.1 | 2.11 |
| 3 | 1 | 6 | 21.8 | 21.5 | -1.26 |
| -3 | 1 | 6 | 26.0 | 26.5 | 2.28 |
| 4 | 1 | 6 | 27.2 | 27.0 | -.55 |
| -4 | 1 | 6 | 32.2 | 32.8 | 2.06 |
| 5 | 1 | 6 | 33.6 | 33.3 | -.65 |
| -5 | 1 | 6 | 39.1 | 39.9 | 2.18 |
| 6 | 1 | 6 | 40.7 | 40.5 | -.40 |
| -6 | 1 | 6 | 47.1 | 48.0 | 2.12 |
| 7 | 1 | 6 | 48.7 | 48.7 | .17 |
| -8 | 1 | 6 | 70.9 | 72.3 | 2.10 |
| 1 | 1 | -6 | 17.8 | 17.6 | -.82 |
| -1 | 1 | -6 | 15.2 | 15.3 | .95 |
| 2 | 1 | -6 | 22.0 | 21.8 | -.66 |
| -2 | 1 | -6 | 17.9 | 17.9 | .12 |
| -3 | 1 | -6 | 21.8 | 22.2 | 1.97 |
| 4 | 1 | -6 | 33.2 | 33.3 | .60 |
| -4 | 1 | -6 | 27.7 | 27.6 | -.19 |
| 5 | 1 | -6 | 40.2 | 40.4 | .61 |
| 6 | 1 | -6 | 48.2 | 48.5 | .81 |
| 8 | 1 | -6 | 72.4 | 73.2 | 1.18 |
| -8 | 1 | -6 | 59.0 | 59.4 | .75 |
| -9 | 1 | -6 | 74.0 | 74.9 | 1.27 |
| 1 | 1 | 7 | 16.3 | 16.6 | 2.27 |
| -1 | 1 | 7 | 18.8 | 19.1 | 1.99 |
| -2 | 1 | 7 | 22.8 | 23.2 | 2.14 |
| 3 | 1 | 7 | 23.2 | 22.9 | -1.18 |
| -3 | 1 | 7 | 27.9 | 28.5 | 2.34 |
| 4 | 1 | 7 | 28.2 | 28.1 | -.29 |
| 5 | 1 | 7 | 34.3 | 34.2 | -.24 |
| -5 | 1 | 7 | 41.0 | 41.7 | 1.93 |
| 6 | 1 | 7 | 41.1 | 41.2 | .26 |
| 1 | 1 | -7 | 20.1 | 20.0 | -.12 |
| -1 | 1 | -7 | 17.8 | 17.6 | -.66 |
| 2 | 1 | -7 | 24.1 | 24.0 | -.15 |
| -2 | 1 | -7 | 19.9 | 19.8 | -.34 |
| 3 | 1 | -7 | 29.2 | 29.2 | .09 |
| -3 | 1 | -7 | 23.7 | 23.7 | .03 |
| -4 | 1 | -7 | 28.8 | 28.7 | -.01 |
| 5 | 1 | -7 | 41.9 | 42.3 | 1.10 |
| -5 | 1 | -7 | 34.7 | 34.8 | .36 |
| -6 | 1 | -7 | 41.8 | 41.7 | -.03 |
| 8 | 1 | -7 | 77.0 | 77.8 | 1.09 |
| -8 | 1 | -7 | 59.8 | 60.0 | .44 |
| -9 | 1 | -7 | 75.0 | 75.8 | 1.11 |
| 1 | 1 | 8 | 18.9 | 19.0 | .86 |
| -1 | 1 | 8 | 21.2 | 21.6 | 2.04 |
| 2 | 1 | 8 | 20.9 | 20.9 | .17 |
| -2 | 1 | 8 | 25.1 | 25.5 | 1.83 |
| -3 | 1 | 8 | 30.1 | 30.6 | 1.88 |
| 4 | 1 | 8 | 29.7 | 29.3 | -1.01 |
| -4 | 1 | 8 | 36.1 | 36.7 | 1.79 |
| 5 | 1 | 8 | 35.3 | 35.2 | -.11 |
| -5 | 1 | 8 | 43.0 | 43.8 | 1.91 |
| 1 | 1 | -8 | 22.7 | 22.5 | -.58 |
| -1 | 1 | -8 | 20.0 | 20.0 | .47 |
| 2 | 1 | -8 | 26.4 | 26.3 | -.04 |
| -2 | 1 | -8 | 22.0 | 21.8 | -.48 |
| 3 | 1 | -8 | 31.4 | 31.4 | .01 |
| -3 | 1 | -8 | 25.2 | 25.3 | .74 |
| -4 | 1 | -8 | 30.2 | 30.1 | -.14 |
| 5 | 1 | -8 | 44.1 | 44.4 | .84 |
| -5 | 1 | -8 | 36.0 | 35.9 | -.14 |
| -6 | 1 | -8 | 42.7 | 42.7 | .10 |
| 7 | 1 | -8 | 63.0 | 63.8 | 1.27 |
| -8 | 1 | -8 | 60.7 | 60.9 | .38 |
| 1 | 1 | 9 | 21.1 | 21.5 | 2.01 |
| -1 | 1 | 9 | 23.8 | 24.1 | 1.51 |
| 2 | 1 | 9 | 22.9 | 23.0 | .83 |
| -2 | 1 | 9 | 27.3 | 27.9 | 2.36 |
| -4 | 1 | 9 | 38.2 | 38.9 | 1.93 |
| -5 | 1 | 9 | 45.2 | 46.0 | 1.88 |
| -6 | 1 | 9 | 53.5 | 54.6 | 2.17 |
| 1 | 1 | -9 | 25.0 | 25.1 | .50 |
| -1 | 1 | -9 | 22.7 | 22.5 | -.53 |
| 2 | 1 | -9 | 28.9 | 28.8 | -.27 |
| -2 | 1 | -9 | 24.0 | 24.0 | .37 |
| 3 | 1 | -9 | 33.8 | 33.7 | -.22 |
| -3 | 1 | -9 | 27.1 | 27.2 | .52 |
| 4 | 1 | -9 | 39.8 | 39.6 | -.28 |
| -4 | 1 | -9 | 31.8 | 31.7 | -.28 |
| 5 | 1 | -9 | 46.4 | 46.7 | .83 |
| -5 | 1 | -9 | 37.1 | 37.2 | .45 |
| -6 | 1 | -9 | 43.8 | 43.9 | .24 |

| h | l | l | $x_o$ | $x_c$ | error% |
|---|---|---|---|---|---|
| 7 | 1 | -9 | 66.4 | 67.1 | 1.12 |
| -7 | 1 | -9 | 51.5 | 51.8 | .73 |
| 1 | 1 | 10 | 23.8 | 24.0 | 1.08 |
| 2 | 1 | 10 | 25.1 | 25.3 | 1.06 |
| -2 | 1 | 10 | 29.8 | 30.4 | 2.13 |
| -3 | 1 | 10 | 34.8 | 35.3 | 1.50 |
| -4 | 1 | 10 | 40.7 | 41.3 | 1.49 |
| -5 | 1 | 10 | 47.8 | 48.4 | 1.45 |
| -6 | 1 | 10 | 56.3 | 57.4 | 1.96 |
| 1 | 1 | -10 | 27.7 | 27.7 | .21 |
| -1 | 1 | -10 | 25.1 | 25.1 | .13 |
| 2 | 1 | -10 | 31.2 | 31.3 | .51 |
| -2 | 1 | -10 | 26.4 | 26.4 | .01 |
| 3 | 1 | -10 | 36.1 | 36.1 | .22 |
| -3 | 1 | -10 | 29.0 | 29.2 | .88 |
| -4 | 1 | -10 | 33.6 | 33.4 | -.46 |
| 5 | 1 | -10 | 49.0 | 49.3 | .65 |
| -5 | 1 | -10 | 38.9 | 38.7 | -.29 |
| 6 | 1 | -10 | 57.8 | 58.3 | .88 |
| -6 | 1 | -10 | 45.0 | 45.2 | .60 |
| 7 | 1 | -10 | 70.2 | 71.2 | 1.50 |
| -7 | 1 | -10 | 52.9 | 53.1 | .53 |
| -8 | 1 | -10 | 62.9 | 63.4 | .93 |
| 1 | 1 | 11 | 26.2 | 26.6 | 1.75 |
| -1 | 1 | 11 | 28.9 | 29.4 | 1.85 |
| -2 | 1 | 11 | 32.5 | 33.0 | 1.65 |
| -3 | 1 | 11 | 37.1 | 37.8 | 2.06 |
| -4 | 1 | 11 | 43.1 | 43.8 | 1.74 |
| -5 | 1 | 11 | 50.2 | 51.1 | 1.94 |
| -6 | 1 | 11 | 59.2 | 60.5 | 2.22 |
| 1 | 1 | -11 | 30.3 | 30.4 | .56 |
| -1 | 1 | -11 | 27.7 | 27.7 | .21 |
| 2 | 1 | -11 | 34.0 | 34.0 | .03 |
| -2 | 1 | -11 | 28.9 | 28.8 | -.25 |
| 3 | 1 | -11 | 38.9 | 38.7 | -.29 |
| -3 | 1 | -11 | 31.2 | 31.4 | .70 |
| 4 | 1 | -11 | 44.2 | 44.7 | 1.24 |
| -5 | 1 | -11 | 39.8 | 40.4 | 1.73 |
| -6 | 1 | -11 | 46.8 | 46.8 | .09 |
| 7 | 1 | -11 | 76.0 | 76.8 | 1.05 |
| 1 | 1 | 12 | 28.9 | 29.3 | 1.51 |
| -1 | 1 | 12 | 31.7 | 32.1 | 1.56 |
| 2 | 1 | 12 | 30.0 | 30.2 | .82 |

| h | k | l | $x_o$ | $x_c$ | error% |
|---|---|---|---|---|---|
| -2 | 1 | 12 | 35.1 | 35.7 | 1.87 |
| -4 | 1 | 12 | 45.8 | 46.5 | 1.74 |
| -5 | 1 | 12 | 53.2 | 54.1 | 1.75 |
| -6 | 1 | 12 | 62.9 | 64.1 | 1.91 |
| 1 | 1 | -12 | 33.1 | 33.2 | .51 |
| -1 | 1 | -12 | 30.4 | 30.4 | .22 |
| 2 | 1 | -12 | 36.8 | 36.7 | -.05 |
| -2 | 1 | -12 | 31.2 | 31.3 | .50 |
| 3 | 1 | -12 | 41.2 | 41.5 | .83 |
| -3 | 1 | -12 | 33.7 | 33.7 | .07 |
| 5 | 1 | -12 | 54.9 | 55.1 | .48 |
| -5 | 1 | -12 | 42.3 | 42.3 | .20 |
| -6 | 1 | -12 | 48.5 | 48.6 | .26 |
| 1 | 1 | 13 | 31.8 | 32.0 | .93 |
| -1 | 1 | 13 | 34.4 | 35.0 | 1.90 |
| 2 | 1 | 13 | 32.7 | 32.8 | .45 |
| -2 | 1 | 13 | 38.1 | 38.6 | 1.31 |
| -3 | 1 | 13 | 41.8 | 43.4 | 3.87 |
| -6 | 1 | 13 | 67.1 | 68.3 | 1.92 |
| 1 | 1 | -13 | 36.1 | 36.1 | .19 |
| -1 | 1 | -13 | 33.2 | 33.2 | .18 |
| 2 | 1 | -13 | 39.8 | 39.6 | -.29 |
| -2 | 1 | -13 | 34.0 | 34.0 | .00 |
| 3 | 1 | -13 | 44.0 | 44.4 | 1.08 |
| -3 | 1 | -13 | 36.0 | 36.1 | .47 |
| 4 | 1 | -13 | 50.5 | 50.6 | .27 |
| -4 | 1 | -13 | 39.8 | 39.6 | -.29 |
| 5 | 1 | -13 | 58.2 | 58.5 | .67 |
| -5 | 1 | -13 | 43.9 | 44.4 | 1.31 |
| -8 | 1 | -13 | 69.2 | 69.9 | 1.13 |
| 1 | 1 | 14 | 34.5 | 34.9 | 1.32 |
| -1 | 1 | 14 | 37.5 | 38.2 | 1.39 |
| 2 | 1 | 14 | 35.3 | 35.5 | .75 |
| -2 | 1 | 14 | 40.9 | 41.5 | 1.69 |
| -3 | 1 | 14 | 45.8 | 46.4 | 1.46 |
| -6 | 1 | 14 | 72.3 | 73.8 | 2.21 |
| 1 | 1 | -14 | 39.1 | 39.1 | .23 |
| -1 | 1 | -14 | 36.0 | 36.1 | .44 |
| 2 | 1 | -14 | 42.6 | 42.7 | .32 |
| -2 | 1 | -14 | 36.9 | 36.7 | -.37 |
| -3 | 1 | -14 | 38.7 | 38.7 | .16 |
| 4 | 1 | -14 | 53.7 | 53.9 | .52 |
| -4 | 1 | -14 | 42.0 | 42.1 | .25 |

| h | k | l | $x_o$ | $x_c$ | error% |
|---|---|---|---|---|---|
| 5 | 1 | -14 | 62.1 | 62.4 | .63 |
| -5 | 1 | -14 | 46.8 | 46.7 | -.06 |
| 6 | 1 | -14 | 75.2 | 76.1 | 1.30 |
| -7 | 1 | -14 | 60.7 | 60.9 | .47 |
| -8 | 1 | -14 | 72.8 | 73.2 | .67 |
| 1 | 1 | 15 | 37.4 | 37.9 | 1.40 |
| -1 | 1 | 15 | 40.7 | 41.1 | 1.04 |
| -2 | 1 | 15 | 44.0 | 44.7 | 1.70 |
| -3 | 1 | 15 | 49.0 | 49.7 | 1.51 |
| -4 | 1 | 15 | 55.3 | 56.3 | 1.90 |
| 1 | 1 | -15 | 42.2 | 42.3 | .36 |
| -1 | 1 | -15 | 39.2 | 39.1 | -.05 |
| 2 | 1 | -15 | 45.8 | 45.9 | .37 |
| -2 | 1 | -15 | 39.8 | 39.6 | -.35 |
| -3 | 1 | -15 | 41.0 | 41.5 | 1.24 |
| 4 | 1 | -15 | 57.5 | 57.6 | .32 |
| -4 | 1 | -15 | 44.7 | 44.7 | .02 |
| 5 | 1 | -15 | 66.3 | 67.1 | 1.20 |
| -5 | 1 | -15 | 49.1 | 49.2 | .37 |
| -7 | 1 | -15 | 63.2 | 63.7 | .90 |
| -8 | 1 | -15 | 77.2 | 77.8 | .80 |
| 1 | 1 | 16 | 40.7 | 41.0 | .79 |
| -1 | 1 | 16 | 43.9 | 44.3 | 1.11 |
| -2 | 1 | 16 | 46.3 | 48.1 | 3.91 |
| -3 | 1 | 16 | 52.3 | 53.2 | 1.90 |
| -4 | 1 | 16 | 59.3 | 60.3 | 1.76 |
| 1 | 1 | -16 | 45.7 | 45.6 | -.02 |
| -1 | 1 | -16 | 42.2 | 42.3 | .32 |
| -2 | 1 | -16 | 42.7 | 42.7 | .00 |
| -3 | 1 | -16 | 44.3 | 44.4 | .30 |
| -6 | 1 | -16 | 57.9 | 58.2 | .60 |
| -7 | 1 | -16 | 66.5 | 67.0 | .86 |
| 1 | 1 | 17 | 43.9 | 44.2 | .87 |
| -1 | 1 | 17 | 47.1 | 47.8 | 1.58 |
| -3 | 1 | 17 | 56.3 | 57.2 | 1.62 |
| -1 | 1 | -17 | 45.7 | 45.6 | -.07 |
| -2 | 1 | -17 | 45.9 | 45.9 | .06 |
| 3 | 1 | -17 | 58.2 | 58.7 | .95 |
| 4 | 1 | -17 | 66.2 | 66.8 | .94 |
| -4 | 1 | -17 | 50.6 | 50.5 | -.05 |
| -5 | 1 | -17 | 55.0 | 55.0 | .15 |
| -7 | 1 | -17 | 70.6 | 71.1 | .74 |
| 1 | 1 | 18 | 47.1 | 47.7 | 1.35 |
| -1 | 1 | 18 | 50.9 | 51.5 | 1.30 |
| 3 | 1 | -18 | 62.9 | 63.4 | .84 |
| -3 | 1 | -18 | 50.2 | 50.9 | 1.43 |
| 4 | 1 | -18 | 72.4 | 73.1 | 1.03 |
| -4 | 1 | -18 | 54.0 | 53.8 | -.18 |
| -5 | 1 | -18 | 58.2 | 58.4 | .49 |
| -7 | 1 | -18 | 76.0 | 76.5 | .75 |
| -1 | 1 | 19 | 54.9 | 55.6 | 1.30 |
| 2 | 1 | -19 | 61.4 | 61.9 | .84 |
| 3 | 1 | -19 | 68.5 | 69.0 | .84 |
| -4 | 1 | -19 | 57.3 | 57.5 | .49 |
| -5 | 1 | -19 | 62.1 | 62.3 | .41 |
| -6 | 1 | -19 | 69.2 | 69.7 | .85 |
| -1 | 1 | 20 | 59.3 | 60.1 | 1.41 |
| 2 | 1 | -20 | 66.8 | 67.4 | .94 |
| 3 | 1 | -20 | 76.1 | 76.9 | 1.05 |
| -3 | 1 | -20 | 58.3 | 58.6 | .60 |
| -5 | 1 | -20 | 66.7 | 66.9 | .32 |
| -6 | 1 | -20 | 75.5 | 75.8 | .49 |
| 2 | 1 | -21 | 74.2 | 74.7 | .71 |
| -2 | 1 | -21 | 61.8 | 61.8 | .04 |
| -3 | 1 | -21 | 63.1 | 63.3 | .32 |
| -4 | 1 | -21 | 66.2 | 66.6 | .68 |
| -2 | 1 | -22 | 66.9 | 67.3 | .62 |
| -3 | 1 | -22 | 68.5 | 68.9 | .59 |
| -4 | 1 | -22 | 72.3 | 72.8 | .81 |
| -2 | 1 | -23 | 74.0 | 74.5 | .75 |
| -3 | 1 | -23 | 76.0 | 76.6 | .82 |
| 1 | 2 | | 6.5 | 6.6 | 2.48 |
| -1 | 2 | | 6.4 | 6.6 | 4.08 |
| 3 | 2 | | 19.5 | 19.4 | -.40 |
| -3 | 2 | | 18.7 | 19.4 | 3.85 |
| 4 | 2 | | 26.1 | 26.2 | .54 |
| -4 | 2 | | 25.6 | 26.2 | 2.51 |
| 5 | 2 | | 33.2 | 33.5 | .92 |
| 6 | 2 | | 40.9 | 41.4 | 1.35 |
| 1 | 2 | 1 | 6.0 | 6.2 | 4.68 |
| 2 | 2 | 1 | 12.5 | 12.4 | -.35 |
| -2 | 2 | 1 | 12.9 | 13.4 | 4.14 |
| 3 | 2 | 1 | 18.8 | 18.9 | .73 |
| -3 | 2 | 1 | 19.5 | 19.9 | 2.36 |
| 4 | 2 | 1 | 25.6 | 25.7 | .49 |
| 5 | 2 | 1 | 32.9 | 32.9 | .14 |

| h | k | l | $x_o$ | $x_c$ | error% |
|---|---|---|---|---|---|
| -5 | 2 | 1 | 33.4 | 34.1 | 2.12 |
| 6 | 2 | 1 | 40.5 | 40.8 | .81 |
| -6 | 2 | 1 | 41.1 | 42.1 | 2.48 |
| 9 | 2 | 1 | 78.5 | 79.7 | 1.52 |
| 1 | 2 | -1 | 8.0 | 7.8 | -1.99 |
| 2 | 2 | -1 | 13.9 | 13.7 | -.72 |
| -2 | 2 | -1 | 12.3 | 12.8 | 4.42 |
| 3 | 2 | -1 | 20.3 | 20.2 | -.39 |
| -3 | 2 | -1 | 18.8 | 19.2 | 2.16 |
| 5 | 2 | -1 | 34.0 | 34.2 | .84 |
| 6 | 2 | -1 | 41.9 | 42.2 | .92 |
| 7 | 2 | -1 | 50.6 | 51.4 | 1.77 |
| 1 | 2 | 2 | 6.6 | 6.8 | 3.51 |
| 2 | 2 | 2 | 12.4 | 12.4 | .78 |
| 3 | 2 | 2 | 18.9 | 18.7 | -.56 |
| -3 | 2 | 2 | 20.1 | 20.8 | 3.52 |
| 4 | 2 | 2 | 25.2 | 25.4 | 1.09 |
| -4 | 2 | 2 | 27.0 | 27.6 | 2.28 |
| 5 | 2 | 2 | 32.6 | 32.6 | .04 |
| -5 | 2 | 2 | 34.0 | 34.9 | 2.73 |
| -6 | 2 | 2 | 42.2 | 42.9 | 1.89 |
| 7 | 2 | 2 | 48.6 | 49.2 | 1.38 |
| -7 | 2 | 2 | 51.2 | 52.3 | 2.21 |
| 9 | 2 | 2 | 76.8 | 77.7 | 1.28 |
|  | 2 | -2 | 6.2 | 6.1 | -.46 |
| 1 | 2 | -2 | 9.5 | 9.5 | .34 |
| 2 | 2 | -2 | 15.3 | 15.0 | -1.52 |
| -2 | 2 | -2 | 12.9 | 13.2 | 2.81 |
| 3 | 2 | -2 | 21.3 | 21.3 | -.01 |
| -3 | 2 | -2 | 18.9 | 19.3 | 2.28 |
| 4 | 2 | -2 | 25.3 | 25.9 | 2.37 |
| 5 | 2 | -2 | 35.0 | 35.2 | .81 |
| -5 | 2 | -2 | 32.1 | 32.9 | 2.74 |
| 6 | 2 | -2 | 42.9 | 43.3 | 1.00 |
| -6 | 2 | -2 | 40.0 | 40.7 | 1.87 |
| -7 | 2 | -2 | 48.8 | 49.6 | 1.66 |
| 2 | 2 | 3 | 12.6 | 13.0 | 3.38 |
| -2 | 2 | 3 | 15.0 | 15.6 | 4.66 |
| 3 | 2 | 3 | 18.6 | 18.9 | 2.10 |
| 4 | 2 | 3 | 25.1 | 25.4 | 1.56 |
| 5 | 2 | 3 | 32.2 | 32.5 | .97 |
| -5 | 2 | 3 | 35.0 | 35.9 | 2.75 |
| 6 | 2 | 3 | 40.0 | 40.2 | .52 |

| h | k | l | $x_o$ | $x_c$ | error% |
|---|---|---|---|---|---|
| -6 | 2 | 3 | 43.0 | 44.0 | 2.52 |
| 7 | 2 | 3 | 48.4 | 48.9 | 1.16 |
| 8 | 2 | 3 | 58.8 | 59.6 | 1.53 |
| 9 | 2 | 3 | 74.6 | 76.5 | 2.66 |
|  | 2 | -3 | 8.5 | 8.5 | .74 |
| 1 | 2 | -3 | 11.6 | 11.5 | -.65 |
| -1 | 2 | -3 | 9.6 | 9.7 | 1.61 |
| 2 | 2 | -3 | 16.7 | 16.6 | -.40 |
| -2 | 2 | -3 | 13.8 | 14.1 | 2.32 |
| 3 | 2 | -3 | 22.5 | 22.6 | .63 |
| -3 | 2 | -3 | 19.4 | 19.7 | 1.99 |
| -4 | 2 | -3 | 25.7 | 26.1 | 1.67 |
| 5 | 2 | -3 | 36.1 | 36.4 | 1.07 |
| -5 | 2 | -3 | 32.5 | 33.0 | 1.72 |
| 6 | 2 | -3 | 44.0 | 44.5 | 1.32 |
| -6 | 2 | -3 | 39.9 | 40.7 | 2.04 |
| 7 | 2 | -3 | 53.2 | 54.0 | 1.68 |
| -7 | 2 | -3 | 48.4 | 49.4 | 2.21 |
| 8 | 2 | -3 | 65.9 | 66.7 | 1.24 |
| 1 | 2 | 4 | 9.5 | 9.8 | 4.12 |
| 2 | 2 | 4 | 13.6 | 13.9 | 2.87 |
| -2 | 2 | 4 | 16.5 | 17.2 | 4.78 |
| 3 | 2 | 4 | 19.2 | 19.5 | 1.67 |
| -3 | 2 | 4 | 22.6 | 23.3 | 3.10 |
| 4 | 2 | 4 | 25.4 | 25.7 | 1.50 |
| 5 | 2 | 4 | 32.3 | 32.6 | 1.05 |
| -5 | 2 | 4 | 36.1 | 37.2 | 3.06 |
| 6 | 2 | 4 | 39.9 | 40.2 | .80 |
| -6 | 2 | 4 | 44.2 | 45.3 | 2.66 |
| 7 | 2 | 4 | 48.2 | 48.8 | 1.38 |
| 8 | 2 | 4 | 58.6 | 59.4 | 1.47 |
| -8 | 2 | 4 | 66.3 | 68.1 | 2.78 |
|  | 2 | -4 | 10.8 | 11.0 | 1.92 |
| -1 | 2 | -4 | 11.6 | 11.7 | .86 |
| -2 | 2 | -4 | 15.4 | 15.3 | -.32 |
| -3 | 2 | -4 | 20.3 | 20.5 | 1.26 |
| 4 | 2 | -4 | 30.3 | 30.6 | 1.29 |
| -4 | 2 | -4 | 26.0 | 26.6 | 2.38 |
| -5 | 2 | -4 | 32.7 | 33.3 | 2.04 |
| 7 | 2 | -4 | 54.9 | 55.7 | 1.57 |
| -7 | 2 | -4 | 48.9 | 49.5 | 1.30 |
| 8 | 2 | -4 | 68.0 | 69.1 | 1.65 |
|  | 2 | 5 | 11.0 | 11.5 | 4.73 |

| h | k | l | $x_o$ | $x_c$ | error% |
|---|---|---|---|---|---|
| 1 | 2 | 5 | 11.5 | 11.9 | 3.69 |
| 2 | 2 | 5 | 15.2 | 15.3 | .76 |
| -2 | 2 | 5 | 18.5 | 19.1 | 3.26 |
| 3 | 2 | 5 | 20.1 | 20.3 | 1.32 |
| -3 | 2 | 5 | 24.1 | 24.8 | 3.27 |
| 4 | 2 | 5 | 26.0 | 26.3 | 1.27 |
| -6 | 2 | 5 | 45.9 | 46.8 | 2.14 |
| 7 | 2 | 5 | 48.4 | 48.9 | 1.20 |
| -7 | 2 | 5 | 55.1 | 56.7 | 3.06 |
| 8 | 2 | 5 | 58.9 | 59.4 | .97 |
| -8 | 2 | 5 | 68.9 | 70.7 | 2.69 |
|  | 2 | -5 | 13.4 | 13.4 | .66 |
| -1 | 2 | -5 | 13.8 | 13.8 | .27 |
| 2 | 2 | -5 | 20.5 | 20.4 | -.43 |
| -2 | 2 | -5 | 16.7 | 16.8 | 1.06 |
| 3 | 2 | -5 | 25.9 | 25.9 | .24 |
| -3 | 2 | -5 | 21.5 | 21.6 | .51 |
| 4 | 2 | -5 | 32.0 | 32.3 | 1.02 |
| -5 | 2 | -5 | 33.1 | 33.9 | 2.43 |
| -6 | 2 | -5 | 40.7 | 41.2 | 1.43 |
| 7 | 2 | -5 | 56.8 | 57.7 | 1.58 |
| 8 | 2 | -5 | 70.8 | 72.1 | 1.88 |
|  | 2 | 6 | 13.4 | 14.0 | 4.55 |
| 2 | 2 | 6 | 16.6 | 16.9 | 1.95 |
| -2 | 2 | 6 | 20.2 | 21.0 | 4.44 |
| -3 | 2 | 6 | 26.0 | 26.6 | 2.57 |
| 4 | 2 | 6 | 26.7 | 27.1 | 1.62 |
| 5 | 2 | 6 | 33.2 | 33.5 | 1.16 |
| -5 | 2 | 6 | 39.3 | 40.2 | 2.50 |
| 6 | 2 | 6 | 40.2 | 40.8 | 1.69 |
| -7 | 2 | 6 | 57.1 | 58.8 | 2.99 |
| -8 | 2 | 6 | 71.7 | 74.1 | 3.36 |
|  | 2 | -6 | 16.0 | 16.0 | .03 |
| 1 | 2 | -6 | 18.4 | 18.3 | -.13 |
| 2 | 2 | -6 | 22.5 | 22.5 | .19 |
| 3 | 2 | -6 | 27.9 | 27.8 | -.01 |
| 4 | 2 | -6 | 33.9 | 34.1 | .72 |
| -5 | 2 | -6 | 34.0 | 34.6 | 1.94 |
| -6 | 2 | -6 | 41.1 | 41.8 | 1.91 |
|  | 2 | 7 | 15.9 | 16.5 | 3.98 |
| 1 | 2 | 7 | 15.9 | 16.4 | 3.36 |
| -1 | 2 | 7 | 18.4 | 19.0 | 3.36 |
| 2 | 2 | 7 | 18.4 | 18.7 | 1.93 |
| 3 | 2 | 7 | 22.7 | 22.8 | .73 |
| -4 | 2 | 7 | 33.8 | 34.9 | 3.27 |
| 5 | 2 | 7 | 33.9 | 34.3 | 1.45 |
| -5 | 2 | 7 | 41.2 | 42.1 | 2.22 |
| 6 | 2 | 7 | 41.9 | 41.5 | -.89 |
| -7 | 2 | 7 | 59.6 | 61.1 | 2.60 |
|  | 2 | -7 | 18.5 | 18.5 | .32 |
| 1 | 2 | -7 | 20.8 | 20.8 | .17 |
| -1 | 2 | -7 | 18.2 | 18.4 | 1.48 |
| 2 | 2 | -7 | 24.7 | 24.8 | .42 |
| -2 | 2 | -7 | 20.4 | 20.5 | .94 |
| 3 | 2 | -7 | 30.0 | 29.9 | -.05 |
| 4 | 2 | -7 | 35.9 | 36.1 | .66 |
| 6 | 2 | -7 | 51.1 | 51.7 | 1.26 |
|  | 2 | 8 | 18.5 | 19.0 | 3.22 |
| 1 | 2 | 8 | 18.4 | 18.8 | 2.36 |
| 2 | 2 | 8 | 20.4 | 20.7 | 1.79 |
| -2 | 2 | 8 | 24.5 | 25.5 | 4.11 |
| 3 | 2 | 8 | 24.0 | 24.4 | 1.92 |
| -4 | 2 | 8 | 36.0 | 36.9 | 2.58 |
| 5 | 2 | 8 | 35.1 | 35.4 | .89 |
| 6 | 2 | 8 | 41.9 | 42.3 | 1.14 |
| 9 | 2 | 8 | 77.1 | 77.8 | .97 |
|  | 2 | -8 | 21.3 | 21.1 | -.67 |
| 1 | 2 | -8 | 23.4 | 23.3 | -.12 |
| -1 | 2 | -8 | 20.8 | 20.9 | .56 |
| -2 | 2 | -8 | 22.5 | 22.7 | .89 |
| 4 | 2 | -8 | 37.9 | 38.3 | 1.07 |
| 6 | 2 | -8 | 53.3 | 54.1 | 1.57 |
|  | 2 | 9 | 21.2 | 21.7 | 2.37 |
| 1 | 2 | 9 | 20.8 | 21.3 | 2.45 |
| -1 | 2 | 9 | 23.1 | 24.0 | 3.98 |
| -2 | 2 | 9 | 27.3 | 27.8 | 2.18 |
| 3 | 2 | 9 | 25.9 | 26.2 | 1.33 |
| -3 | 2 | 9 | 32.1 | 32.9 | 2.76 |
| 4 | 2 | 9 | 30.3 | 30.9 | 1.98 |
| -4 | 2 | 9 | 38.3 | 39.1 | 2.15 |
| 5 | 2 | 9 | 36.1 | 36.6 | 1.49 |
| -5 | 2 | 9 | 45.0 | 46.3 | 3.08 |
| 6 | 2 | 9 | 43.0 | 43.4 | 1.03 |
| 7 | 2 | 9 | 51.1 | 51.5 | .94 |
| -7 | 2 | 9 | 65.2 | 67.1 | 2.98 |
|  | 2 | -9 | 23.8 | 23.8 | .01 |

| h | k | l | $x_o$ | $x_c$ | error% |
|---|---|---|---|---|---|
| 1 | 2 | -9 | 25.9 | 25.9 | .29 |
| -1 | 2 | -9 | 23.4 | 23.4 | .16 |
| 2 | 2 | -9 | 29.6 | 29.6 | .24 |
| -2 | 2 | -9 | 24.7 | 24.9 | .97 |
| 4 | 2 | -9 | 40.0 | 40.6 | 1.61 |
| 5 | 2 | -9 | 47.2 | 47.8 | 1.46 |
| 6 | 2 | -9 | 56.0 | 56.8 | 1.48 |
|  | 2 | 10 | 23.5 | 24.3 | 3.66 |
| 1 | 2 | 10 | 23.2 | 23.8 | 2.83 |
| 2 | 2 | 10 | 24.7 | 25.2 | 2.03 |
| -2 | 2 | 10 | 29.2 | 30.3 | 4.10 |
| -3 | 2 | 10 | 34.5 | 35.3 | 2.57 |
| -4 | 2 | 10 | 40.4 | 41.4 | 2.71 |
| 6 | 2 | 10 | 44.1 | 44.7 | 1.39 |
| 7 | 2 | 10 | 52.1 | 52.7 | 1.30 |
|  | 2 | -10 | 26.7 | 26.5 | -.72 |
| -1 | 2 | -10 | 25.9 | 26.0 | .51 |
| 2 | 2 | -10 | 32.1 | 32.2 | .53 |
| -2 | 2 | -10 | 27.0 | 27.3 | 1.11 |
| 3 | 2 | -10 | 36.9 | 37.1 | .63 |
| 4 | 2 | -10 | 42.5 | 43.1 | 1.57 |
| 5 | 2 | -10 | 49.9 | 50.5 | 1.26 |
| 6 | 2 | -10 | 58.8 | 59.8 | 1.83 |
|  | 2 | 11 | 26.3 | 27.0 | 2.95 |
| 2 | 2 | 11 | 27.0 | 27.6 | 2.22 |
| -3 | 2 | 11 | 37.0 | 37.9 | 2.54 |
| 4 | 2 | 11 | 33.9 | 34.4 | 1.47 |
| 5 | 2 | 11 | 39.1 | 39.6 | 1.51 |
| -5 | 2 | 11 | 50.4 | 51.5 | 2.28 |
| 6 | 2 | 11 | 45.7 | 46.1 | 1.08 |
|  | 2 | -11 | 29.3 | 29.2 | -.08 |
| 1 | 2 | -11 | 31.1 | 31.4 | 1.03 |
| 2 | 2 | -11 | 34.9 | 34.9 | .24 |
| -2 | 2 | -11 | 29.4 | 29.7 | 1.27 |
| 6 | 2 | -11 | 62.1 | 63.3 | 2.07 |
| 2 | 2 | 12 | 29.8 | 30.1 | 1.03 |
| 3 | 2 | 12 | 32.1 | 32.5 | 1.48 |
| 4 | 2 | 12 | 36.0 | 36.4 | 1.16 |
| 5 | 2 | 12 | 41.0 | 41.5 | 1.25 |
| -5 | 2 | 12 | 53.2 | 54.5 | 2.51 |
| -6 | 2 | 12 | 63.1 | 64.8 | 2.76 |
| 7 | 2 | 12 | 55.1 | 55.9 | 1.46 |
| 8 | 2 | 12 | 66.0 | 66.8 | 1.28 |

| h | k | l | $x_o$ | $x_c$ | error% |
|---|---|---|---|---|---|
|  | 2 | -12 | 31.8 | 32.1 | 1.01 |
| 1 | 2 | -12 | 34.0 | 34.2 | .83 |
| -1 | 2 | -12 | 31.0 | 31.4 | 1.50 |
| 2 | 2 | -12 | 37.2 | 37.8 | 1.68 |
| -2 | 2 | -12 | 32.0 | 32.3 | 1.12 |
| 3 | 2 | -12 | 42.0 | 42.6 | 1.57 |
| 4 | 2 | -12 | 48.0 | 48.8 | 1.72 |
|  | 2 | 13 | 31.7 | 32.7 | 3.23 |
| -1 | 2 | 13 | 34.0 | 34.9 | 2.88 |
| 3 | 2 | 13 | 34.3 | 34.9 | 1.98 |
| 4 | 2 | 13 | 38.0 | 38.6 | 1.60 |
| -5 | 2 | 13 | 56.2 | 57.8 | 2.96 |
| -6 | 2 | 13 | 67.1 | 69.2 | 3.25 |
| 7 | 2 | 13 | 57.1 | 57.8 | 1.34 |
| 8 | 2 | 13 | 68.6 | 69.2 | .99 |
|  | 2 | -13 | 34.6 | 35.0 | 1.33 |
| 1 | 2 | -13 | 36.8 | 37.2 | 1.23 |
| -1 | 2 | -13 | 34.0 | 34.3 | .94 |
| -2 | 2 | -13 | 35.0 | 35.0 | .17 |
| 3 | 2 | -13 | 45.1 | 45.6 | 1.31 |
|  | 2 | 14 | 34.8 | 35.6 | 2.55 |
| 1 | 2 | 14 | 34.0 | 34.8 | 2.46 |
| -2 | 2 | 14 | 40.7 | 41.6 | 2.26 |
| 3 | 2 | 14 | 37.1 | 37.5 | 1.16 |
| 4 | 2 | 14 | 40.6 | 40.9 | .91 |
| 5 | 2 | 14 | 45.0 | 45.7 | 1.66 |
| -6 | 2 | 14 | 72.5 | 75.1 | 3.62 |
| 7 | 2 | 14 | 59.6 | 60.1 | .89 |
| 8 | 2 | 14 | 71.5 | 72.3 | 1.17 |
|  | 2 | -14 | 37.8 | 38.1 | .83 |
| -1 | 2 | -14 | 36.5 | 37.2 | 2.15 |
| -2 | 2 | -14 | 37.2 | 37.8 | 1.86 |
| 4 | 2 | -14 | 54.5 | 55.5 | 1.89 |
|  | 2 | 15 | 38.0 | 38.7 | 2.01 |
| 4 | 2 | 15 | 43.1 | 43.5 | .97 |
| 7 | 2 | 15 | 62.1 | 62.7 | 1.08 |
| 8 | 2 | 15 | 75.3 | 76.4 | 1.46 |
| 1 | 2 | -15 | 42.9 | 43.6 | 1.65 |
| 4 | 2 | -15 | 58.2 | 59.4 | 2.16 |
|  | 2 | 16 | 41.0 | 41.9 | 2.39 |
| 5 | 2 | 16 | 50.2 | 50.8 | 1.30 |
| 7 | 2 | 16 | 65.1 | 65.8 | 1.19 |
|  | 2 | -16 | 43.9 | 44.6 | 1.70 |

| h | k | l | $x_o$ | $x_c$ | error% |
|---|---|---|---|---|---|
| 1 | 2 | -16 | 46.5 | 47.0 | 1.20 |
| -1 | 2 | -16 | 42.8 | 43.6 | 1.94 |
| 2 | 2 | -16 | 50.2 | 50.8 | 1.38 |
| 4 | 2 | -16 | 62.6 | 63.9 | 2.20 |
| | 2 | 17 | 44.2 | 45.3 | 2.64 |
| -1 | 2 | 17 | 46.8 | 47.8 | 2.32 |
| -2 | 2 | 17 | 50.9 | 51.8 | 1.87 |
| 5 | 2 | 17 | 53.1 | 53.7 | 1.31 |
| 7 | 2 | 17 | 68.9 | 69.6 | 1.07 |
| -1 | 2 | -17 | 46.3 | 47.0 | 1.67 |
| 2 | 2 | -17 | 53.9 | 54.8 | 1.68 |
| 1 | 2 | 18 | 46.9 | 47.7 | 1.78 |
| -1 | 2 | 18 | 50.6 | 51.6 | 2.06 |
| -2 | 2 | 18 | 54.6 | 55.8 | 2.29 |
| 5 | 2 | 18 | 56.3 | 57.0 | 1.37 |
| 6 | 2 | 18 | 63.0 | 63.7 | 1.19 |
| 2 | 2 | -18 | 58.4 | 59.1 | 1.30 |
| -2 | 2 | -18 | 50.0 | 50.9 | 1.86 |
| -1 | 2 | 19 | 54.5 | 55.7 | 2.28 |
| 2 | 2 | 19 | 50.6 | 51.5 | 1.85 |
| -2 | 2 | 19 | 58.9 | 60.3 | 2.43 |
| 5 | 2 | 19 | 59.9 | 60.7 | 1.45 |
| 6 | 2 | 19 | 67.0 | 67.9 | 1.48 |
| -2 | 2 | -19 | 54.0 | 54.8 | 1.54 |
| 2 | 2 | 20 | 54.8 | 55.5 | 1.30 |
| 6 | 2 | 20 | 72.2 | 73.4 | 1.67 |
| 2 | 2 | 21 | 59.2 | 59.9 | 1.28 |
| 1 | 3 | | 7.2 | 7.1 | -.34 |
| 2 | 3 | | 13.6 | 13.3 | -1.76 |
| 4 | 3 | | 27.1 | 26.8 | -.76 |
| -4 | 3 | | 25.8 | 26.8 | 4.23 |
| 5 | 3 | | 34.7 | 34.3 | -1.08 |
| -5 | 3 | | 33.0 | 34.3 | 4.01 |
| -6 | 3 | | 41.7 | 42.5 | 1.93 |
| 8 | 3 | | 64.0 | 64.1 | .16 |
| -8 | 3 | | 62.9 | 64.1 | 1.92 |
| 1 | 3 | 1 | 6.7 | 6.6 | -1.13 |
| 2 | 3 | 1 | 13.0 | 12.8 | -1.45 |
| 3 | 3 | 1 | 19.7 | 19.3 | -1.57 |
| 4 | 3 | 1 | 26.7 | 26.3 | -1.45 |
| -4 | 3 | 1 | 26.2 | 27.4 | 4.63 |
| 5 | 3 | 1 | 34.0 | 33.7 | -.86 |
| 7 | 3 | 1 | 51.3 | 51.1 | -.30 |
| -8 | 3 | 1 | 63.9 | 65.2 | 2.08 |
| 1 | 3 | -1 | 8.7 | 8.4 | -2.62 |
| 2 | 3 | -1 | 14.7 | 14.3 | -2.37 |
| 3 | 3 | -1 | 21.2 | 20.8 | -1.77 |
| 4 | 3 | -1 | 28.0 | 27.7 | -.96 |
| -4 | 3 | -1 | 26.1 | 26.6 | 2.05 |
| 6 | 3 | -1 | 43.8 | 43.4 | -.87 |
| -6 | 3 | -1 | 41.2 | 42.0 | 2.13 |
| 8 | 3 | -1 | 65.7 | 65.5 | -.19 |
| -8 | 3 | -1 | 62.0 | 63.2 | 2.08 |
| 1 | 3 | 2 | 6.9 | 6.9 | 1.32 |
| 2 | 3 | 2 | 12.9 | 12.7 | -1.13 |
| 3 | 3 | 2 | 19.4 | 19.1 | -1.17 |
| 4 | 3 | 2 | 26.2 | 25.9 | -.76 |
| -4 | 3 | 2 | 26.9 | 28.1 | 4.80 |
| 5 | 3 | 2 | 33.3 | 33.3 | .04 |
| -5 | 3 | 2 | 34.4 | 35.6 | 3.76 |
| 6 | 3 | 2 | 41.8 | 41.3 | -1.08 |
| -6 | 3 | 2 | 43.1 | 44.0 | 2.13 |
| 7 | 3 | 2 | 50.9 | 50.5 | -.68 |
| -8 | 3 | 2 | 65.2 | 66.6 | 2.28 |
| 1 | 3 | -2 | 10.3 | 10.2 | -.57 |
| -1 | 3 | -2 | 8.5 | 8.8 | 4.53 |
| 2 | 3 | -2 | 16.0 | 15.7 | -1.83 |
| -2 | 3 | -2 | 13.4 | 13.9 | 3.79 |
| 3 | 3 | -2 | 22.1 | 21.9 | -.51 |
| -3 | 3 | -2 | 19.1 | 19.9 | 4.67 |
| 4 | 3 | -2 | 29.0 | 28.8 | -.65 |
| -4 | 3 | -2 | 26.2 | 26.6 | 1.72 |
| -5 | 3 | -2 | 33.2 | 33.8 | 2.04 |
| 8 | 3 | -2 | 67.2 | 67.4 | .31 |
| 1 | 3 | 3 | 8.0 | 8.1 | 1.96 |
| 2 | 3 | 3 | 13.2 | 13.1 | -.03 |
| 3 | 3 | 3 | 19.5 | 19.3 | -1.00 |
| 4 | 3 | 3 | 26.1 | 25.9 | -.52 |
| -4 | 3 | 3 | 28.0 | 29.2 | 4.32 |
| 5 | 3 | 3 | 33.3 | 33.1 | -.41 |
| -5 | 3 | 3 | 35.5 | 36.7 | 3.42 |
| 6 | 3 | 3 | 41.3 | 41.0 | -.50 |
| -6 | 3 | 3 | 44.2 | 45.1 | 2.04 |
| 7 | 3 | 3 | 50.2 | 50.1 | -.03 |
| 1 | 3 | -3 | 12.4 | 12.2 | -.87 |
| -1 | 3 | -3 | 10.4 | 10.5 | 1.70 |

| h | k | l | $x_o$ | $x_c$ | error% |
|---|---|---|---|---|---|
| 2 | 3 | -3 | 17.7 | 17.3 | -1.97 |
| -2 | 3 | -3 | 14.5 | 14.8 | 2.40 |
| 3 | 3 | -3 | 23.8 | 23.4 | -1.67 |
| -3 | 3 | -3 | 19.9 | 20.5 | 3.10 |
| 4 | 3 | -3 | 30.1 | 30.1 | .05 |
| -4 | 3 | -3 | 26.7 | 26.9 | .89 |
| 5 | 3 | -3 | 37.8 | 37.5 | -.73 |
| -5 | 3 | -3 | 33.4 | 34.0 | 1.81 |
| -6 | 3 | -3 | 41.0 | 41.8 | 2.13 |
| 2 | 3 | 4 | 14.2 | 14.0 | -.74 |
| 3 | 3 | 4 | 20.0 | 19.7 | -1.09 |
| 4 | 3 | 4 | 26.5 | 26.2 | -1.11 |
| -4 | 3 | 4 | 29.2 | 30.4 | 4.31 |
| -5 | 3 | 4 | 36.6 | 37.9 | 3.68 |
| -7 | 3 | 4 | 55.1 | 56.5 | 2.61 |
| -8 | 3 | 4 | 68.0 | 70.8 | 4.24 |
| 1 | 3 | -4 | 14.7 | 14.5 | -1.23 |
| -1 | 3 | -4 | 12.5 | 12.5 | .53 |
| 2 | 3 | -4 | 19.6 | 19.2 | -1.92 |
| -2 | 3 | -4 | 15.9 | 16.1 | 1.57 |
| 3 | 3 | -4 | 25.2 | 25.0 | -.63 |
| -3 | 3 | -4 | 21.0 | 21.3 | 1.69 |
| -4 | 3 | -4 | 27.1 | 27.4 | 1.43 |
| 5 | 3 | -4 | 39.1 | 39.0 | -.22 |
| -5 | 3 | -4 | 33.8 | 34.3 | 1.68 |
| 6 | 3 | -4 | 47.7 | 47.4 | -.54 |
| -6 | 3 | -4 | 41.2 | 42.1 | 2.19 |
| 7 | 3 | -4 | 57.9 | 57.6 | -.38 |
| -7 | 3 | -4 | 50.0 | 51.0 | 2.18 |
| -8 | 3 | -4 | 60.9 | 62.4 | 2.62 |
| 2 | 3 | 5 | 15.4 | 15.3 | -.17 |
| 3 | 3 | 5 | 20.8 | 20.5 | -1.04 |
| 4 | 3 | 5 | 27.0 | 26.7 | -1.05 |
| -4 | 3 | 5 | 30.6 | 31.9 | 4.32 |
| -5 | 3 | 5 | 38.0 | 39.3 | 3.65 |
| 6 | 3 | 5 | 41.3 | 41.2 | -.12 |
| -7 | 3 | 5 | 56.9 | 58.3 | 2.52 |
| -8 | 3 | 5 | 71.5 | 73.9 | 3.36 |
| 1 | 3 | -5 | 17.0 | 16.8 | -.79 |
| -1 | 3 | -5 | 14.8 | 14.7 | -.36 |
| 2 | 3 | -5 | 21.6 | 21.2 | -1.50 |
| -2 | 3 | -5 | 17.7 | 17.7 | .25 |
| 3 | 3 | -5 | 27.0 | 26.8 | -.46 |
| -3 | 3 | -5 | 22.2 | 22.4 | 1.25 |
| 4 | 3 | -5 | 33.8 | 33.3 | -1.33 |
| -4 | 3 | -5 | 28.0 | 28.2 | 1.05 |
| 5 | 3 | -5 | 41.0 | 40.7 | -.72 |
| -5 | 3 | -5 | 34.7 | 34.9 | .75 |
| 6 | 3 | -5 | 49.5 | 49.2 | -.54 |
| -6 | 3 | -5 | 41.3 | 42.5 | 3.02 |
| -7 | 3 | -5 | 50.7 | 51.4 | 1.44 |
| 2 | 3 | 6 | 16.8 | 16.9 | .94 |
| 3 | 3 | 6 | 21.9 | 21.6 | -1.01 |
| 4 | 3 | 6 | 27.8 | 27.4 | -1.13 |
| -4 | 3 | 6 | 32.1 | 33.5 | 4.63 |
| -5 | 3 | 6 | 39.8 | 41.0 | 3.11 |
| 6 | 3 | 6 | 41.9 | 41.6 | -.58 |
| -7 | 3 | 6 | 59.2 | 60.4 | 2.10 |
| -8 | 3 | 6 | 75.1 | 78.0 | 3.96 |
| 1 | 3 | -6 | 19.7 | 19.3 | -2.00 |
| -1 | 3 | -6 | 17.0 | 17.0 | .33 |
| 2 | 3 | -6 | 23.7 | 23.4 | -.93 |
| -2 | 3 | -6 | 19.4 | 19.5 | .88 |
| 3 | 3 | -6 | 29.1 | 28.8 | -.73 |
| -3 | 3 | -6 | 23.7 | 23.8 | .65 |
| 4 | 3 | -6 | 35.6 | 35.2 | -.97 |
| -4 | 3 | -6 | 29.0 | 29.3 | 1.18 |
| 5 | 3 | -6 | 42.9 | 42.6 | -.69 |
| 7 | 3 | -6 | 62.5 | 62.2 | -.33 |
| -7 | 3 | -6 | 51.1 | 52.0 | 1.76 |
| 1 | 3 | 7 | 15.7 | 16.3 | 4.28 |
| 2 | 3 | 7 | 18.3 | 18.7 | 2.64 |
| 3 | 3 | 7 | 23.1 | 23.0 | -.28 |
| -3 | 3 | 7 | 27.8 | 28.9 | 4.19 |
| 4 | 3 | 7 | 28.5 | 28.5 | .01 |
| -4 | 3 | 7 | 34.0 | 35.4 | 4.24 |
| 5 | 3 | 7 | 34.9 | 34.9 | .03 |
| -5 | 3 | 7 | 41.4 | 42.8 | 3.60 |
| -6 | 3 | 7 | 49.9 | 51.6 | 3.55 |
| 1 | 3 | -7 | 22.0 | 21.8 | -.78 |
| -1 | 3 | -7 | 19.3 | 19.4 | .88 |
| 2 | 3 | -7 | 26.0 | 25.8 | -.71 |
| -2 | 3 | -7 | 21.5 | 21.5 | .39 |
| 3 | 3 | -7 | 31.3 | 31.0 | -.77 |
| -3 | 3 | -7 | 25.3 | 25.4 | .61 |
| 4 | 3 | -7 | 37.8 | 37.3 | -1.21 |

| h | k | l | $x_o$ | $x_c$ | error% | h | k | l | $x_o$ | $x_c$ | error% |
|---|---|---|---|---|---|---|---|---|---|---|---|
| -4 | 3 | -7 | 30.3 | 30.6 | 1.04 | 1 | 3 | -10 | 29.9 | 29.8 | -.13 |
| 5 | 3 | -7 | 45.0 | 44.7 | -.65 | -1 | 3 | -10 | 27.2 | 27.2 | .04 |
| 6 | 3 | -7 | 53.8 | 53.5 | -.46 | 2 | 3 | -10 | 33.7 | 33.5 | -.51 |
| -7 | 3 | -7 | 52.1 | 52.7 | 1.33 | -2 | 3 | -10 | 28.5 | 28.4 | -.03 |
| -8 | 3 | -7 | 62.8 | 64.1 | 2.14 | 3 | 3 | -10 | 38.7 | 38.4 | -.52 |
| 1 | 3 | 8 | 18.0 | 18.7 | 4.41 | -3 | 3 | -10 | 31.1 | 31.3 | .90 |
| -1 | 3 | 8 | 20.6 | 21.5 | 4.56 | -4 | 3 | -10 | 35.2 | 35.6 | 1.32 |
| -2 | 3 | 8 | 24.5 | 25.7 | 4.91 | 5 | 3 | -10 | 52.6 | 52.4 | -.37 |
| -4 | 3 | 8 | 36.2 | 37.4 | 3.54 | -5 | 3 | -10 | 40.9 | 41.2 | .74 |
| 5 | 3 | 8 | 36.1 | 35.9 | -.50 | 6 | 3 | -10 | 62.7 | 62.4 | -.43 |
| -5 | 3 | 8 | 43.5 | 44.9 | 3.34 | -6 | 3 | -10 | 47.6 | 48.0 | .94 |
| -6 | 3 | 8 | 52.3 | 53.9 | 3.11 | -7 | 3 | -10 | 55.3 | 56.6 | 2.41 |
| 1 | 3 | -8 | 24.5 | 24.4 | -.30 | -8 | 3 | -10 | 67.5 | 68.6 | 1.66 |
| -1 | 3 | -8 | 22.0 | 21.9 | -.13 | 1 | 3 | 11 | 25.9 | 26.5 | 2.47 |
| 2 | 3 | -8 | 28.5 | 28.2 | -.81 | -1 | 3 | 11 | 28.4 | 29.4 | 3.83 |
| -2 | 3 | -8 | 23.8 | 23.7 | -.19 | 2 | 3 | 11 | 27.1 | 27.7 | 2.23 |
| -3 | 3 | -8 | 27.0 | 27.2 | .95 | -3 | 3 | 11 | 37.0 | 38.3 | 3.77 |
| 4 | 3 | -8 | 40.0 | 39.6 | -.97 | -4 | 3 | 11 | 43.5 | 44.7 | 2.82 |
| -5 | 3 | -8 | 37.7 | 38.0 | .99 | -6 | 3 | 11 | 60.4 | 62.7 | 3.83 |
| 6 | 3 | -8 | 56.2 | 56.1 | -.11 | -1 | 3 | -11 | 30.0 | 29.9 | -.13 |
| -8 | 3 | -8 | 64.2 | 65.2 | 1.68 | 2 | 3 | -11 | 36.6 | 36.3 | -.70 |
| 1 | 3 | 9 | 20.5 | 21.3 | 3.90 | -2 | 3 | -11 | 31.0 | 31.0 | .12 |
| -1 | 3 | 9 | 23.1 | 24.1 | 4.36 | 3 | 3 | -11 | 41.5 | 41.2 | -.49 |
| 2 | 3 | 9 | 22.4 | 22.9 | 2.54 | -3 | 3 | -11 | 32.9 | 33.6 | 2.37 |
| -2 | 3 | 9 | 27.0 | 28.1 | 4.13 | -4 | 3 | -11 | 37.5 | 37.7 | .60 |
| -3 | 3 | 9 | 32.0 | 33.3 | 4.27 | -5 | 3 | -11 | 42.9 | 43.0 | .41 |
| -6 | 3 | 9 | 54.9 | 56.4 | 2.87 | 6 | 3 | -11 | 66.3 | 66.3 | .13 |
| 1 | 3 | -9 | 27.2 | 27.1 | -.36 | -6 | 3 | -11 | 49.5 | 49.8 | .64 |
| -1 | 3 | -9 | 24.6 | 24.5 | -.20 | -7 | 3 | -11 | 57.7 | 58.4 | 1.29 |
| 2 | 3 | -9 | 31.0 | 30.8 | -.52 | 1 | 3 | 12 | 28.5 | 29.2 | 2.74 |
| -2 | 3 | -9 | 26.1 | 26.0 | -.15 | 2 | 3 | 12 | 29.6 | 30.2 | 2.19 |
| -3 | 3 | -9 | 29.0 | 29.2 | .81 | -2 | 3 | 12 | 34.9 | 36.0 | 3.38 |
| 4 | 3 | -9 | 42.2 | 42.0 | -.32 | -3 | 3 | 12 | 39.9 | 41.1 | 3.14 |
| -4 | 3 | -9 | 33.7 | 33.7 | .26 | 2 | 3 | -12 | 39.5 | 39.2 | -.52 |
| -5 | 3 | -9 | 39.1 | 39.5 | 1.11 | -2 | 3 | -12 | 33.7 | 33.7 | .03 |
| -6 | 3 | -9 | 45.6 | 46.5 | 1.99 | 3 | 3 | -12 | 44.3 | 44.2 | -.05 |
| -8 | 3 | -9 | 65.8 | 66.7 | 1.45 | -3 | 3 | -12 | 35.0 | 36.1 | 3.24 |
| 1 | 3 | 10 | 23.1 | 23.8 | 3.38 | -4 | 3 | -12 | 39.8 | 39.9 | .43 |
| -1 | 3 | 10 | 25.8 | 26.7 | 3.70 | -5 | 3 | -12 | 45.0 | 45.1 | .35 |
| 2 | 3 | 10 | 24.8 | 25.2 | 1.92 | 6 | 3 | -12 | 71.2 | 71.3 | .14 |
| -2 | 3 | 10 | 29.9 | 30.6 | 2.50 | -7 | 3 | -12 | 59.9 | 60.5 | 1.12 |
| -3 | 3 | 10 | 34.5 | 35.8 | 3.77 | -2 | 3 | 13 | 37.9 | 38.9 | 2.89 |
| -4 | 3 | 10 | 41.0 | 42.1 | 2.73 | -3 | 3 | 13 | 43.0 | 44.0 | 2.54 |

| h | k | l | $x_o$ | $x_c$ | error% |
|---|---|---|---|---|---|
| 2 | 3 | -13 | 42.5 | 42.4 | -.22 |
| -2 | 3 | -13 | 36.3 | 36.5 | .57 |
| 3 | 3 | -13 | 47.8 | 47.4 | -.69 |
| -3 | 3 | -13 | 38.7 | 38.7 | .12 |
| -4 | 3 | -13 | 42.2 | 42.4 | .48 |
| -5 | 3 | -13 | 48.5 | 47.4 | -2.13 |
| -6 | 3 | -13 | 53.8 | 54.1 | .57 |
| -7 | 3 | -13 | 62.2 | 63.0 | 1.40 |
| -8 | 3 | -13 | 76.6 | 78.2 | 2.18 |
| 2 | 3 | 14 | 35.2 | 35.6 | 1.41 |
| -5 | 3 | 14 | 60.9 | 63.0 | 3.57 |
| 2 | 3 | -14 | 45.9 | 45.7 | -.42 |
| -2 | 3 | -14 | 39.2 | 39.4 | .63 |
| 3 | 3 | -14 | 51.1 | 50.9 | -.37 |
| -3 | 3 | -14 | 41.7 | 41.5 | -.40 |
| 5 | 3 | -14 | 67.9 | 67.8 | -.02 |
| -5 | 3 | -14 | 48.4 | 50.0 | 3.31 |
| -6 | 3 | -14 | 56.2 | 56.6 | .86 |
| 1 | 3 | 15 | 37.2 | 38.1 | 2.42 |
| 2 | 3 | 15 | 37.9 | 38.6 | 1.89 |
| 1 | 3 | -15 | 45.6 | 45.3 | -.46 |
| -2 | 3 | -15 | 42.6 | 42.5 | -.11 |
| 3 | 3 | -15 | 55.0 | 54.6 | -.58 |
| -3 | 3 | -15 | 44.2 | 44.4 | .67 |
| 4 | 3 | -15 | 62.2 | 62.2 | .05 |
| 5 | 3 | -15 | 74.0 | 74.1 | .20 |
| -5 | 3 | -15 | 52.5 | 52.8 | .59 |
| -1 | 3 | 16 | 43.9 | 44.8 | 2.19 |
| -2 | 3 | 16 | 47.8 | 48.8 | 2.12 |
| 1 | 3 | -16 | 49.1 | 49.0 | -.16 |
| -1 | 3 | -16 | 45.2 | 45.4 | .56 |
| -2 | 3 | -16 | 45.7 | 45.8 | .31 |
| -3 | 3 | -16 | 47.7 | 47.6 | -.04 |
| 4 | 3 | -16 | 67.6 | 67.3 | -.33 |
| -6 | 3 | -16 | 62.2 | 62.9 | 1.27 |
| -7 | 3 | -16 | 73.0 | 74.2 | 1.74 |
| 1 | 3 | 17 | 43.9 | 44.6 | 1.74 |
| 1 | 3 | -17 | 53.0 | 52.9 | -.09 |
| -1 | 3 | -17 | 49.1 | 49.0 | -.03 |
| -3 | 3 | -17 | 51.0 | 51.0 | .22 |
| 4 | 3 | -17 | 74.0 | 74.0 | .11 |
| -6 | 3 | -17 | 66.2 | 66.9 | 1.19 |
| 1 | 3 | -18 | 57.4 | 57.2 | -.21 |
| -1 | 3 | -18 | 52.9 | 53.0 | .20 |
| 2 | 3 | -18 | 62.0 | 62.0 | .09 |
| -3 | 3 | -18 | 54.9 | 54.8 | -.04 |
| -6 | 3 | -18 | 71.0 | 71.9 | 1.40 |
| 1 | 3 | -19 | 62.1 | 62.1 | .14 |
| -1 | 3 | -19 | 57.5 | 57.3 | -.28 |
| 2 | 3 | -19 | 67.7 | 67.7 | .11 |
| -2 | 3 | -19 | 56.0 | 57.3 | 2.49 |
| -4 | 3 | -19 | 62.1 | 62.5 | .68 |
| -5 | 3 | -19 | 67.8 | 68.3 | .79 |
| 1 | 3 | -20 | 67.9 | 68.0 | .28 |
| -1 | 3 | -20 | 62.1 | 62.2 | .24 |
| -2 | 3 | -20 | 61.9 | 62.1 | .45 |
| -4 | 3 | -20 | 67.5 | 67.6 | .28 |
| -5 | 3 | -20 | 74.0 | 74.7 | .97 |
| 1 | 3 | -21 | 75.9 | 76.1 | .37 |
| -1 | 3 | -21 | 68.0 | 68.1 | .23 |
| -2 | 3 | -21 | 67.8 | 67.9 | .71 |
| -4 | 3 | -21 | 74.0 | 74.4 | .65 |
| -1 | 3 | -22 | 76.0 | 76.2 | .36 |
| 2 | 4 | | 14.1 | 13.8 | -1.89 |
| 3 | 4 | | 21.0 | 20.6 | -1.89 |
| 4 | 4 | | 28.2 | 27.7 | -1.51 |
| 5 | 4 | | 35.9 | 35.4 | -1.13 |
| -5 | 4 | | 34.1 | 35.4 | 4.08 |
| 6 | 4 | | 44.4 | 44.0 | -.74 |
| -6 | 4 | | 43.1 | 44.0 | 2.24 |
| 7 | 4 | | 54.4 | 54.1 | -.45 |
| 1 | 4 | 1 | 6.8 | 6.7 | -.26 |
| 2 | 4 | 1 | 13.5 | 13.1 | -2.47 |
| 3 | 4 | 1 | 20.2 | 19.9 | -1.20 |
| -3 | 4 | 1 | 20.3 | 21.0 | 3.60 |
| 4 | 4 | 1 | 27.4 | 27.1 | -1.03 |
| -4 | 4 | 1 | 27.5 | 28.2 | 2.75 |
| 5 | 4 | 1 | 35.2 | 34.7 | -1.14 |
| -5 | 4 | 1 | 35.1 | 36.0 | 2.68 |
| 6 | 4 | 1 | 43.8 | 43.2 | -1.15 |
| -6 | 4 | 1 | 43.8 | 44.7 | 2.06 |
| 7 | 4 | 1 | 53.7 | 53.2 | -.89 |
| -8 | 4 | 1 | 66.8 | 69.0 | 3.37 |
| 1 | 4 | -1 | 9.3 | 8.9 | -3.32 |
| 2 | 4 | -1 | 15.3 | 14.9 | -2.35 |
| 4 | 4 | -1 | 29.0 | 28.6 | -1.05 |

| h | k | l | $x_o$ | $x_c$ | error% |
|---|---|---|---|---|---|
| -4 | 4 | -1 | 27.0 | 27.5 | 2.08 |
| 5 | 4 | -1 | 36.9 | 36.4 | -1.28 |
| -5 | 4 | -1 | 34.5 | 35.1 | 1.98 |
| -6 | 4 | -1 | 42.9 | 43.6 | 1.77 |
| 7 | 4 | -1 | 55.8 | 55.3 | -.82 |
| -8 | 4 | -1 | 64.8 | 66.8 | 3.20 |
| 1 | 4 | 2 | 7.1 | 6.9 | -1.76 |
| 2 | 4 | 2 | 13.2 | 13.0 | -1.48 |
| 4 | 4 | 2 | 27.1 | 26.7 | -1.34 |
| -4 | 4 | 2 | 28.1 | 29.0 | 3.24 |
| -6 | 4 | 2 | 44.7 | 45.5 | 1.95 |
| 7 | 4 | 2 | 52.9 | 52.5 | -.69 |
| -8 | 4 | 2 | 68.7 | 70.7 | 3.00 |
|  | 4 | -2 | 7.8 | 7.7 | -.40 |
| 1 | 4 | -2 | 11.1 | 10.8 | -1.87 |
| -1 | 4 | -2 | 9.1 | 9.5 | 4.89 |
| 2 | 4 | -2 | 16.9 | 16.4 | -2.90 |
| -2 | 4 | -2 | 14.0 | 14.5 | 4.15 |
| 3 | 4 | -2 | 23.2 | 22.8 | -1.59 |
| -3 | 4 | -2 | 20.2 | 20.7 | 2.90 |
| 4 | 4 | -2 | 30.1 | 29.8 | -.78 |
| -4 | 4 | -2 | 27.1 | 27.6 | 1.97 |
| -5 | 4 | -2 | 34.6 | 35.1 | 1.51 |
| 6 | 4 | -2 | 46.7 | 46.3 | -.84 |
| -6 | 4 | -2 | 42.5 | 43.4 | 2.31 |
| -7 | 4 | -2 | 52.2 | 53.2 | 2.09 |
| 1 | 4 | 3 | 7.9 | 8.0 | 1.80 |
| 2 | 4 | 3 | 13.6 | 13.3 | -1.74 |
| 4 | 4 | 3 | 27.0 | 26.6 | -1.32 |
| 5 | 4 | 3 | 34.6 | 34.1 | -1.34 |
| -5 | 4 | 3 | 36.8 | 37.8 | 2.83 |
| 6 | 4 | 3 | 42.9 | 42.4 | -1.07 |
| -6 | 4 | 3 | 45.7 | 46.6 | 2.13 |
| -7 | 4 | 3 | 56.0 | 57.3 | 2.37 |
| -8 | 4 | 3 | 70.8 | 73.0 | 3.13 |
|  | 4 | -3 | 10.3 | 10.2 | -.70 |
| 1 | 4 | -3 | 13.6 | 13.0 | -4.02 |
| -1 | 4 | -3 | 11.0 | 11.3 | 3.14 |
| 2 | 4 | -3 | 18.8 | 18.1 | -3.39 |
| -2 | 4 | -3 | 15.2 | 15.6 | 2.79 |
| 3 | 4 | -3 | 24.8 | 24.3 | -1.82 |
| -3 | 4 | -3 | 21.0 | 21.3 | 1.86 |
| 4 | 4 | -3 | 31.7 | 31.2 | -1.35 |
| -4 | 4 | -3 | 27.6 | 27.9 | 1.39 |
| 5 | 4 | -3 | 39.3 | 38.9 | -.83 |
| 6 | 4 | -3 | 48.0 | 47.7 | -.47 |
| -6 | 4 | -3 | 42.7 | 43.5 | 1.96 |
| 2 | 4 | 4 | 14.3 | 14.2 | -.66 |
| 3 | 4 | 4 | 20.2 | 20.1 | -.24 |
| -4 | 4 | 4 | 30.1 | 31.2 | 3.87 |
| 5 | 4 | 4 | 34.5 | 34.1 | -.94 |
| -5 | 4 | 4 | 38.2 | 39.0 | 2.32 |
| 6 | 4 | 4 | 42.8 | 42.3 | -1.03 |
| -6 | 4 | 4 | 47.0 | 48.0 | 2.14 |
| -7 | 4 | 4 | 57.5 | 58.9 | 2.51 |
| -8 | 4 | 4 | 73.2 | 76.0 | 3.92 |
|  | 4 | -4 | 13.0 | 12.7 | -1.81 |
| 1 | 4 | -4 | 15.8 | 15.3 | -2.65 |
| -1 | 4 | -4 | 13.3 | 13.4 | .97 |
| -2 | 4 | -4 | 16.8 | 17.0 | 1.33 |
| 3 | 4 | -4 | 26.6 | 26.0 | -1.92 |
| -3 | 4 | -4 | 22.0 | 22.3 | 1.43 |
| 4 | 4 | -4 | 34.2 | 32.8 | -3.82 |
| -4 | 4 | -4 | 28.2 | 28.6 | 1.44 |
| 5 | 4 | -4 | 41.0 | 40.5 | -1.03 |
| -5 | 4 | -4 | 35.0 | 35.7 | 2.09 |
| 6 | 4 | -4 | 49.8 | 49.4 | -.63 |
| -7 | 4 | -4 | 52.2 | 53.4 | 2.30 |
| 2 | 4 | 5 | 15.2 | 15.4 | 1.70 |
| 3 | 4 | 5 | 21.2 | 20.9 | -1.34 |
| 4 | 4 | 5 | 27.5 | 27.3 | -.69 |
| -4 | 4 | 5 | 31.4 | 32.7 | 4.27 |
| 5 | 4 | 5 | 34.8 | 34.4 | -.96 |
| -5 | 4 | 5 | 39.6 | 40.5 | 2.41 |
| 6 | 4 | 5 | 42.9 | 42.5 | -.91 |
| -6 | 4 | 5 | 48.6 | 49.5 | 2.02 |
| -7 | 4 | 5 | 59.2 | 60.8 | 2.83 |
| -8 | 4 | 5 | 77.0 | 80.6 | 4.68 |
|  | 4 | -5 | 15.7 | 15.3 | -2.19 |
| 1 | 4 | -5 | 18.1 | 17.8 | -1.51 |
| -1 | 4 | -5 | 15.7 | 15.6 | -.01 |
| 2 | 4 | -5 | 22.8 | 22.2 | -2.20 |
| -2 | 4 | -5 | 18.7 | 18.7 | .60 |
| -3 | 4 | -5 | 23.1 | 23.5 | 1.84 |
| -4 | 4 | -5 | 29.0 | 29.4 | 1.70 |
| 5 | 4 | -5 | 42.9 | 42.3 | -1.17 |

| h | k | l | $x_o$ | $x_c$ | error% |
|---|---|---|---|---|---|
| -5 | 4 | -5 | 36.0 | 36.3 | 1.10 |
| 6 | 4 | -5 | 51.8 | 51.4 | -.68 |
| -6 | 4 | -5 | 43.7 | 44.3 | 1.46 |
| -7 | 4 | -5 | 53.0 | 53.8 | 1.54 |
| -8 | 4 | -5 | 65.0 | 66.5 | 2.33 |
| 2 | 4 | 6 | 16.7 | 17.0 | 2.05 |
| 4 | 4 | 6 | 28.2 | 28.0 | -.50 |
| -4 | 4 | 6 | 33.1 | 34.4 | 4.02 |
| 5 | 4 | 6 | 35.2 | 34.9 | -.58 |
| -5 | 4 | 6 | 41.2 | 42.2 | 2.53 |
| -7 | 4 | 6 | 61.5 | 63.1 | 2.73 |
| | 4 | -6 | 18.2 | 17.9 | -1.11 |
| 1 | 4 | -6 | 20.9 | 20.3 | -2.56 |
| -1 | 4 | -6 | 18.1 | 18.0 | -.02 |
| -2 | 4 | -6 | 20.7 | 20.6 | -.32 |
| -3 | 4 | -6 | 24.8 | 24.9 | .77 |
| 4 | 4 | -6 | 37.1 | 36.7 | -.94 |
| -4 | 4 | -6 | 30.1 | 30.6 | 1.74 |
| 5 | 4 | -6 | 44.9 | 44.4 | -1.02 |
| -5 | 4 | -6 | 36.8 | 37.2 | 1.35 |
| 6 | 4 | -6 | 53.7 | 53.6 | -.03 |
| -6 | 4 | -6 | 44.3 | 45.0 | 1.77 |
| 7 | 4 | -6 | 66.5 | 66.0 | -.72 |
| -7 | 4 | -6 | 53.8 | 54.4 | 1.26 |
| -8 | 4 | -6 | 65.8 | 67.2 | 2.16 |
| 1 | 4 | 7 | 15.7 | 16.3 | 4.07 |
| 2 | 4 | 7 | 18.3 | 18.8 | 3.20 |
| -4 | 4 | 7 | 35.0 | 36.3 | 3.78 |
| | 4 | -7 | 20.9 | 20.6 | -1.00 |
| 1 | 4 | -7 | 23.3 | 22.9 | -1.34 |
| -1 | 4 | -7 | 20.8 | 20.6 | -.96 |
| 2 | 4 | -7 | 27.5 | 27.0 | -1.62 |
| -2 | 4 | -7 | 22.8 | 22.7 | -.26 |
| 3 | 4 | -7 | 32.9 | 32.4 | -1.37 |
| -3 | 4 | -7 | 26.5 | 26.6 | .70 |
| 4 | 4 | -7 | 39.2 | 38.9 | -.58 |
| -4 | 4 | -7 | 31.7 | 31.9 | .91 |
| 5 | 4 | -7 | 47.1 | 46.7 | -.82 |
| 7 | 4 | -7 | 70.0 | 69.5 | -.57 |
| -7 | 4 | -7 | 54.6 | 55.3 | 1.45 |
| -8 | 4 | -7 | 66.8 | 68.2 | 2.22 |
| 1 | 4 | 8 | 18.0 | 18.8 | 4.57 |
| 2 | 4 | 8 | 20.3 | 20.9 | 3.13 |
| 3 | 4 | 8 | 24.7 | 24.9 | 1.01 |
| -4 | 4 | 8 | 36.9 | 38.4 | 4.10 |
| -5 | 4 | 8 | 44.9 | 46.2 | 3.09 |
| -6 | 4 | 8 | 54.6 | 55.8 | 2.36 |
| | 4 | -8 | 23.8 | 23.4 | -1.52 |
| -1 | 4 | -8 | 23.3 | 23.1 | -.44 |
| 2 | 4 | -8 | 30.0 | 29.6 | -1.25 |
| -2 | 4 | -8 | 25.1 | 25.0 | -.36 |
| 3 | 4 | -8 | 35.2 | 34.9 | -.84 |
| -3 | 4 | -8 | 28.4 | 28.5 | .65 |
| 4 | 4 | -8 | 41.8 | 41.3 | -.98 |
| -4 | 4 | -8 | 33.1 | 33.5 | 1.43 |
| -5 | 4 | -8 | 39.2 | 39.7 | 1.48 |
| -6 | 4 | -8 | 46.8 | 47.2 | 1.01 |
| 7 | 4 | -8 | 74.8 | 74.2 | -.74 |
| -7 | 4 | -8 | 56.0 | 56.5 | 1.02 |
| -8 | 4 | -8 | 68.1 | 69.7 | 2.40 |
| | 4 | 9 | 20.9 | 21.8 | 4.43 |
| 1 | 4 | 9 | 20.4 | 21.3 | 4.88 |
| 2 | 4 | 9 | 22.7 | 23.1 | 2.00 |
| 3 | 4 | 9 | 26.3 | 26.7 | 1.77 |
| -3 | 4 | 9 | 32.8 | 34.0 | 3.82 |
| -4 | 4 | 9 | 39.1 | 40.7 | 4.10 |
| -5 | 4 | 9 | 47.8 | 48.6 | 1.80 |
| -6 | 4 | 9 | 57.1 | 58.6 | 2.66 |
| | 4 | -9 | 26.5 | 26.2 | -.94 |
| 1 | 4 | -9 | 28.9 | 28.4 | -1.44 |
| -1 | 4 | -9 | 26.0 | 25.8 | -.46 |
| 2 | 4 | -9 | 32.8 | 32.3 | -1.46 |
| -2 | 4 | -9 | 27.7 | 27.4 | -1.02 |
| 4 | 4 | -9 | 44.2 | 44.0 | -.42 |
| -5 | 4 | -9 | 41.0 | 41.3 | .87 |
| 6 | 4 | -9 | 62.9 | 62.4 | -.69 |
| -6 | 4 | -9 | 48.3 | 48.7 | .87 |
| -7 | 4 | -9 | 56.8 | 58.0 | 2.15 |
| -8 | 4 | -9 | 69.3 | 71.6 | 3.41 |
| | 4 | 10 | 23.6 | 24.6 | 4.23 |
| 1 | 4 | 10 | 23.1 | 24.0 | 4.12 |
| -1 | 4 | 10 | 25.9 | 27.0 | 4.52 |
| 2 | 4 | 10 | 25.0 | 25.5 | 2.07 |
| 3 | 4 | 10 | 28.2 | 28.7 | 2.04 |
| -3 | 4 | 10 | 35.1 | 36.5 | 4.15 |
| -4 | 4 | 10 | 41.2 | 43.2 | 4.85 |

| h | k | l | $x_o$ | $x_c$ | error% |
|---|---|---|---|---|---|
| -5 | 4 | 10 | 50.3 | 51.3 | 1.99 |
| -6 | 4 | 10 | 60.1 | 61.7 | 2.77 |
| | 4 | -10 | 29.3 | 29.1 | -.55 |
| 1 | 4 | -10 | 31.8 | 31.3 | -1.36 |
| -1 | 4 | -10 | 28.8 | 28.6 | -.51 |
| 2 | 4 | -10 | 35.4 | 35.1 | -.71 |
| -2 | 4 | -10 | 29.9 | 29.9 | .19 |
| 3 | 4 | -10 | 40.8 | 40.3 | -1.19 |
| -3 | 4 | -10 | 32.8 | 32.9 | .39 |
| 4 | 4 | -10 | 47.2 | 46.8 | -.72 |
| -4 | 4 | -10 | 37.0 | 37.3 | .98 |
| -5 | 4 | -10 | 42.8 | 43.1 | .82 |
| -6 | 4 | -10 | 50.0 | 50.4 | .82 |
| | 4 | 11 | 26.4 | 27.4 | 3.94 |
| 1 | 4 | 11 | 26.0 | 26.7 | 3.04 |
| -1 | 4 | 11 | 28.7 | 29.8 | 4.13 |
| -3 | 4 | 11 | 37.8 | 39.2 | 3.79 |
| -6 | 4 | 11 | 63.7 | 65.4 | 2.77 |
| | 4 | -11 | 32.5 | 32.1 | -1.19 |
| 1 | 4 | -11 | 34.7 | 34.3 | -.99 |
| -1 | 4 | -11 | 31.8 | 31.5 | -.88 |
| 2 | 4 | -11 | 38.3 | 38.1 | -.48 |
| -2 | 4 | -11 | 32.8 | 32.6 | -.51 |
| -3 | 4 | -11 | 35.2 | 35.3 | .44 |
| 4 | 4 | -11 | 50.3 | 49.9 | -.68 |
| -4 | 4 | -11 | 39.2 | 39.5 | .91 |
| -5 | 4 | -11 | 44.8 | 45.1 | .82 |
| 6 | 4 | -11 | 71.8 | 71.3 | -.62 |
| -6 | 4 | -11 | 51.9 | 52.3 | .88 |
| -7 | 4 | -11 | 60.7 | 61.8 | 1.93 |
| | 4 | 12 | 29.4 | 30.3 | 3.27 |
| 1 | 4 | 12 | 28.8 | 29.6 | 2.83 |
| -1 | 4 | 12 | 31.8 | 32.8 | 3.14 |
| 3 | 4 | 12 | 32.8 | 33.3 | 1.56 |
| | 4 | -12 | 35.2 | 35.1 | -.04 |
| 1 | 4 | -12 | 37.8 | 37.4 | -.88 |
| -1 | 4 | -12 | 34.6 | 34.4 | -.29 |
| 2 | 4 | -12 | 41.5 | 41.2 | -.62 |
| -2 | 4 | -12 | 35.5 | 35.4 | -.18 |
| -3 | 4 | -12 | 38.0 | 37.9 | -.13 |
| 4 | 4 | -12 | 53.7 | 53.3 | -.64 |
| -4 | 4 | -12 | 41.7 | 41.9 | .60 |
| -5 | 4 | -12 | 47.1 | 47.4 | .68 |
| 6 | 4 | -12 | 79.2 | 78.4 | -1.00 |
| -6 | 4 | -12 | 54.2 | 54.5 | .71 |
| | 4 | 13 | 32.2 | 33.3 | 3.65 |
| 1 | 4 | 13 | 31.8 | 32.5 | 2.32 |
| -2 | 4 | 13 | 38.5 | 39.7 | 3.31 |
| 3 | 4 | 13 | 35.2 | 35.8 | 1.78 |
| -4 | 4 | 13 | 50.3 | 52.0 | 3.57 |
| -5 | 4 | 13 | 59.7 | 61.2 | 2.66 |
| -1 | 4 | -13 | 37.8 | 37.5 | -.53 |
| 2 | 4 | -13 | 45.0 | 44.5 | -.99 |
| -2 | 4 | -13 | 38.5 | 38.3 | -.30 |
| -3 | 4 | -13 | 40.8 | 40.7 | -.20 |
| 4 | 4 | -13 | 57.4 | 57.1 | -.46 |
| -4 | 4 | -13 | 44.2 | 44.5 | .79 |
| 5 | 4 | -13 | 67.8 | 67.3 | -.61 |
| -7 | 4 | -13 | 66.4 | 67.3 | 1.47 |
| | 4 | 14 | 35.5 | 36.5 | 2.81 |
| 1 | 4 | 14 | 34.6 | 35.5 | 2.81 |
| -2 | 4 | 14 | 41.8 | 42.9 | 2.79 |
| 3 | 4 | 14 | 37.8 | 38.5 | 1.87 |
| | 4 | -14 | 42.0 | 41.7 | -.63 |
| 1 | 4 | -14 | 44.3 | 44.1 | -.33 |
| -2 | 4 | -14 | 41.6 | 41.4 | -.24 |
| 3 | 4 | -14 | 54.1 | 53.6 | -.77 |
| 4 | 4 | -14 | 61.9 | 61.4 | -.76 |
| -4 | 4 | -14 | 47.1 | 47.3 | .60 |
| 5 | 4 | -14 | 74.0 | 73.5 | -.59 |
| -7 | 4 | -14 | 70.0 | 71.1 | 1.60 |
| | 4 | 15 | 38.6 | 39.7 | 3.00 |
| 1 | 4 | 15 | 37.6 | 38.7 | 3.03 |
| -1 | 4 | 15 | 41.0 | 42.3 | 3.19 |
| 2 | 4 | 15 | 38.4 | 39.2 | 2.29 |
| -2 | 4 | 15 | 45.0 | 46.3 | 3.04 |
| -4 | 4 | 15 | 57.2 | 59.6 | 4.36 |
| | 4 | -15 | 45.3 | 45.2 | -.06 |
| 1 | 4 | -15 | 48.0 | 47.7 | -.41 |
| -1 | 4 | -15 | 44.2 | 44.2 | .15 |
| -2 | 4 | -15 | 44.9 | 44.7 | -.22 |
| 3 | 4 | -15 | 58.2 | 57.8 | -.58 |
| -4 | 4 | -15 | 50.2 | 50.4 | .54 |
| -6 | 4 | -15 | 63.0 | 63.4 | .68 |
| -7 | 4 | -15 | 74.9 | 76.1 | 1.63 |
| 1 | 4 | 16 | 41.1 | 42.0 | 2.33 |

| h | k | l | $x_o$ | $x_c$ | error% | h | k | l | $x_o$ | $x_c$ | error% |
|---|---|---|---|---|---|---|---|---|---|---|---|
| -1 | 4 | 16 | 44.7 | 45.8 | 2.51 | | 4 | 21 | 64.0 | 65.2 | 1.96 |
| 2 | 4 | 16 | 41.8 | 42.4 | 1.60 | 1 | 4 | 21 | 61.8 | 63.0 | 2.07 |
| -2 | 4 | 16 | 48.7 | 50.0 | 2.71 | | 4 | -21 | 78.4 | 78.2 | -.15 |
| | 4 | -16 | 49.1 | 49.0 | -.11 | -1 | 4 | -21 | 74.5 | 74.5 | .06 |
| 1 | 4 | -16 | 52.0 | 51.7 | -.51 | -2 | 4 | -21 | 74.0 | 74.2 | .27 |
| -1 | 4 | -16 | 48.0 | 47.9 | -.17 | | 4 | 22 | 70.8 | 72.3 | 2.20 |
| -2 | 4 | -16 | 47.8 | 48.3 | 1.10 | 2 | 5 | | 15.2 | 14.5 | -3.96 |
| -3 | 4 | -16 | 50.3 | 50.2 | -.01 | 3 | 5 | | 22.3 | 21.5 | -3.15 |
| -4 | 4 | -16 | 53.7 | 53.8 | .31 | 4 | 5 | | 29.8 | 29.0 | -2.41 |
| 1 | 4 | 17 | 44.8 | 45.5 | 1.72 | 5 | 5 | | 37.9 | 37.2 | -1.81 |
| 2 | 4 | 17 | 45.0 | 45.8 | 1.92 | -5 | 5 | | 36.1 | 37.2 | 3.08 |
| -2 | 4 | 17 | 52.3 | 54.0 | 3.25 | -7 | 5 | | 56.2 | 57.4 | 2.29 |
| | 4 | -17 | 53.1 | 53.1 | .04 | 2 | 5 | 1 | 14.3 | 13.8 | -3.45 |
| 1 | 4 | -17 | 55.8 | 56.0 | .44 | 3 | 5 | 1 | 21.7 | 20.8 | -3.90 |
| -1 | 4 | -17 | 51.8 | 51.8 | .09 | 5 | 5 | 1 | 37.0 | 36.4 | -1.55 |
| -2 | 4 | -17 | 52.0 | 52.1 | .29 | -5 | 5 | 1 | 36.2 | 37.7 | 4.26 |
| -3 | 4 | -17 | 53.8 | 54.0 | .46 | 6 | 5 | 1 | 46.0 | 45.4 | -1.09 |
| -4 | 4 | -17 | 57.4 | 57.6 | .44 | -7 | 5 | 1 | 57.0 | 58.3 | 2.35 |
| -6 | 4 | -17 | 71.8 | 72.6 | 1.11 | 1 | 5 | -1 | 10.2 | 9.8 | -3.83 |
| 1 | 4 | 18 | 47.9 | 49.3 | 2.97 | 2 | 5 | -1 | 16.4 | 15.8 | -3.47 |
| 2 | 4 | 18 | 48.7 | 49.5 | 1.65 | 4 | 5 | -1 | 30.8 | 30.1 | -2.26 |
| | 4 | -18 | 57.6 | 57.6 | .07 | -4 | 5 | -1 | 27.9 | 28.9 | 3.65 |
| -1 | 4 | -18 | 56.2 | 56.1 | -.05 | 5 | 5 | -1 | 38.8 | 38.2 | -1.41 |
| 2 | 4 | -18 | 66.5 | 66.4 | -.03 | 6 | 5 | -1 | 48.1 | 47.5 | -1.21 |
| -3 | 4 | -18 | 58.2 | 58.2 | .05 | -7 | 5 | -1 | 55.8 | 56.9 | 2.01 |
| -4 | 4 | -18 | 61.7 | 61.9 | .44 | 2 | 5 | 2 | 14.0 | 13.5 | -3.35 |
| -5 | 4 | -18 | 67.7 | 68.2 | .75 | 3 | 5 | 2 | 21.2 | 20.4 | -3.45 |
| -6 | 4 | -18 | 79.1 | 80.3 | 1.59 | 4 | 5 | 2 | 28.8 | 27.8 | -3.21 |
| | 4 | 19 | 52.8 | 54.9 | 4.06 | -5 | 5 | 2 | 36.8 | 38.5 | 4.69 |
| 2 | 4 | 19 | 52.2 | 53.4 | 2.41 | 6 | 5 | 2 | 45.4 | 44.8 | -1.18 |
| | 4 | -19 | 62.7 | 62.8 | .18 | -7 | 5 | 2 | 58.0 | 59.4 | 2.56 |
| 1 | 4 | -19 | 66.8 | 66.7 | -.14 | 1 | 5 | -2 | 12.2 | 11.8 | -2.99 |
| 2 | 4 | -19 | 73.8 | 73.8 | .05 | -1 | 5 | -2 | 10.0 | 10.4 | 4.99 |
| -2 | 4 | -19 | 60.9 | 61.1 | .35 | 2 | 5 | -2 | 18.2 | 17.4 | -4.26 |
| -4 | 4 | -19 | 66.6 | 67.1 | .76 | -2 | 5 | -2 | 15.0 | 15.5 | 3.73 |
| -5 | 4 | -19 | 73.9 | 74.6 | .97 | 3 | 5 | -2 | 24.8 | 24.0 | -3.03 |
| | 4 | 20 | 58.2 | 59.6 | 2.57 | -3 | 5 | -2 | 21.2 | 21.9 | 3.44 |
| -1 | 4 | 20 | 60.5 | 63.4 | 4.82 | 4 | 5 | -2 | 32.1 | 31.3 | -2.22 |
| | 4 | -20 | 69.0 | 69.1 | .17 | -4 | 5 | -2 | 28.2 | 29.0 | 3.02 |
| 1 | 4 | -20 | 74.3 | 74.3 | .08 | 5 | 5 | -2 | 40.1 | 39.5 | -1.40 |
| -1 | 4 | -20 | 66.9 | 66.8 | -.09 | -5 | 5 | -2 | 35.3 | 36.9 | 4.60 |
| -2 | 4 | -20 | 66.5 | 66.7 | .38 | 6 | 5 | -2 | 49.6 | 48.9 | -1.40 |
| -4 | 4 | -20 | 73.2 | 73.8 | .82 | -6 | 5 | -2 | 44.8 | 45.8 | 2.33 |

| h | k | l | $x_o$ | $x_c$ | error% |
|---|---|---|---|---|---|
| -8 | 5 | -2 | 69.8 | 72.4 | 3.77 |
| 1 | 5 | 3 | 8.2 | 8.2 | .00 |
| 2 | 5 | 3 | 14.2 | 13.7 | -2.83 |
| 3 | 5 | 3 | 21.1 | 20.4 | -3.02 |
| 4 | 5 | 3 | 28.5 | 27.7 | -2.75 |
| -5 | 5 | 3 | 37.8 | 39.5 | 4.65 |
| 6 | 5 | 3 | 44.9 | 44.4 | -.94 |
| -7 | 5 | 3 | 59.1 | 60.9 | 3.14 |
| 1 | 5 | -3 | 14.8 | 14.1 | -4.64 |
| -1 | 5 | -3 | 12.1 | 12.4 | 2.54 |
| 2 | 5 | -3 | 20.1 | 19.3 | -3.96 |
| -2 | 5 | -3 | 16.3 | 16.7 | 2.53 |
| 3 | 5 | -3 | 26.5 | 25.6 | -3.06 |
| -3 | 5 | -3 | 22.2 | 22.6 | 1.92 |
| 4 | 5 | -3 | 33.8 | 32.9 | -2.62 |
| 5 | 5 | -3 | 41.7 | 41.0 | -1.53 |
| 6 | 5 | -3 | 51.3 | 50.5 | -1.44 |
| -6 | 5 | -3 | 45.0 | 45.9 | 2.12 |
| -8 | 5 | -3 | 69.9 | 72.1 | 3.26 |
| 2 | 5 | 4 | 14.3 | 14.5 | 1.95 |
| 3 | 5 | 4 | 21.4 | 20.8 | -2.65 |
| 4 | 5 | 4 | 28.3 | 27.8 | -1.56 |
| -5 | 5 | 4 | 39.0 | 40.8 | 4.71 |
| -6 | 5 | 4 | 48.8 | 50.4 | 3.40 |
| 1 | 5 | -4 | 17.2 | 16.5 | -3.75 |
| -1 | 5 | -4 | 14.8 | 14.5 | -1.40 |
| 2 | 5 | -4 | 22.1 | 21.4 | -3.13 |
| -2 | 5 | -4 | 18.0 | 18.2 | 1.23 |
| -4 | 5 | -4 | 29.6 | 30.1 | 1.97 |
| -5 | 5 | -4 | 36.9 | 37.6 | 2.08 |
| 6 | 5 | -4 | 53.1 | 52.4 | -1.15 |
| -6 | 5 | -4 | 45.2 | 46.3 | 2.46 |
| -8 | 5 | -4 | 70.0 | 72.3 | 3.37 |
| 3 | 5 | 5 | 21.2 | 21.5 | 1.71 |
| -6 | 5 | 5 | 50.7 | 52.1 | 2.83 |
| -7 | 5 | 5 | 63.2 | 65.0 | 2.86 |
| 1 | 5 | -5 | 19.8 | 19.1 | -3.44 |
| -1 | 5 | -5 | 17.2 | 16.9 | -1.37 |
| 2 | 5 | -5 | 24.2 | 23.6 | -2.07 |
| -2 | 5 | -5 | 20.0 | 20.0 | .11 |
| 3 | 5 | -5 | 30.2 | 29.6 | -1.86 |
| -3 | 5 | -5 | 24.7 | 24.9 | 1.06 |
| 4 | 5 | -5 | 37.2 | 36.6 | -1.47 |
| -4 | 5 | -5 | 30.7 | 31.1 | 1.51 |
| -5 | 5 | -5 | 37.7 | 38.4 | 1.92 |
| 6 | 5 | -5 | 55.3 | 54.7 | -1.05 |
| -6 | 5 | -5 | 45.9 | 46.9 | 2.22 |
| -8 | 5 | -5 | 70.7 | 72.9 | 3.22 |
| -6 | 5 | 6 | 52.4 | 54.1 | 3.25 |
| -7 | 5 | 6 | 65.3 | 67.7 | 3.74 |
| 1 | 5 | -6 | 22.5 | 21.7 | -3.18 |
| -1 | 5 | -6 | 19.7 | 19.4 | -1.15 |
| 2 | 5 | -6 | 26.9 | 26.1 | -2.80 |
| -2 | 5 | -6 | 22.0 | 22.0 | .25 |
| 3 | 5 | -6 | 32.8 | 31.9 | -2.71 |
| -3 | 5 | -6 | 26.2 | 26.5 | 1.30 |
| 4 | 5 | -6 | 39.7 | 38.8 | -2.14 |
| -4 | 5 | -6 | 32.0 | 32.4 | 1.25 |
| -5 | 5 | -6 | 38.8 | 39.4 | 1.62 |
| 1 | 5 | 7 | 15.8 | 16.5 | 4.80 |
| 2 | 5 | 7 | 19.1 | 19.2 | .88 |
| -6 | 5 | 7 | 54.7 | 56.3 | 3.07 |
| -7 | 5 | 7 | 68.6 | 71.1 | 3.77 |
| 1 | 5 | -7 | 25.2 | 24.5 | -2.62 |
| -1 | 5 | -7 | 22.3 | 22.0 | -.92 |
| 2 | 5 | -7 | 29.5 | 28.7 | -2.58 |
| -2 | 5 | -7 | 24.2 | 24.2 | .35 |
| 3 | 5 | -7 | 35.0 | 34.3 | -1.81 |
| 4 | 5 | -7 | 41.9 | 41.2 | -1.53 |
| -4 | 5 | -7 | 33.6 | 33.8 | .85 |
| -5 | 5 | -7 | 40.2 | 40.6 | 1.19 |
| -6 | 5 | -7 | 48.1 | 48.8 | 1.64 |
| -7 | 5 | -7 | 57.7 | 59.2 | 2.76 |
| -8 | 5 | -7 | 73.2 | 75.7 | 3.52 |
| 2 | 5 | 8 | 20.8 | 21.3 | 2.74 |
| -6 | 5 | 8 | 57.1 | 59.0 | 3.36 |
| 1 | 5 | -8 | 27.9 | 27.3 | -1.83 |
| -1 | 5 | -8 | 25.0 | 24.8 | -.72 |
| 2 | 5 | -8 | 32.1 | 31.4 | -1.97 |
| -2 | 5 | -8 | 26.8 | 26.6 | -.43 |
| 3 | 5 | -8 | 37.8 | 36.9 | -2.11 |
| -3 | 5 | -8 | 30.1 | 30.3 | .95 |
| -5 | 5 | -8 | 41.7 | 42.1 | 1.13 |
| -6 | 5 | -8 | 49.6 | 50.2 | 1.33 |
| 2 | 5 | 9 | 22.8 | 23.6 | 3.75 |
| -6 | 5 | 9 | 60.1 | 62.0 | 3.32 |

| h | k | l | $x_o$ | $x_c$ | error% |
|---|---|---|---|---|---|
| 1 | 5 | -9 | 31.0 | 30.3 | -2.14 |
| -1 | 5 | -9 | 28.0 | 27.6 | -1.28 |
| -2 | 5 | -9 | 29.3 | 29.2 | -.23 |
| -3 | 5 | -9 | 32.5 | 32.6 | .35 |
| -4 | 5 | -9 | 37.2 | 37.5 | .92 |
| 5 | 5 | -9 | 56.2 | 55.5 | -1.13 |
| -6 | 5 | -9 | 50.5 | 51.9 | 2.77 |
| 2 | 5 | 10 | 25.2 | 26.1 | 3.58 |
| -5 | 5 | 10 | 51.8 | 53.7 | 3.81 |
| 1 | 5 | -10 | 33.9 | 33.3 | -1.49 |
| -1 | 5 | -10 | 31.0 | 30.5 | -1.39 |
| 2 | 5 | -10 | 38.0 | 37.3 | -1.68 |
| -2 | 5 | -10 | 32.0 | 31.9 | -.23 |
| -3 | 5 | -10 | 34.8 | 35.0 | .65 |
| 4 | 5 | -10 | 50.5 | 49.9 | -1.17 |
| -4 | 5 | -10 | 39.5 | 39.7 | .51 |
| 5 | 5 | -10 | 59.8 | 59.1 | -1.10 |
| -5 | 5 | -10 | 45.3 | 45.8 | 1.29 |
| -6 | 5 | -10 | 53.0 | 53.8 | 1.55 |
| -4 | 5 | 11 | 45.8 | 47.8 | 4.43 |
| -5 | 5 | 11 | 54.8 | 56.9 | 4.00 |
| 1 | 5 | -11 | 37.1 | 36.5 | -1.41 |
| -1 | 5 | -11 | 33.9 | 33.6 | -.86 |
| 2 | 5 | -11 | 41.2 | 40.5 | -1.58 |
| -3 | 5 | -11 | 37.7 | 37.6 | -.18 |
| 4 | 5 | -11 | 53.9 | 53.3 | -.98 |
| -4 | 5 | -11 | 41.9 | 42.0 | .43 |
| 5 | 5 | -11 | 64.0 | 63.2 | -1.11 |
| -6 | 5 | -11 | 55.2 | 56.0 | 1.56 |
| 1 | 5 | 12 | 29.1 | 30.3 | 4.26 |
| -3 | 5 | 12 | 41.8 | 43.6 | 4.44 |
| -4 | 5 | 12 | 49.0 | 50.9 | 4.07 |
| -5 | 5 | 12 | 58.2 | 60.6 | 4.23 |
| 1 | 5 | -12 | 40.2 | 39.9 | -.72 |
| -1 | 5 | -12 | 37.0 | 36.7 | -.60 |
| 2 | 5 | -12 | 44.2 | 43.9 | -.60 |
| -2 | 5 | -12 | 37.8 | 37.7 | -.09 |
| -3 | 5 | -12 | 40.4 | 40.4 | .05 |
| -4 | 5 | -12 | 43.8 | 44.6 | 2.03 |
| 5 | 5 | -12 | 69.0 | 68.3 | -1.01 |
| -6 | 5 | -12 | 57.2 | 58.6 | 2.53 |
| 1 | 5 | 13 | 32.0 | 33.3 | 4.36 |
| -5 | 5 | 13 | 62.3 | 64.9 | 4.30 |
| 1 | 5 | -13 | 43.8 | 43.4 | -.86 |
| -1 | 5 | -13 | 40.5 | 40.0 | -.98 |
| -2 | 5 | -13 | 41.0 | 40.9 | -.16 |
| -4 | 5 | -13 | 47.2 | 47.5 | .73 |
| -5 | 5 | -13 | 53.2 | 53.4 | .44 |
| -6 | 5 | -13 | 60.2 | 61.6 | 2.42 |
| 1 | 5 | 14 | 35.2 | 36.5 | 3.92 |
| -2 | 5 | 14 | 42.7 | 44.5 | 4.22 |
| 1 | 5 | -14 | 47.7 | 47.1 | -1.13 |
| -1 | 5 | -14 | 44.0 | 43.6 | -.89 |
| -2 | 5 | -14 | 44.2 | 44.3 | .23 |
| -4 | 5 | -14 | 50.4 | 50.6 | .56 |
| -5 | 5 | -14 | 56.2 | 56.6 | .72 |
| -7 | 5 | -14 | 79.2 | 81.9 | 3.49 |
| 1 | 5 | 15 | 38.2 | 39.9 | 4.48 |
| -1 | 5 | 15 | 42.1 | 43.7 | 3.90 |
| -3 | 5 | 15 | 52.2 | 54.3 | 4.04 |
| -1 | 5 | -15 | 47.0 | 47.3 | .72 |
| 3 | 5 | -15 | 63.1 | 62.6 | -.72 |
| -4 | 5 | -15 | 53.9 | 54.1 | .46 |
| -5 | 5 | -15 | 59.8 | 60.2 | .70 |
| 1 | 5 | 16 | 42.0 | 43.4 | 3.39 |
| -3 | 5 | 16 | 56.5 | 58.6 | 3.81 |
| -1 | 5 | -16 | 50.9 | 51.3 | .92 |
| 3 | 5 | -16 | 69.0 | 68.6 | -.54 |
| -3 | 5 | -16 | 53.2 | 54.0 | 1.50 |
| -4 | 5 | -16 | 57.8 | 58.0 | .42 |
| -5 | 5 | -16 | 64.0 | 64.4 | .70 |
| -3 | 5 | 17 | 61.3 | 63.6 | 3.89 |
| 3 | 5 | -17 | 77.5 | 77.0 | -.57 |
| -3 | 5 | -17 | 58.1 | 58.3 | .35 |
| -5 | 5 | -17 | 68.8 | 69.6 | 1.21 |
| -3 | 5 | 18 | 67.3 | 69.9 | 3.86 |
| -2 | 5 | -18 | 60.8 | 61.0 | .40 |
| -3 | 5 | -18 | 63.0 | 63.2 | .42 |
| -4 | 5 | -18 | 66.9 | 67.9 | 1.51 |
| -2 | 5 | -19 | 66.1 | 66.8 | 1.19 |
| -3 | 5 | -19 | 69.0 | 69.3 | .52 |
| -4 | 5 | -19 | 74.5 | 75.1 | .89 |
| -2 | 5 | -20 | 74.1 | 74.7 | .83 |
| -3 | 5 | -20 | 77.7 | 78.2 | .65 |

APPENDIX D

Table XXXVI. List of Observed and Calculated Structure Factors

| h | k | l | $F_o$ | $F_c$ | h | k | l | $F_o$ | $F_c$ |
|---|---|---|---|---|---|---|---|---|---|
| 2 | | | 537 | 467 | 2 | | -4 | 660 | -705 |
| 3 | | | 326 | -304 | 3 | | -4 | 148 | 161 |
| 4 | | | 256 | 275 | 6 | | -4 | 139 | -149 |
| 7 | | | 162 | -125 | 0 | | 5 | 474 | -411 |
| 8 | | | 102 | 99 | 1 | | 5 | 605 | 586 |
| 2 | | 1 | 879 | -890 | 2 | | 5 | 743 | -776 |
| 3 | | 1 | 271 | -254 | 4 | | 5 | 177 | 187 |
| 4 | | 1 | 129 | 131 | 6 | | 5 | 166 | -164 |
| 6 | | 1 | 178 | -168 | 1 | | -5 | 337 | 345 |
| 7 | | 1 | 115 | -95 | 2 | | -5 | 301 | -275 |
| 8 | | 1 | 124 | 107 | 3 | | -5 | 154 | 158 |
| 1 | | -1 | 348 | -281 | 4 | | -5 | 40 | -37 |
| 3 | | -1 | 254 | -269 | 5 | | -5 | 257 | 281 |
| 4 | | -1 | 171 | 173 | 6 | | -5 | 254 | -257 |
| 5 | | -1 | 175 | -159 | 0 | | 6 | 330 | -311 |
| 7 | | -1 | 247 | -216 | 1 | | 6 | 337 | 375 |
| 1 | | 2 | 363 | -296 | 3 | | 6 | 88 | 76 |
| 2 | | 2 | 527 | 465 | 4 | | 6 | 398 | 452 |
| 3 | | 2 | 271 | -251 | 5 | | 6 | 151 | -160 |
| 6 | | 2 | 298 | -306 | 7 | | 6 | 115 | -105 |
| 1 | | -2 | 392 | 314 | 1 | | -6 | 137 | 108 |
| 2 | | -2 | 492 | -525 | 2 | | -6 | 65 | -96 |
| 4 | | -2 | 402 | 423 | 3 | | -6 | 169 | -175 |
| 6 | | -2 | 115 | 146 | 5 | | -6 | 239 | 275 |
| 7 | | -2 | 204 | -193 | 6 | | -6 | 259 | -250 |
| 0 | | 3 | 471 | 451 | 1 | | 7 | 137 | 121 |
| 1 | | 3 | 383 | 307 | 2 | | 7 | 297 | -264 |
| 3 | | 3 | 316 | -278 | 3 | | 7 | 140 | 149 |
| 4 | | 3 | 129 | 120 | 4 | | 7 | 162 | 175 |
| 6 | | 3 | 313 | -313 | 7 | | 7 | 127 | -141 |
| 1 | | -3 | 780 | 744 | 8 | | 7 | 102 | 113 |
| 2 | | -3 | 792 | -770 | 2 | | -7 | 77 | 81 |
| 3 | | -3 | 103 | 101 | 3 | | -7 | 221 | -228 |
| 4 | | -3 | 163 | 156 | 5 | | -7 | 168 | 157 |
| | | 4 | 599 | -647 | 6 | | -7 | 115 | -131 |
| 1 | | 4 | 804 | 753 | | | 8 | 236 | 239 |
| 2 | | 4 | 506 | -524 | 2 | | 8 | 75 | -99 |
| 3 | | 4 | 268 | -265 | 3 | | 8 | 158 | 163 |
| 4 | | 4 | 274 | 285 | 6 | | 8 | 120 | 143 |
| 6 | | 4 | 311 | -291 | 7 | | 8 | 254 | -222 |
| 1 | | -4 | 596 | 588 | 8 | | 8 | 102 | 99 |

| h | k | l | $F_o$ | $F_c$ |
|---|---|---|---|---|
| 4 | | -8 | 117 | -153 |
| 7 | | -8 | 96 | -95 |
| 2 | | 9 | 83 | 91 |
| 3 | | 9 | 181 | -186 |
| 7 | | 9 | 210 | -188 |
| 1 | | -9 | 166 | -152 |
| 2 | | -9 | 96 | 107 |
| 7 | | -9 | 123 | -104 |
| 0 | | 10 | 468 | 450 |
| 1 | | 10 | 162 | -150 |
| 3 | | 10 | 216 | -229 |
| 5 | | 10 | 290 | 298 |
| 6 | | 10 | 122 | -164 |
| 3 | | -10 | 68 | -102 |
| 4 | | -10 | 119 | 153 |
| 5 | | -10 | 115 | -122 |
| 7 | | -10 | 123 | -95 |
| | | 11 | 384 | 402 |
| 2 | | 11 | 97 | 109 |
| 5 | | 11 | 281 | 286 |
| 6 | | 11 | 279 | -264 |
| 1 | | -11 | 137 | 130 |
| 2 | | -11 | 106 | -122 |
| 4 | | -11 | 297 | 286 |
| 7 | | -11 | 113 | -85 |
| | | 12 | 77 | 98 |
| 1 | | 12 | 102 | 118 |
| 4 | | 12 | 149 | -160 |
| 5 | | 12 | 164 | 170 |
| 6 | | 12 | 264 | -263 |
| 2 | | -12 | 336 | -328 |
| 3 | | -12 | 228 | -221 |
| 4 | | -12 | 210 | 197 |
| | | 13 | 198 | 226 |
| 2 | | 13 | 103 | -130 |
| 6 | | 13 | 115 | -129 |
| 1 | | -13 | 229 | 236 |
| 0 | | 14 | 77 | -63 |
| 1 | | 14 | 198 | 213 |
| 2 | | 14 | 290 | -310 |
| 4 | | 14 | 115 | 165 |
| 4 | | -14 | 113 | 109 |
| 6 | | -14 | 77 | -92 |

| h | k | l | $F_o$ | $F_c$ |
|---|---|---|---|---|
| 3 | | 15 | 201 | -214 |
| 4 | | 15 | 254 | 284 |
| 5 | | 15 | 117 | -128 |
| 7 | | 15 | 96 | -97 |
| 1 | | -15 | 115 | -121 |
| 2 | | -15 | 223 | -192 |
| 5 | | -15 | 70 | 86 |
| 0 | | 16 | 349 | 307 |
| 1 | | 16 | 96 | -121 |
| 4 | | 16 | 205 | 199 |
| 7 | | 16 | 100 | -113 |
| 5 | | -16 | 119 | 101 |
| 0 | | 17 | 198 | 186 |
| 2 | | 17 | 210 | -202 |
| 7 | | 17 | 115 | -101 |
| 0 | | 18 | 174 | 159 |
| 7 | | 18 | 79 | -74 |
| 1 | 1 | | 863 | 825 |
| -1 | 1 | | 699 | 652 |
| -2 | 1 | | 150 | 91 |
| 3 | 1 | | 288 | 325 |
| -3 | 1 | | 595 | -617 |
| -4 | 1 | | 55 | 53 |
| -5 | 1 | | 224 | 229 |
| -6 | 1 | | 80 | 86 |
| -7 | 1 | | 61 | -74 |
| 8 | 1 | | 114 | 110 |
| -8 | 1 | | 69 | 68 |
| 1 | 1 | 1 | 731 | -655 |
| 3 | 1 | 1 | 126 | 99 |
| -3 | 1 | 1 | 176 | -166 |
| 4 | 1 | 1 | 69 | -69 |
| -4 | 1 | 1 | 316 | -376 |
| 5 | 1 | 1 | 52 | -51 |
| -5 | 1 | 1 | 286 | 278 |
| -6 | 1 | 1 | 61 | 68 |
| -7 | 1 | 1 | 61 | -79 |
| 8 | 1 | 1 | 110 | 118 |
| -8 | 1 | 1 | 38 | 41 |
| 1 | 1 | -1 | 312 | -275 |
| -1 | 1 | -1 | 768 | -822 |
| 2 | 1 | -1 | 406 | -455 |
| 3 | 1 | -1 | 129 | 121 |

| h | k | l | $F_o$ | $F_c$ |
|---|---|---|---|---|
| -3 | 1 | -1 | 492 | -521 |
| -4 | 1 | -1 | 45 | -59 |
| -5 | 1 | -1 | 174 | 174 |
| 6 | 1 | -1 | 259 | -224 |
| -6 | 1 | -1 | 122 | 113 |
| -7 | 1 | -1 | 75 | -70 |
| -1 | 1 | 2 | 340 | -246 |
| 2 | 1 | 2 | 228 | -109 |
| -2 | 1 | 2 | 228 | -217 |
| 3 | 1 | 2 | 505 | 537 |
| -3 | 1 | 2 | 292 | -263 |
| 4 | 1 | 2 | 133 | 148 |
| -4 | 1 | 2 | 298 | -324 |
| 5 | 1 | 2 | 66 | -73 |
| -5 | 1 | 2 | 310 | 320 |
| 6 | 1 | 2 | 131 | -116 |
| -6 | 1 | 2 | 61 | 75 |
| 8 | 1 | 2 | 149 | 137 |
| -8 | 1 | 2 | 26 | -42 |
| 1 | 1 | -2 | 193 | -198 |
| -1 | 1 | -2 | 325 | 278 |
| 2 | 1 | -2 | 113 | -134 |
| 3 | 1 | -2 | 134 | 142 |
| -3 | 1 | -2 | 121 | -100 |
| 4 | 1 | -2 | 231 | 234 |
| -4 | 1 | -2 | 141 | -150 |
| -5 | 1 | -2 | 160 | 156 |
| 6 | 1 | -2 | 100 | -111 |
| -6 | 1 | -2 | 60 | 74 |
| 7 | 1 | -2 | 72 | 59 |
| -7 | 1 | -2 | 73 | -68 |
| 1 | 1 | 3 | 283 | 258 |
| -1 | 1 | 3 | 701 | 728 |
| -2 | 1 | 3 | 518 | -465 |
| 3 | 1 | 3 | 566 | 630 |
| -3 | 1 | 3 | 268 | -287 |
| -4 | 1 | 3 | 220 | -219 |
| 5 | 1 | 3 | 158 | -169 |
| -5 | 1 | 3 | 283 | 317 |
| -6 | 1 | 3 | 81 | 96 |
| 8 | 1 | 3 | 184 | 156 |
| -8 | 1 | 3 | 135 | -115 |
| 1 | 1 | -3 | 457 | -493 |
| -1 | 1 | -3 | 198 | 188 |
| 2 | 1 | -3 | 146 | 165 |
| -2 | 1 | -3 | 430 | 467 |
| -3 | 1 | -3 | 302 | -326 |
| 4 | 1 | -3 | 215 | 231 |
| -4 | 1 | -3 | 66 | 75 |
| 5 | 1 | -3 | 174 | -186 |
| -5 | 1 | -3 | 45 | 72 |
| 6 | 1 | -3 | 104 | -98 |
| 7 | 1 | -3 | 75 | 73 |
| -7 | 1 | -3 | 68 | -59 |
| 1 | 1 | 4 | 682 | -730 |
| -1 | 1 | 4 | 274 | 301 |
| 2 | 1 | 4 | 221 | 230 |
| -2 | 1 | 4 | 413 | -402 |
| 3 | 1 | 4 | 155 | 153 |
| -4 | 1 | 4 | 157 | -136 |
| 5 | 1 | 4 | 181 | -184 |
| 6 | 1 | 4 | 81 | -76 |
| -6 | 1 | 4 | 73 | 88 |
| 7 | 1 | 4 | 68 | 59 |
| 8 | 1 | 4 | 93 | 83 |
| -8 | 1 | 4 | 135 | -129 |
| 1 | 1 | -4 | 141 | 132 |
| -1 | 1 | -4 | 480 | 505 |
| 2 | 1 | -4 | 160 | 121 |
| -2 | 1 | -4 | 115 | 138 |
| 3 | 1 | -4 | 131 | 131 |
| -3 | 1 | -4 | 139 | -115 |
| 4 | 1 | -4 | 269 | 294 |
| 5 | 1 | -4 | 194 | -184 |
| 6 | 1 | -4 | 143 | -130 |
| -6 | 1 | -4 | 94 | 101 |
| -8 | 1 | -4 | 90 | -96 |
| -9 | 1 | -4 | 48 | 44 |
| 1 | 1 | 5 | 278 | -299 |
| -1 | 1 | 5 | 446 | 450 |
| 2 | 1 | 5 | 448 | 464 |
| -2 | 1 | 5 | 170 | 184 |
| 3 | 1 | 5 | 257 | 266 |
| -3 | 1 | 5 | 255 | -266 |
| 4 | 1 | 5 | 306 | 353 |
| -4 | 1 | 5 | 171 | 204 |

| h | k | l | $F_o$ | $F_c$ |
|---|---|---|---|---|
| 5 | 1 | 5 | 215 | -217 |
| -5 | 1 | 5 | 92 | -104 |
| 6 | 1 | 5 | 131 | -122 |
| -6 | 1 | 5 | 62 | 78 |
| 7 | 1 | 5 | 68 | 67 |
| -8 | 1 | 5 | 127 | -105 |
| 1 | 1 | -5 | 124 | 107 |
| -1 | 1 | -5 | 136 | -128 |
| 2 | 1 | -5 | 143 | 125 |
| -2 | 1 | -5 | 150 | -170 |
| 3 | 1 | -5 | 66 | 67 |
| -3 | 1 | -5 | 127 | -167 |
| 4 | 1 | -5 | 239 | 290 |
| 5 | 1 | -5 | 131 | -154 |
| 6 | 1 | -5 | 122 | -124 |
| 8 | 1 | -5 | 52 | 48 |
| -8 | 1 | -5 | 148 | -156 |
| -9 | 1 | -5 | 89 | 73 |
| 1 | 1 | 6 | 444 | -460 |
| -1 | 1 | 6 | 72 | 54 |
| 2 | 1 | 6 | 390 | 415 |
| -2 | 1 | 6 | 114 | 95 |
| 3 | 1 | 6 | 251 | 280 |
| -3 | 1 | 6 | 321 | -371 |
| 4 | 1 | 6 | 286 | 321 |
| -4 | 1 | 6 | 271 | 267 |
| 5 | 1 | 6 | 263 | -277 |
| -5 | 1 | 6 | 60 | -68 |
| 6 | 1 | 6 | 76 | -80 |
| -6 | 1 | 6 | 114 | 112 |
| 7 | 1 | 6 | 68 | 65 |
| -8 | 1 | 6 | 56 | -37 |
| 1 | 1 | -6 | 244 | 235 |
| -1 | 1 | -6 | 128 | -118 |
| 2 | 1 | -6 | 120 | 141 |
| -2 | 1 | -6 | 156 | -130 |
| 3 | 1 | -6 | 256 | 288 |
| -3 | 1 | -6 | 38 | -34 |
| 4 | 1 | -6 | 90 | 112 |
| -4 | 1 | -6 | 222 | -248 |
| 5 | 1 | -6 | 73 | -71 |
| 6 | 1 | -6 | 63 | -77 |
| 8 | 1 | -6 | 75 | 70 |
| -8 | 1 | -6 | 137 | -140 |
| -9 | 1 | -6 | 82 | 81 |
| 1 | 1 | 7 | 63 | -48 |
| -1 | 1 | 7 | 170 | 156 |
| -2 | 1 | 7 | 187 | 211 |
| -3 | 1 | 7 | 291 | -329 |
| 4 | 1 | 7 | 216 | 211 |
| 5 | 1 | 7 | 305 | -314 |
| -5 | 1 | 7 | 49 | 67 |
| 6 | 1 | 7 | 52 | -65 |
| -1 | 1 | -7 | 230 | -239 |
| 2 | 1 | -7 | 251 | 292 |
| -2 | 1 | -7 | 143 | -126 |
| 3 | 1 | -7 | 158 | 182 |
| -3 | 1 | -7 | 117 | -129 |
| -4 | 1 | -7 | 220 | -214 |
| 5 | 1 | -7 | 77 | -63 |
| -6 | 1 | -7 | 214 | 246 |
| 8 | 1 | -7 | 65 | 56 |
| -8 | 1 | -7 | 141 | -116 |
| -9 | 1 | -7 | 80 | 68 |
| 1 | 1 | 8 | 169 | -181 |
| -1 | 1 | 8 | 50 | 58 |
| -3 | 1 | 8 | 227 | -245 |
| 4 | 1 | 8 | 142 | 141 |
| -4 | 1 | 8 | 80 | -85 |
| 5 | 1 | 8 | 275 | -307 |
| -5 | 1 | 8 | 102 | 109 |
| 1 | 1 | -8 | 237 | -277 |
| 2 | 1 | -8 | 120 | 107 |
| -2 | 1 | -8 | 115 | -140 |
| 3 | 1 | -8 | 243 | 251 |
| -3 | 1 | -8 | 80 | -80 |
| -4 | 1 | -8 | 272 | -294 |
| 5 | 1 | -8 | 59 | -35 |
| -5 | 1 | -8 | 178 | 185 |
| -6 | 1 | -8 | 117 | 118 |
| 7 | 1 | -8 | 66 | 53 |
| -8 | 1 | -8 | 109 | -102 |
| 1 | 1 | 9 | 40 | -69 |
| -1 | 1 | 9 | 50 | 60 |
| -2 | 1 | 9 | 191 | 212 |
| -4 | 1 | 9 | 183 | -205 |

| h | k | l | $F_o$ | $F_c$ |
|---|---|---|---|---|
| -5 | 1 | 9 | 99 | 105 |
| -6 | 1 | 9 | 76 | 85 |
| 1 | 1 | -9 | 80 | -102 |
| -1 | 1 | -9 | 238 | 291 |
| 2 | 1 | -9 | 205 | -226 |
| -2 | 1 | -9 | 243 | -279 |
| 3 | 1 | -9 | 276 | 294 |
| -3 | 1 | -9 | 238 | -294 |
| 4 | 1 | -9 | 122 | -141 |
| -4 | 1 | -9 | 238 | -288 |
| 5 | 1 | -9 | 97 | -116 |
| -5 | 1 | -9 | 180 | 186 |
| -6 | 1 | -9 | 108 | 111 |
| 7 | 1 | -9 | 47 | 38 |
| -7 | 1 | -9 | 59 | -68 |
| 1 | 1 | 10 | 43 | -59 |
| -2 | 1 | 10 | 53 | -70 |
| -3 | 1 | 10 | 193 | 217 |
| -4 | 1 | 10 | 247 | -271 |
| -5 | 1 | 10 | 124 | 143 |
| -6 | 1 | 10 | 65 | 53 |
| 1 | 1 | -10 | 243 | -248 |
| -1 | 1 | -10 | 86 | 100 |
| 2 | 1 | -10 | 150 | -167 |
| -2 | 1 | -10 | 117 | -117 |
| 3 | 1 | -10 | 319 | 364 |
| -3 | 1 | -10 | 150 | -194 |
| -4 | 1 | -10 | 109 | -121 |
| 5 | 1 | -10 | 89 | -88 |
| -5 | 1 | -10 | 143 | 151 |
| 6 | 1 | -10 | 74 | -66 |
| -6 | 1 | -10 | 119 | 128 |
| 7 | 1 | -10 | 36 | 32 |
| -7 | 1 | -10 | 60 | -74 |
| -8 | 1 | -10 | 50 | 49 |
| 1 | 1 | 11 | 46 | -55 |
| -1 | 1 | 11 | 139 | 152 |
| -2 | 1 | 11 | 232 | -253 |
| -3 | 1 | 11 | 115 | 120 |
| -4 | 1 | 11 | 189 | -201 |
| -5 | 1 | 11 | 124 | 99 |
| -6 | 1 | 11 | 45 | 45 |
| 1 | 1 | -11 | 131 | -117 |
| -1 | 1 | -11 | 238 | 257 |
| 2 | 1 | -11 | 200 | -230 |
| -2 | 1 | -11 | 203 | 206 |
| 3 | 1 | -11 | 262 | 287 |
| -3 | 1 | -11 | 212 | -235 |
| 4 | 1 | -11 | 83 | 70 |
| -5 | 1 | -11 | 72 | 72 |
| -6 | 1 | -11 | 92 | 120 |
| 7 | 1 | -11 | 46 | 40 |
| 1 | 1 | 12 | 144 | -145 |
| -1 | 1 | 12 | 121 | 130 |
| -2 | 1 | 12 | 247 | -260 |
| -4 | 1 | 12 | 86 | -103 |
| -6 | 1 | 12 | 42 | 49 |
| 1 | 1 | -12 | 171 | -184 |
| -1 | 1 | -12 | 133 | 128 |
| 2 | 1 | -12 | 156 | -164 |
| -2 | 1 | -12 | 137 | 152 |
| 3 | 1 | -12 | 52 | -42 |
| -3 | 1 | -12 | 243 | -290 |
| 5 | 1 | -12 | 151 | -122 |
| -5 | 1 | -12 | 75 | 60 |
| -6 | 1 | -12 | 62 | 60 |
| 1 | 1 | 13 | 146 | -146 |
| -1 | 1 | 13 | 182 | 196 |
| -2 | 1 | 13 | 135 | -116 |
| -3 | 1 | 13 | 193 | -192 |
| -6 | 1 | 13 | 73 | 56 |
| 1 | 1 | -13 | 150 | -155 |
| -1 | 1 | -13 | 166 | 182 |
| 2 | 1 | -13 | 204 | 183 |
| -2 | 1 | -13 | 174 | 214 |
| 3 | 1 | -13 | 69 | 56 |
| -3 | 1 | -13 | 308 | -353 |
| 4 | 1 | -13 | 150 | 127 |
| -4 | 1 | -13 | 123 | 129 |
| 5 | 1 | -13 | 167 | -132 |
| -5 | 1 | -13 | 58 | 41 |
| -8 | 1 | -13 | 58 | -52 |
| 1 | 1 | 14 | 190 | -204 |
| -1 | 1 | 14 | 270 | 241 |
| -2 | 1 | 14 | 131 | 119 |
| -3 | 1 | 14 | 163 | -185 |

| h | k | l | $F_o$ | $F_c$ |
|---|---|---|---|---|
| -4 | 1 | 14 | 65 | 53 |
| -6 | 1 | 14 | 69 | 42 |
| 1 | 1 | -14 | 278 | -225 |
| -1 | 1 | -14 | 153 | 157 |
| 2 | 1 | -14 | 77 | 116 |
| -2 | 1 | -14 | 149 | 169 |
| -3 | 1 | -14 | 276 | -288 |
| 4 | 1 | -14 | 182 | 160 |
| -4 | 1 | -14 | 66 | 57 |
| 5 | 1 | -14 | 72 | -78 |
| -5 | 1 | -14 | 96 | 105 |
| 6 | 1 | -14 | 33 | -43 |
| -7 | 1 | -14 | 45 | -38 |
| -8 | 1 | -14 | 83 | -68 |
| 1 | 1 | 15 | 269 | -247 |
| -1 | 1 | 15 | 269 | -236 |
| -2 | 1 | 15 | 134 | 149 |
| -3 | 1 | 15 | 258 | -262 |
| -4 | 1 | 15 | 74 | 85 |
| 1 | 1 | -15 | 133 | -147 |
| -1 | 1 | -15 | 255 | 236 |
| 2 | 1 | -15 | 68 | 86 |
| -2 | 1 | -15 | 189 | -184 |
| -3 | 1 | -15 | 61 | 37 |
| 4 | 1 | -15 | 147 | 115 |
| -4 | 1 | -15 | 90 | -76 |
| 5 | 1 | -15 | 45 | -57 |
| -5 | 1 | -15 | 87 | 100 |
| -7 | 1 | -15 | 62 | -50 |
| -8 | 1 | -15 | 83 | -61 |
| -1 | 1 | 16 | 62 | 51 |
| -2 | 1 | 16 | 114 | 120 |
| -3 | 1 | 16 | 200 | -196 |
| -4 | 1 | 16 | 74 | 56 |
| 1 | 1 | -16 | 101 | -105 |
| -1 | 1 | -16 | 134 | 140 |
| -2 | 1 | -16 | 81 | -99 |
| -3 | 1 | -16 | 75 | -76 |
| -6 | 1 | -16 | 75 | 67 |
| -7 | 1 | -16 | 52 | -42 |
| -1 | 1 | 17 | 143 | 133 |
| -2 | 1 | 17 | 69 | 75 |
| -3 | 1 | 17 | 110 | -106 |

| h | k | l | $F_o$ | $F_c$ |
|---|---|---|---|---|
| -1 | 1 | -17 | 122 | 99 |
| -2 | 1 | -17 | 82 | -77 |
| 3 | 1 | -17 | 96 | 95 |
| 4 | 1 | -17 | 40 | -39 |
| -4 | 1 | -17 | 153 | -138 |
| -5 | 1 | -17 | 142 | 130 |
| -7 | 1 | -17 | 41 | -31 |
| -1 | 1 | 18 | 60 | 76 |
| 3 | 1 | -18 | 127 | 103 |
| -3 | 1 | -18 | 54 | 48 |
| 4 | 1 | -18 | 49 | -40 |
| -4 | 1 | -18 | 177 | -167 |
| -5 | 1 | -18 | 157 | 138 |
| -7 | 1 | -18 | 54 | -44 |
| -1 | 1 | 19 | 97 | 115 |
| 2 | 1 | -19 | 82 | -86 |
| 3 | 1 | -19 | 137 | 114 |
| -4 | 1 | -19 | 144 | -120 |
| -5 | 1 | -19 | 102 | 81 |
| -6 | 1 | -19 | 42 | 33 |
| -2 | 1 | 20 | 35 | -49 |
| 3 | 1 | -20 | 79 | 76 |
| -3 | 1 | -20 | 100 | -94 |
| -5 | 1 | -20 | 65 | 57 |
| -6 | 1 | -20 | 63 | 54 |
| 2 | 1 | -21 | 61 | -53 |
| -2 | 1 | -21 | 101 | 86 |
| -3 | 1 | -21 | 137 | -113 |
| -4 | 1 | -21 | 59 | 43 |
| -2 | 1 | -22 | 86 | 76 |
| -3 | 1 | -22 | 141 | -118 |
| -4 | 1 | -22 | 50 | 44 |
| -2 | 1 | -23 | 75 | 48 |
| -3 | 1 | -23 | 95 | -76 |
| 2 | 2 | | 49 | 50 |
| -2 | 2 | | 114 | -97 |
| 3 | 2 | | 168 | 181 |
| -3 | 2 | | 616 | 634 |
| 4 | 2 | | 119 | 107 |
| -4 | 2 | | 521 | -566 |
| 5 | 2 | | 117 | -115 |
| -5 | 2 | | 61 | -57 |
| 6 | 2 | | 239 | 232 |

| h | k | l | $F_o$ | $F_c$ |
|---|---|---|---|---|
| 2 | 2 | 1 | 151 | 150 |
| -2 | 2 | 1 | 645 | 626 |
| 3 | 2 | 1 | 151 | 123 |
| -3 | 2 | 1 | 170 | -184 |
| 4 | 2 | 1 | 237 | -234 |
| 5 | 2 | 1 | 110 | 116 |
| -5 | 2 | 1 | 162 | -179 |
| 6 | 2 | 1 | 89 | 84 |
| -6 | 2 | 1 | 160 | 178 |
| 9 | 2 | 1 | 93 | -70 |
| 1 | 2 | -1 | 40 | 36 |
| 2 | 2 | -1 | 154 | -110 |
| -2 | 2 | -1 | 126 | 145 |
| 3 | 2 | -1 | 419 | 414 |
| -3 | 2 | -1 | 150 | 147 |
| 4 | 2 | -1 | 67 | 43 |
| -4 | 2 | -1 | 86 | -75 |
| 5 | 2 | -1 | 207 | -210 |
| 6 | 2 | -1 | 302 | 312 |
| 7 | 2 | -1 | 76 | -87 |
| 1 | 2 | 2 | 892 | -802 |
| -1 | 2 | 2 | 222 | 166 |
| 2 | 2 | 2 | 124 | -107 |
| -2 | 2 | 2 | 255 | 268 |
| 3 | 2 | 2 | 157 | 142 |
| -3 | 2 | 2 | 188 | -213 |
| 4 | 2 | 2 | 171 | -177 |
| -4 | 2 | 2 | 154 | 152 |
| 5 | 2 | 2 | 134 | 120 |
| -5 | 2 | 2 | 247 | -270 |
| -6 | 2 | 2 | 289 | 283 |
| 7 | 2 | 2 | 92 | 99 |
| -7 | 2 | 2 | 73 | -81 |
| 9 | 2 | 2 | 102 | -75 |
| 1 | 2 | -2 | 140 | 154 |
| -1 | 2 | -2 | 49 | -11 |
| 2 | 2 | -2 | 352 | -320 |
| -2 | 2 | -2 | 59 | 51 |
| 3 | 2 | -2 | 460 | 479 |
| -3 | 2 | -2 | 142 | 126 |
| 4 | 2 | -2 | 52 | -71 |
| -4 | 2 | -2 | 205 | -171 |
| 5 | 2 | -2 | 128 | -128 |
| -5 | 2 | -2 | 117 | 118 |
| 6 | 2 | -2 | 223 | 236 |
| -6 | 2 | -2 | 168 | -173 |
| -7 | 2 | -2 | 175 | 196 |
| 0 | 2 | 3 | 163 | -133 |
| -1 | 2 | 3 | 236 | 207 |
| 2 | 2 | 3 | 573 | 616 |
| -2 | 2 | 3 | 281 | 266 |
| 3 | 2 | 3 | 595 | 638 |
| 4 | 2 | 3 | 70 | -64 |
| 5 | 2 | 3 | 123 | 115 |
| -5 | 2 | 3 | 193 | -204 |
| 6 | 2 | 3 | 164 | -177 |
| 7 | 2 | 3 | 245 | 229 |
| 8 | 2 | 3 | 73 | -72 |
| 9 | 2 | 3 | 52 | -41 |
| 1 | 2 | -3 | 198 | 200 |
| -1 | 2 | -3 | 146 | 161 |
| 2 | 2 | -3 | 200 | -177 |
| -2 | 2 | -3 | 137 | -127 |
| 3 | 2 | -3 | 218 | 198 |
| -3 | 2 | -3 | 156 | 201 |
| -4 | 2 | -3 | 218 | -222 |
| 5 | 2 | -3 | 80 | -81 |
| -5 | 2 | -3 | 142 | 124 |
| 6 | 2 | -3 | 83 | 76 |
| -6 | 2 | -3 | 153 | -174 |
| 7 | 2 | -3 | 81 | 81 |
| -7 | 2 | -3 | 248 | 250 |
| 8 | 2 | -3 | 61 | -58 |
| 0 | 2 | 4 | 783 | -738 |
| 1 | 2 | 4 | 230 | 226 |
| -1 | 2 | 4 | 92 | -115 |
| 2 | 2 | 4 | 251 | 252 |
| -2 | 2 | 4 | 333 | 309 |
| 3 | 2 | 4 | 164 | -169 |
| -3 | 2 | 4 | 182 | -192 |
| 4 | 2 | 4 | 537 | -581 |
| 5 | 2 | 4 | 76 | -84 |
| -5 | 2 | 4 | 119 | -111 |
| 6 | 2 | 4 | 173 | -175 |
| -6 | 2 | 4 | 255 | 265 |
| 7 | 2 | 4 | 284 | 258 |

| h | k | l | $F_o$ | $F_c$ |
|---|---|---|---|---|
| 8 | 2 | 4 | 124 | -104 |
| -8 | 2 | 4 | 73 | -75 |
| 9 | 2 | 4 | 54 | -39 |
| | 2 | -4 | 852 | -909 |
| 1 | 2 | -4 | 184 | 235 |
| -1 | 2 | -4 | 197 | 216 |
| -2 | 2 | -4 | 336 | -318 |
| -3 | 2 | -4 | 397 | 411 |
| 4 | 2 | -4 | 90 | -92 |
| -4 | 2 | -4 | 95 | 108 |
| -5 | 2 | -4 | 117 | 119 |
| 7 | 2 | -4 | 128 | 123 |
| -7 | 2 | -4 | 212 | 222 |
| 8 | 2 | -4 | 69 | -62 |
| | 2 | 5 | 425 | -495 |
| 1 | 2 | 5 | 88 | -126 |
| 2 | 2 | 5 | 271 | 274 |
| -2 | 2 | 5 | 498 | 485 |
| 3 | 2 | 5 | 189 | -228 |
| -3 | 2 | 5 | 73 | 95 |
| 4 | 2 | 5 | 73 | -71 |
| -6 | 2 | 5 | 144 | 129 |
| 7 | 2 | 5 | 228 | 192 |
| 8 | 2 | 5 | 117 | -101 |
| -8 | 2 | 5 | 85 | -77 |
| 9 | 2 | 5 | 56 | -44 |
| -1 | 2 | -5 | 200 | 228 |
| 2 | 2 | -5 | 445 | 498 |
| -2 | 2 | -5 | 200 | -194 |
| 3 | 2 | -5 | 189 | -202 |
| -3 | 2 | -5 | 410 | 475 |
| 4 | 2 | -5 | 176 | -208 |
| -4 | 2 | -5 | 46 | 40 |
| -5 | 2 | -5 | 119 | -117 |
| 7 | 2 | -5 | 116 | 111 |
| 8 | 2 | -5 | 68 | -63 |
| | 2 | 6 | 803 | -809 |
| -1 | 2 | 6 | 319 | -318 |
| 2 | 2 | 6 | 321 | 302 |
| -2 | 2 | 6 | 436 | 441 |
| -3 | 2 | 6 | 178 | 185 |
| 4 | 2 | 6 | 190 | 182 |
| 5 | 2 | 6 | 158 | -165 |

| h | k | l | $F_o$ | $F_c$ |
|---|---|---|---|---|
| -5 | 2 | 6 | 89 | 110 |
| 6 | 2 | 6 | 67 | 89 |
| -7 | 2 | 6 | 160 | 148 |
| 8 | 2 | 6 | 25 | -33 |
| -8 | 2 | 6 | 77 | -75 |
| 9 | 2 | 6 | 53 | -37 |
| | 2 | -6 | 445 | -489 |
| 1 | 2 | -6 | 141 | -175 |
| 3 | 2 | -6 | 70 | -85 |
| 4 | 2 | -6 | 234 | -248 |
| -5 | 2 | -6 | 208 | -212 |
| -6 | 2 | -6 | 228 | 233 |
| 7 | 2 | -6 | 45 | 41 |
| 8 | 2 | -6 | 55 | -38 |
| | 2 | 7 | 600 | -646 |
| 1 | 2 | 7 | 297 | -289 |
| -1 | 2 | 7 | 399 | -448 |
| 2 | 2 | 7 | 490 | 494 |
| 3 | 2 | 7 | 197 | -203 |
| -4 | 2 | 7 | 153 | -142 |
| 5 | 2 | 7 | 268 | -257 |
| -5 | 2 | 7 | 126 | 112 |
| 6 | 2 | 7 | 177 | 170 |
| -7 | 2 | 7 | 153 | 141 |
| | 2 | -7 | 261 | -269 |
| 1 | 2 | -7 | 431 | -484 |
| -1 | 2 | -7 | 129 | -172 |
| 2 | 2 | -7 | 398 | 462 |
| -2 | 2 | -7 | 441 | 497 |
| 3 | 2 | -7 | 61 | -95 |
| 4 | 2 | -7 | 190 | -210 |
| 0 | 2 | 8 | 65 | -52 |
| 1 | 2 | 8 | 390 | -392 |
| -1 | 2 | 8 | 150 | -159 |
| 2 | 2 | 8 | 421 | 428 |
| -2 | 2 | 8 | 322 | 353 |
| 3 | 2 | 8 | 76 | 91 |
| -4 | 2 | 8 | 171 | -173 |
| 5 | 2 | 8 | 201 | -197 |
| -5 | 2 | 8 | 67 | 66 |
| 6 | 2 | 8 | 322 | 284 |
| -7 | 2 | 8 | 42 | 63 |
| 9 | 2 | 8 | 76 | -59 |

| h | k | l | $F_o$ | $F_c$ |
|---|---|---|---|---|
| 1 | 2 | -8 | 367 | -434 |
| -1 | 2 | -8 | 406 | -482 |
| 2 | 2 | -8 | 431 | 517 |
| 4 | 2 | -8 | 117 | -126 |
| 6 | 2 | -8 | 156 | 157 |
| 1 | 2 | 9 | 127 | -163 |
| -1 | 2 | 9 | 87 | -97 |
| 2 | 2 | 9 | 42 | 68 |
| -2 | 2 | 9 | 212 | 204 |
| 3 | 2 | 9 | 158 | 171 |
| -3 | 2 | 9 | 123 | 138 |
| 4 | 2 | 9 | 59 | -78 |
| -4 | 2 | 9 | 225 | -235 |
| 5 | 2 | 9 | 103 | -112 |
| -5 | 2 | 9 | 106 | 89 |
| 6 | 2 | 9 | 328 | 306 |
| 7 | 2 | 9 | 86 | -85 |
| -7 | 2 | 9 | 72 | 71 |
| 9 | 2 | 9 | 109 | -88 |
|  | 2 | -9 | 128 | 160 |
| 1 | 2 | -9 | 248 | -272 |
| -1 | 2 | -9 | 359 | -414 |
| 2 | 2 | -9 | 244 | 276 |
| -2 | 2 | -9 | 382 | 463 |
| 4 | 2 | -9 | 89 | -103 |
| 5 | 2 | -9 | 178 | -201 |
| 6 | 2 | -9 | 77 | 94 |
|  | 2 | 10 | 302 | -322 |
| 1 | 2 | 10 | 68 | -100 |
| 2 | 2 | 10 | 312 | 377 |
| -2 | 2 | 10 | 140 | 159 |
| -3 | 2 | 10 | 120 | 142 |
| -4 | 2 | 10 | 168 | -181 |
| -5 | 2 | 10 | 54 | -56 |
| 6 | 2 | 10 | 266 | 248 |
|  | 2 | -10 | 95 | -118 |
| -1 | 2 | -10 | 252 | -273 |
| 2 | 2 | -10 | 107 | 110 |
| -2 | 2 | -10 | 421 | 500 |
| 3 | 2 | -10 | 49 | 76 |
| 4 | 2 | -10 | 101 | 116 |
| 5 | 2 | -10 | 94 | -104 |
| 6 | 2 | -10 | 142 | 121 |

| h | k | l | $F_o$ | $F_c$ |
|---|---|---|---|---|
|  | 2 | 11 | 202 | -215 |
| 2 | 2 | 11 | 193 | 214 |
| -3 | 2 | 11 | 123 | 130 |
| 4 | 2 | 11 | 150 | -161 |
| 5 | 2 | 11 | 87 | 107 |
| -5 | 2 | 11 | 119 | -127 |
| 6 | 2 | 11 | 144 | 128 |
| -6 | 2 | 11 | 38 | 50 |
| 7 | 2 | 11 | 61 | -22 |
|  | 2 | -11 | 325 | -356 |
| 1 | 2 | -11 | 191 | 210 |
| -2 | 2 | -11 | 241 | 274 |
| 6 | 2 | -11 | 127 | 98 |
| 2 | 2 | 12 | 131 | 167 |
| 3 | 2 | 12 | 100 | 134 |
| -3 | 2 | 12 | 53 | 71 |
| 4 | 2 | 12 | 163 | -175 |
| 5 | 2 | 12 | 116 | 117 |
| -5 | 2 | 12 | 94 | -108 |
| -6 | 2 | 12 | 106 | 91 |
| 7 | 2 | 12 | 61 | 86 |
| 8 | 2 | 12 | 70 | -70 |
| 1 | 2 | -12 | 252 | 246 |
| -1 | 2 | -12 | 175 | 200 |
| -2 | 2 | -12 | 73 | 112 |
| 3 | 2 | -12 | 96 | 107 |
| 4 | 2 | -12 | 104 | -107 |
| 0 | 2 | 13 | 107 | -91 |
| -1 | 2 | 13 | 150 | 122 |
| 3 | 2 | 13 | 114 | 129 |
| 4 | 2 | 13 | 243 | -240 |
| 5 | 2 | 13 | 67 | 59 |
| -5 | 2 | 13 | 76 | -97 |
| -6 | 2 | 13 | 89 | 85 |
| 7 | 2 | 13 | 151 | 143 |
| 8 | 2 | 13 | 96 | -68 |
|  | 2 | -13 | 414 | -445 |
| 1 | 2 | -13 | 114 | 107 |
| -1 | 2 | -13 | 252 | 223 |
| 3 | 2 | -13 | 122 | 120 |
| 6 | 2 | -13 | 62 | -51 |
| 0 | 2 | 14 | 121 | -118 |
| 1 | 2 | 14 | 124 | 118 |

| h | k | l | $F_o$ | $F_c$ |
|---|---|---|---|---|
| -1 | 2 | 14 | 85 | 68 |
| -2 | 2 | 14 | 93 | 98 |
| 3 | 2 | 14 | 120 | 126 |
| 4 | 2 | 14 | 156 | -160 |
| 5 | 2 | 14 | 65 | 76 |
| -6 | 2 | 14 | 55 | 66 |
| 7 | 2 | 14 | 139 | 142 |
| 8 | 2 | 14 | 86 | -72 |
|  | 2 | -14 | 209 | -211 |
| -1 | 2 | -14 | 86 | 98 |
| 3 | 2 | -14 | 83 | 88 |
| 4 | 2 | -14 | 96 | -82 |
| 0 | 2 | 15 | 386 | -358 |
| 4 | 2 | 15 | 67 | -90 |
| 7 | 2 | 15 | 62 | 61 |
| 8 | 2 | 15 | 55 | -58 |
| 1 | 2 | -15 | 75 | -94 |
| 4 | 2 | -15 | 86 | -86 |
|  | 2 | 16 | 160 | -174 |
| 1 | 2 | 16 | 67 | 86 |
| 3 | 2 | 16 | 90 | 75 |
| -3 | 2 | 16 | 86 | 82 |
| 5 | 2 | 16 | 130 | -136 |
| 7 | 2 | 16 | 70 | 67 |
| 1 | 2 | -16 | 126 | -134 |
| 2 | 2 | -16 | 147 | 130 |
| 4 | 2 | -16 | 70 | -62 |
| 0 | 2 | 17 | 90 | 70 |
| -1 | 2 | 17 | 154 | -133 |
| -2 | 2 | 17 | 153 | 142 |
| 5 | 2 | 17 | 86 | -97 |
| -1 | 2 | -17 | 116 | -132 |
| 2 | 2 | -17 | 113 | 106 |
|  | 2 | 18 | 86 | -95 |
| 1 | 2 | 18 | 90 | -124 |
| -1 | 2 | 18 | 86 | -107 |
| -2 | 2 | 18 | 116 | 121 |
| 5 | 2 | 18 | 61 | -92 |
| 6 | 2 | 18 | 76 | 95 |
| 2 | 2 | -18 | 63 | 67 |
| -2 | 2 | -18 | 114 | 130 |
| 1 | 2 | 19 | 87 | -91 |
| -1 | 2 | 19 | 81 | -95 |
| 2 | 2 | 19 | 119 | 136 |
| -2 | 2 | 19 | 106 | 121 |
| 3 | 2 | 19 | 86 | 84 |
| 5 | 2 | 19 | 58 | -64 |
| 6 | 2 | 19 | 70 | 76 |
| 2 | 2 | 20 | 79 | 125 |
| 6 | 2 | 20 | 61 | 61 |
| 2 | 2 | 21 | 109 | 127 |
| 2 | 3 |  | 429 | -387 |
| -2 | 3 |  | 520 | 474 |
| -3 | 3 |  | 115 | -129 |
| 4 | 3 |  | 264 | -286 |
| -4 | 3 |  | 297 | 247 |
| 5 | 3 |  | 182 | 181 |
| -5 | 3 |  | 42 | -16 |
| -6 | 3 |  | 218 | -192 |
| 8 | 3 |  | 108 | -110 |
| -8 | 3 |  | 83 | 79 |
| 2 | 3 | 1 | 767 | -740 |
| -2 | 3 | 1 | 313 | 210 |
| 3 | 3 | 1 | 43 | 38 |
| -3 | 3 | 1 | 359 | 301 |
| 4 | 3 | 1 | 305 | -297 |
| -4 | 3 | 1 | 113 | 109 |
| 5 | 3 | 1 | 234 | 226 |
| 6 | 3 | 1 | 53 | 61 |
| 7 | 3 | 1 | 54 | -56 |
| -8 | 3 | 1 | 162 | 149 |
| 1 | 3 | -1 | 205 | 219 |
| 2 | 3 | -1 | 316 | 335 |
| -2 | 3 | -1 | 733 | 726 |
| 3 | 3 | -1 | 387 | -377 |
| -3 | 3 | -1 | 79 | 70 |
| 4 | 3 | -1 | 100 | 93 |
| -4 | 3 | -1 | 329 | 288 |
| -6 | 3 | -1 | 256 | -222 |
| -7 | 3 | -1 | 48 | -37 |
| 8 | 3 | -1 | 113 | -101 |
| -8 | 3 | -1 | 101 | 97 |
| 1 | 3 | 2 | 249 | 248 |
| -1 | 3 | 2 | 270 | 192 |

| h | k | l | $F_o$ | $F_c$ |
|---|---|---|---|---|
| 2 | 3 | 2 | 452 | -430 |
| -2 | 3 | 2 | 402 | -350 |
| 3 | 3 | 2 | 72 | -74 |
| -3 | 3 | 2 | 653 | 678 |
| 4 | 3 | 2 | 346 | -359 |
| -4 | 3 | 2 | 297 | -280 |
| 5 | 3 | 2 | 281 | 276 |
| -5 | 3 | 2 | 185 | 156 |
| 6 | 3 | 2 | 70 | 59 |
| -6 | 3 | 2 | 191 | -168 |
| 7 | 3 | 2 | 85 | -74 |
| -8 | 3 | 2 | 123 | 108 |
| 1 | 3 | -2 | 386 | 304 |
| -1 | 3 | -2 | 205 | -222 |
| 2 | 3 | -2 | 207 | 150 |
| -2 | 3 | -2 | 440 | 365 |
| 3 | 3 | -2 | 464 | -457 |
| -3 | 3 | -2 | 58 | -40 |
| 4 | 3 | -2 | 257 | 240 |
| -4 | 3 | -2 | 406 | 385 |
| -5 | 3 | -2 | 298 | -284 |
| -6 | 3 | -2 | 65 | -65 |
| 8 | 3 | -2 | 55 | -70 |
| -8 | 3 | -2 | 86 | 87 |
| 1 | 3 | 3 | 217 | -203 |
| -1 | 3 | 3 | 475 | 389 |
| 2 | 3 | 3 | 237 | -235 |
| -2 | 3 | 3 | 612 | -530 |
| 3 | 3 | 3 | 95 | 118 |
| -3 | 3 | 3 | 375 | 335 |
| 4 | 3 | 3 | 262 | -281 |
| -4 | 3 | 3 | 137 | -140 |
| 5 | 3 | 3 | 294 | 282 |
| -5 | 3 | 3 | 59 | 75 |
| 6 | 3 | 3 | 86 | 91 |
| -6 | 3 | 3 | 120 | -126 |
| 7 | 3 | 3 | 62 | -70 |
| 1 | 3 | -3 | 350 | 346 |
| -1 | 3 | -3 | 389 | -318 |
| 2 | 3 | -3 | 232 | 200 |
| -2 | 3 | -3 | 343 | -326 |
| 3 | 3 | -3 | 429 | -393 |
| -3 | 3 | -3 | 68 | 65 |
| 4 | 3 | -3 | 277 | 278 |
| -4 | 3 | -3 | 366 | 314 |
| 5 | 3 | -3 | 59 | 78 |
| -5 | 3 | -3 | 279 | -266 |
| -6 | 3 | -3 | 88 | -95 |
| 1 | 3 | 4 | 420 | -383 |
| -1 | 3 | 4 | 163 | 123 |
| 2 | 3 | 4 | 346 | 358 |
| -2 | 3 | 4 | 527 | -459 |
| 3 | 3 | 4 | 296 | -275 |
| -3 | 3 | 4 | 333 | 306 |
| 4 | 3 | 4 | 242 | -216 |
| -4 | 3 | 4 | 54 | -48 |
| -5 | 3 | 4 | 43 | -47 |
| -7 | 3 | 4 | 101 | 92 |
| -8 | 3 | 4 | 34 | -35 |
| 1 | 3 | -4 | 321 | 311 |
| -1 | 3 | -4 | 362 | -345 |
| 2 | 3 | -4 | 86 | 84 |
| -2 | 3 | -4 | 215 | -172 |
| 3 | 3 | -4 | 498 | -482 |
| -3 | 3 | -4 | 410 | 385 |
| -4 | 3 | -4 | 272 | 270 |
| 5 | 3 | -4 | 119 | 116 |
| -5 | 3 | -4 | 234 | -229 |
| 6 | 3 | -4 | 56 | 57 |
| -6 | 3 | -4 | 67 | -67 |
| 7 | 3 | -4 | 62 | -52 |
| -7 | 3 | -4 | 67 | 69 |
| -8 | 3 | -4 | 53 | -51 |
| 1 | 3 | 5 | 154 | -116 |
| 2 | 3 | 5 | 526 | 540 |
| -2 | 3 | 5 | 120 | -128 |
| -3 | 3 | 5 | 95 | 75 |
| 4 | 3 | 5 | 112 | -104 |
| -4 | 3 | 5 | 146 | 120 |
| -5 | 3 | 5 | 197 | -178 |
| 6 | 3 | 5 | 234 | 220 |
| -7 | 3 | 5 | 103 | 104 |
| -8 | 3 | 5 | 50 | -47 |
| -1 | 3 | -5 | 329 | -300 |
| 2 | 3 | -5 | 318 | 312 |
| -2 | 3 | -5 | 241 | -230 |

| h | k | l | $F_o$ | $F_c$ |
|---|---|---|---|---|
| 3 | 3 | -5 | 227 | -224 |
| -3 | 3 | -5 | 468 | 469 |
| 4 | 3 | -5 | 117 | -128 |
| -4 | 3 | -5 | 103 | -104 |
| 5 | 3 | -5 | 150 | 144 |
| -5 | 3 | -5 | 176 | -166 |
| 6 | 3 | -5 | 68 | 79 |
| -6 | 3 | -5 | 58 | -64 |
| -7 | 3 | -5 | 88 | 89 |
| -1 | 3 | 6 | 207 | -154 |
| -2 | 3 | 6 | 135 | 78 |
| 3 | 3 | 6 | 326 | -336 |
| 4 | 3 | 6 | 257 | 267 |
| -4 | 3 | 6 | 257 | 250 |
| -5 | 3 | 6 | 288 | -298 |
| 6 | 3 | 6 | 216 | 194 |
| -7 | 3 | 6 | 87 | 74 |
| -8 | 3 | 6 | 34 | -14 |
| 1 | 3 | -6 | 86 | 90 |
| -2 | 3 | -6 | 86 | -92 |
| 3 | 3 | -6 | 68 | -90 |
| -3 | 3 | -6 | 429 | 399 |
| 4 | 3 | -6 | 169 | -164 |
| -4 | 3 | -6 | 259 | -249 |
| 5 | 3 | -6 | 161 | 163 |
| 7 | 3 | -6 | 46 | -56 |
| -7 | 3 | -6 | 61 | 58 |
| 1 | 3 | 7 | 184 | 154 |
| -2 | 3 | 7 | 229 | 246 |
| 3 | 3 | 7 | 276 | -301 |
| -3 | 3 | 7 | 114 | -110 |
| 4 | 3 | 7 | 122 | 119 |
| -4 | 3 | 7 | 284 | 323 |
| 5 | 3 | 7 | 154 | -149 |
| -5 | 3 | 7 | 254 | -271 |
| -6 | 3 | 7 | 45 | -38 |
| 1 | 3 | -7 | 115 | 113 |
| -1 | 3 | -7 | 92 | -89 |
| 2 | 3 | -7 | 210 | -221 |
| -2 | 3 | -7 | 331 | -307 |
| 3 | 3 | -7 | 65 | -91 |

| h | k | l | $F_o$ | $F_c$ |
|---|---|---|---|---|
| -3 | 3 | -7 | 497 | 485 |
| 4 | 3 | -7 | 166 | -158 |
| -4 | 3 | -7 | 282 | -292 |
| 5 | 3 | -7 | 101 | 90 |
| 6 | 3 | -7 | 115 | 118 |
| -7 | 3 | -7 | 56 | 59 |
| -8 | 3 | -7 | 62 | 61 |
| -1 | 3 | 8 | 188 | -232 |
| -2 | 3 | 8 | 237 | 223 |
| -4 | 3 | 8 | 203 | 194 |
| 5 | 3 | 8 | 66 | -79 |
| -5 | 3 | 8 | 120 | -136 |
| -6 | 3 | 8 | 95 | -85 |
| 1 | 3 | -8 | 239 | 234 |
| -1 | 3 | -8 | 120 | -109 |
| 2 | 3 | -8 | 154 | -156 |
| -2 | 3 | -8 | 50 | -49 |
| -3 | 3 | -8 | 218 | 229 |
| 4 | 3 | -8 | 147 | -138 |
| -5 | 3 | -8 | 68 | -79 |
| 6 | 3 | -8 | 124 | 135 |
| -8 | 3 | -8 | 103 | 115 |
| 1 | 3 | 9 | 232 | 212 |
| -1 | 3 | 9 | 121 | -155 |
| -2 | 3 | 9 | 177 | 192 |
| -3 | 3 | 9 | 187 | 225 |
| -6 | 3 | 9 | 55 | -60 |
| 1 | 3 | -9 | 203 | 185 |
| -1 | 3 | -9 | 227 | -241 |
| 2 | 3 | -9 | 223 | -235 |
| -2 | 3 | -9 | 211 | 224 |
| -3 | 3 | -9 | 63 | 85 |
| 4 | 3 | -9 | 154 | -155 |
| -4 | 3 | -9 | 110 | 141 |
| -5 | 3 | -9 | 120 | -127 |
| -6 | 3 | -9 | 52 | -43 |
| -8 | 3 | -9 | 109 | 110 |
| 1 | 3 | 10 | 113 | 150 |
| -1 | 3 | 10 | 259 | -322 |
| -2 | 3 | 10 | 60 | 72 |
| -3 | 3 | 10 | 263 | 311 |

| h | k | l | $F_o$ | $F_c$ |
|---|---|---|---|---|
| -4 | 3 | 10 | 69 | -105 |
| 1 | 3 | -10 | 160 | 131 |
| -1 | 3 | -10 | 193 | -187 |
| 2 | 3 | -10 | 47 | -48 |
| -2 | 3 | -10 | 149 | 151 |
| 3 | 3 | -10 | 94 | -99 |
| -3 | 3 | -10 | 68 | 97 |
| -4 | 3 | -10 | 156 | 167 |
| 5 | 3 | -10 | 69 | 59 |
| -5 | 3 | -10 | 154 | -154 |
| 6 | 3 | -10 | 59 | 55 |
| -6 | 3 | -10 | 65 | -61 |
| -7 | 3 | -10 | 40 | 34 |
| -8 | 3 | -10 | 68 | 76 |
| 1 | 3 | 11 | 248 | 333 |
| -1 | 3 | 11 | 117 | -148 |
| -4 | 3 | 11 | 119 | -149 |
| -6 | 3 | 11 | 52 | -67 |
| -1 | 3 | -11 | 154 | -152 |
| 2 | 3 | -11 | 129 | 127 |
| -2 | 3 | -11 | 217 | 225 |
| 3 | 3 | -11 | 162 | -146 |
| -4 | 3 | -11 | 155 | 169 |
| -5 | 3 | -11 | 157 | -169 |
| 6 | 3 | -11 | 59 | 56 |
| -6 | 3 | -11 | 77 | -82 |
| -7 | 3 | -11 | 62 | 60 |
| 1 | 3 | 12 | 101 | 152 |
| -2 | 3 | 12 | 108 | -141 |
| -3 | 3 | 12 | 252 | 337 |
| 2 | 3 | -12 | 142 | 140 |
| -2 | 3 | -12 | 49 | 45 |
| 3 | 3 | -12 | 143 | -127 |
| -3 | 3 | -12 | 55 | 8 |
| -4 | 3 | -12 | 137 | 148 |
| -5 | 3 | -12 | 94 | -91 |
| 6 | 3 | -12 | 43 | 31 |
| -6 | 3 | -12 | 47 | -37 |
| -7 | 3 | -12 | 52 | 63 |
| -2 | 3 | 13 | 113 | -158 |
| -3 | 3 | 13 | 109 | 143 |

| h | k | l | $F_o$ | $F_c$ |
|---|---|---|---|---|
| 2 | 3 | -13 | 134 | 117 |
| -2 | 3 | -13 | 128 | -130 |
| 3 | 3 | -13 | 141 | -122 |
| -3 | 3 | -13 | 81 | 96 |
| -4 | 3 | -13 | 139 | 156 |
| -6 | 3 | -13 | 115 | -124 |
| -7 | 3 | -13 | 53 | 59 |
| -8 | 3 | -13 | 54 | -45 |
| -5 | 3 | 14 | 63 | -87 |
| 2 | 3 | -14 | 119 | 109 |
| -2 | 3 | -14 | 140 | -139 |
| 3 | 3 | -14 | 121 | -101 |
| -3 | 3 | -14 | 143 | 138 |
| 5 | 3 | -14 | 65 | 52 |
| -5 | 3 | -14 | 61 | -41 |
| -6 | 3 | -14 | 129 | -141 |
| 1 | 3 | 15 | 96 | 27 |
| 1 | 3 | -15 | 137 | 132 |
| -2 | 3 | -15 | 135 | -114 |
| 3 | 3 | -15 | 85 | -67 |
| -3 | 3 | -15 | 135 | 125 |
| 4 | 3 | -15 | 56 | -45 |
| 5 | 3 | -15 | 103 | 80 |
| -5 | 3 | -15 | 79 | -70 |
| -1 | 3 | 16 | 85 | -185 |
| -2 | 3 | 16 | 69 | 155 |
| 1 | 3 | -16 | 136 | 107 |
| -1 | 3 | -16 | 137 | -133 |
| -2 | 3 | -16 | 115 | -108 |
| -3 | 3 | -16 | 142 | 124 |
| 4 | 3 | -16 | 92 | -79 |
| -6 | 3 | -16 | 67 | -55 |
| -7 | 3 | -16 | 39 | 42 |
| 1 | 3 | -17 | 60 | 61 |
| -1 | 3 | -17 | 130 | -109 |
| -3 | 3 | -17 | 120 | 101 |
| 4 | 3 | -17 | 103 | -76 |
| -6 | 3 | -17 | 63 | -49 |
| 1 | 3 | -18 | 142 | 111 |
| -1 | 3 | -18 | 67 | -60 |
| 2 | 3 | -18 | 40 | -46 |

| h | k | l | $F_o$ | $F_c$ |
|---|---|---|---|---|
| -3 | 3 | -18 | 83 | 67 |
| -6 | 3 | -18 | 43 | -28 |
| 1 | 3 | -19 | 113 | 94 |
| -1 | 3 | -19 | 139 | -104 |
| 2 | 3 | -19 | 56 | -46 |
| -2 | 3 | -19 | 41 | 33 |
| -4 | 3 | -19 | 55 | 43 |
| -5 | 3 | -19 | 69 | -47 |
| -6 | 3 | -19 | 34 | -22 |
| 1 | 3 | -20 | 129 | 77 |
| -1 | 3 | -20 | 106 | -94 |
| -2 | 3 | -20 | 47 | 46 |
| -4 | 3 | -20 | 93 | 73 |
| -5 | 3 | -20 | 109 | -78 |
| 1 | 3 | -21 | 56 | 48 |
| -1 | 3 | -21 | 131 | -80 |
| -2 | 3 | -21 | 66 | 44 |
| -4 | 3 | -21 | 108 | 72 |
| -1 | 3 | -22 | 56 | -47 |
| -1 | 4 | | 137 | -138 |
| 2 | 4 | | 306 | -287 |
| -2 | 4 | | 378 | -356 |
| 3 | 4 | | 93 | -83 |
| 4 | 4 | | 305 | 313 |
| 5 | 4 | | 154 | -139 |
| -5 | 4 | | 169 | 143 |
| 6 | 4 | | 66 | 79 |
| -6 | 4 | | 188 | -165 |
| 7 | 4 | | 128 | -115 |
| 1 | 4 | 1 | 197 | -176 |
| -1 | 4 | 1 | 70 | 92 |
| 2 | 4 | 1 | 134 | -131 |
| -2 | 4 | 1 | 377 | -354 |
| 3 | 4 | 1 | 188 | -201 |
| -3 | 4 | 1 | 96 | 92 |
| 4 | 4 | 1 | 310 | 306 |
| -4 | 4 | 1 | 170 | -165 |
| 5 | 4 | 1 | 90 | -83 |
| -5 | 4 | 1 | 281 | 294 |
| 6 | 4 | 1 | 81 | 80 |
| -6 | 4 | 1 | 167 | -148 |
| 7 | 4 | 1 | 195 | -168 |
| -8 | 4 | 1 | 39 | 32 |
| 0 | 4 | -1 | 467 | 441 |
| 1 | 4 | -1 | 103 | -76 |
| -1 | 4 | -1 | 16 | 9 |
| 2 | 4 | -1 | 394 | -400 |
| -2 | 4 | -1 | 153 | -141 |
| 4 | 4 | -1 | 242 | 246 |
| -4 | 4 | -1 | 176 | 160 |
| 5 | 4 | -1 | 191 | -171 |
| -5 | 4 | -1 | 156 | 147 |
| -6 | 4 | -1 | 257 | -242 |
| 7 | 4 | -1 | 72 | -62 |
| -8 | 4 | -1 | 33 | -29 |
| 1 | 4 | 2 | 86 | 85 |
| -1 | 4 | 2 | 154 | 138 |
| 2 | 4 | 2 | 326 | -330 |
| -2 | 4 | 2 | 291 | -248 |
| -3 | 4 | 2 | 77 | 63 |
| 4 | 4 | 2 | 277 | 284 |
| -4 | 4 | 2 | 195 | -171 |
| -6 | 4 | 2 | 158 | -149 |
| 7 | 4 | 2 | 158 | -124 |
| -8 | 4 | 2 | 45 | 47 |
| 1 | 4 | -2 | 102 | -66 |
| -1 | 4 | -2 | 97 | -86 |
| 2 | 4 | -2 | 216 | -197 |
| -2 | 4 | -2 | 342 | -302 |
| 3 | 4 | -2 | 61 | -59 |
| -3 | 4 | -2 | 200 | -202 |
| 4 | 4 | -2 | 242 | 253 |
| -4 | 4 | -2 | 328 | 300 |
| -5 | 4 | -2 | 122 | 117 |
| 6 | 4 | -2 | 120 | -95 |
| -6 | 4 | -2 | 197 | -200 |
| -7 | 4 | -2 | 70 | 68 |
| 1 | 4 | 3 | 162 | 141 |
| -1 | 4 | 3 | 135 | 83 |
| 2 | 4 | 3 | 317 | -341 |
| -2 | 4 | 3 | 230 | -223 |
| -3 | 4 | 3 | 52 | -42 |

| h | k | l | $F_o$ | $F_c$ |
|---|---|---|---|---|
| 4 | 4 | 3 | 154 | 146 |
| 5 | 4 | 3 | 113 | 86 |
| -5 | 4 | 3 | 62 | -54 |
| 6 | 4 | 3 | 130 | -111 |
| -6 | 4 | 3 | 59 | -52 |
| -7 | 4 | 3 | 191 | -175 |
| -8 | 4 | 3 | 62 | 50 |
| 0 | 4 | -3 | 308 | 301 |
| 1 | 4 | -3 | 62 | 39 |
| -1 | 4 | -3 | 89 | -68 |
| 2 | 4 | -3 | 176 | -175 |
| -2 | 4 | -3 | 411 | -395 |
| 3 | 4 | -3 | 232 | -233 |
| -3 | 3 | -3 | 97 | -88 |
| 4 | 4 | -3 | 130 | 123 |
| -4 | 4 | -3 | 318 | 328 |
| 5 | 4 | -3 | 130 | 119 |
| 6 | 4 | -3 | 134 | -118 |
| -6 | 4 | -3 | 115 | -110 |
| | 4 | 4 | 355 | 379 |
| -1 | 4 | 4 | 363 | 344 |
| 2 | 4 | 4 | 252 | -240 |
| -2 | 4 | 4 | 130 | -114 |
| 3 | 4 | 4 | 86 | 84 |
| -3 | 4 | 4 | 158 | -153 |
| -4 | 4 | 4 | 104 | 80 |
| 5 | 4 | 4 | 140 | 148 |
| -5 | 4 | 4 | 52 | 59 |
| 6 | 4 | 4 | 218 | -205 |
| -6 | 4 | 4 | 68 | 76 |
| -7 | 4 | 4 | 168 | -151 |
| -8 | 4 | 4 | 68 | 54 |
| | 4 | -4 | 214 | 281 |
| 1 | 4 | -4 | 154 | 179 |
| -1 | 4 | -4 | 50 | 39 |
| -2 | 4 | -4 | 225 | -197 |
| 3 | 4 | -4 | 269 | -274 |
| -3 | 4 | -4 | 47 | -46 |
| 4 | 4 | -4 | 110 | -105 |
| -4 | 4 | -4 | 303 | 330 |
| 5 | 4 | -4 | 142 | 132 |

| h | k | l | $F_o$ | $F_c$ |
|---|---|---|---|---|
| -5 | 4 | -4 | 95 | -80 |
| 6 | 4 | -4 | 207 | -185 |
| -7 | 4 | -4 | 56 | -56 |
| 0 | 4 | 5 | 117 | 98 |
| 1 | 4 | 5 | 313 | 318 |
| -1 | 4 | 5 | 383 | 389 |
| -2 | 4 | 5 | 123 | -107 |
| 3 | 4 | 5 | 75 | 82 |
| -3 | 4 | 5 | 133 | -142 |
| 4 | 4 | 5 | 162 | -150 |
| -4 | 4 | 5 | 46 | 59 |
| 5 | 4 | 5 | 144 | 119 |
| -6 | 4 | 5 | 101 | 96 |
| -7 | 4 | 5 | 137 | -123 |
| -8 | 4 | 5 | 58 | 51 |
| | 4 | -5 | 189 | 211 |
| 1 | 4 | -5 | 90 | 131 |
| -1 | 4 | -5 | 160 | 176 |
| 2 | 4 | -5 | 61 | 54 |
| -2 | 4 | -5 | 180 | -163 |
| -3 | 4 | -5 | 62 | -55 |
| -4 | 4 | -5 | 239 | 257 |
| 5 | 4 | -5 | 161 | 157 |
| -5 | 4 | -5 | 154 | -135 |
| 6 | 4 | -5 | 141 | -138 |
| -6 | 4 | -5 | 85 | 75 |
| -7 | 4 | -5 | 134 | -124 |
| -8 | 4 | -5 | 72 | 55 |
| 1 | 4 | 6 | 355 | 390 |
| -1 | 4 | 6 | 205 | 176 |
| -2 | 4 | 6 | 47 | -42 |
| -3 | 4 | 6 | 161 | -154 |
| 4 | 4 | 6 | 169 | -168 |
| -4 | 4 | 6 | 97 | 101 |
| -5 | 4 | 6 | 48 | -48 |
| -7 | 4 | 6 | 86 | -76 |
| | 4 | -6 | 352 | 397 |
| 1 | 4 | -6 | 96 | -101 |
| -1 | 4 | -6 | 90 | 128 |
| -2 | 4 | -6 | 42 | -33 |
| -3 | 4 | -6 | 223 | -232 |

| h | k | l | $F_o$ | $F_c$ |
|---|---|---|---|---|
| 4 | 4 | -6 | 74 | -70 |
| -4 | 4 | -6 | 241 | 235 |
| 5 | 4 | -6 | 156 | 127 |
| -5 | 4 | -6 | 180 | -182 |
| 6 | 4 | -6 | 60 | -56 |
| -6 | 4 | -6 | 69 | 74 |
| 7 | 4 | -6 | 67 | -65 |
| -7 | 4 | -6 | 169 | -164 |
| -8 | 4 | -6 | 103 | 97 |
| 0 | 4 | 7 | 135 | -69 |
| 1 | 4 | 7 | 201 | 194 |
| -1 | 4 | 7 | 197 | 197 |
| -2 | 4 | 7 | 54 | -97 |
| -3 | 4 | 7 | 69 | -73 |
| -4 | 4 | 7 | 183 | 165 |
|  | 4 | -7 | 376 | 411 |
| 1 | 4 | -7 | 112 | -106 |
| -1 | 4 | -7 | 90 | -90 |
| 2 | 4 | -7 | 55 | -70 |
| -2 | 4 | -7 | 67 | 55 |
| 3 | 4 | -7 | 60 | 67 |
| -3 | 4 | -7 | 245 | -284 |
| 4 | 4 | -7 | 94 | -103 |
| -4 | 4 | -7 | 128 | 129 |
| 5 | 4 | -7 | 139 | 146 |
| 7 | 4 | -7 | 65 | -51 |
| -7 | 4 | -7 | 127 | -122 |
| -8 | 4 | -7 | 123 | 113 |
| 0 | 4 | 8 | 139 | 101 |
| 1 | 4 | 8 | 185 | 184 |
| -2 | 4 | 8 | 171 | -177 |
| -4 | 4 | 8 | 151 | 142 |
| -5 | 4 | 8 | 102 | 102 |
| -6 | 4 | 8 | 127 | -115 |
| 1 | 4 | -8 | 72 | -82 |
| -1 | 4 | -8 | 102 | -101 |
| 2 | 4 | -8 | 61 | -42 |
| -2 | 4 | -8 | 29 | -44 |
| 3 | 4 | -8 | 72 | -88 |
| -3 | 4 | -8 | 32 | -39 |
| 4 | 4 | -8 | 107 | 120 |

| h | k | l | $F_o$ | $F_c$ |
|---|---|---|---|---|
| -4 | 4 | -8 | 103 | -95 |
| -5 | 4 | -8 | 124 | 119 |
| -6 | 4 | -8 | 109 | -101 |
| 7 | 4 | -8 | 106 | -82 |
| -7 | 4 | -8 | 83 | -74 |
| -8 | 4 | -8 | 95 | 83 |
| -1 | 4 | 9 | 169 | -155 |
| -3 | 4 | 9 | 157 | -171 |
| -4 | 4 | 9 | 154 | 139 |
| -5 | 4 | 9 | 134 | 119 |
| -6 | 4 | 9 | 142 | -124 |
| 0 | 4 | -9 | 95 | 79 |
| 1 | 4 | -9 | 164 | 152 |
| -1 | 4 | -9 | 70 | -69 |
| 2 | 4 | -9 | 174 | -172 |
| -2 | 4 | -9 | 55 | -64 |
| 4 | 4 | -9 | 142 | 145 |
| -5 | 4 | -9 | 133 | 125 |
| 6 | 4 | -9 | 34 | 41 |
| -6 | 4 | -9 | 128 | -126 |
| -7 | 4 | -9 | 43 | -52 |
| -8 | 4 | -9 | 38 | 47 |
|  | 4 | 10 | 46 | 63 |
| 1 | 4 | 10 | 146 | -151 |
| -1 | 4 | 10 | 110 | -83 |
| -3 | 4 | 10 | 140 | -136 |
| -4 | 4 | 10 | 86 | 70 |
| -5 | 4 | 10 | 96 | 102 |
| -6 | 4 | 10 | 127 | -113 |
|  | 4 | -10 | 217 | -222 |
| 1 | 4 | -10 | 254 | 234 |
| -1 | 4 | -10 | 160 | 150 |
| 2 | 4 | -10 | 254 | -246 |
| -2 | 4 | -10 | 55 | -51 |
| 3 | 4 | -10 | 53 | 43 |
| -3 | 4 | -10 | 60 | 63 |
| 4 | 4 | -10 | 89 | 81 |
| -4 | 4 | -10 | 72 | -73 |
| -5 | 4 | -10 | 163 | 165 |
| -6 | 4 | -10 | 193 | -192 |
|  | 4 | 11 | 243 | 288 |

| h | k | l | $F_o$ | $F_c$ |
|---|---|---|---|---|
| 1 | 4 | 11 | 102 | -94 |
| -1 | 4 | 11 | 127 | -131 |
| -3 | 4 | 11 | 88 | -81 |
| -6 | 4 | 11 | 104 | -79 |
| 0 | 4 | -11 | 201 | -197 |
| 1 | 4 | -11 | 204 | 180 |
| -1 | 4 | -11 | 215 | 221 |
| 2 | 4 | -11 | 224 | -223 |
| -2 | 4 | -11 | 161 | -186 |
| -3 | 4 | -11 | 67 | -75 |
| 4 | 4 | -11 | 92 | 87 |
| -4 | 4 | -11 | 86 | -97 |
| -5 | 4 | -11 | 147 | 142 |
| 6 | 4 | -11 | 40 | -38 |
| -6 | 4 | -11 | 135 | -142 |
| -7 | 4 | -11 | 40 | 34 |
| 1 | 4 | 12 | 117 | -150 |
| -1 | 4 | 12 | 117 | -123 |
| -6 | 4 | 12 | 46 | -30 |
| 0 | 4 | -12 | 82 | -55 |
| 1 | 4 | -12 | 157 | 144 |
| -1 | 4 | -12 | 188 | 186 |
| 2 | 4 | -12 | 150 | -127 |
| -2 | 4 | -12 | 241 | -242 |
| -3 | 4 | -12 | 34 | -31 |
| 4 | 4 | -12 | 60 | 66 |
| -4 | 4 | -12 | 97 | 118 |
| -5 | 4 | -12 | 142 | 157 |
| 6 | 4 | -12 | 89 | -88 |
| -6 | 4 | -12 | 66 | -65 |
| 1 | 4 | 13 | 121 | -129 |
| -1 | 4 | 13 | 50 | -76 |
| -2 | 4 | 13 | 120 | -153 |
| -4 | 4 | 13 | 61 | 71 |
| -1 | 4 | -13 | 144 | 141 |
| 2 | 4 | -13 | 92 | -83 |
| -2 | 4 | -13 | 214 | -223 |
| -3 | 4 | -13 | 50 | 43 |
| 4 | 4 | -13 | 62 | 63 |
| -4 | 4 | -13 | 124 | 143 |
| 5 | 4 | -13 | 43 | 48 |

| h | k | l | $F_o$ | $F_c$ |
|---|---|---|---|---|
| -7 | 4 | -13 | 69 | -72 |
|  | 4 | 14 | 188 | 254 |
| 1 | 4 | 14 | 53 | -95 |
| -1 | 4 | 14 | 50 | 79 |
| -2 | 4 | 14 | 166 | -185 |
| 0 | 4 | -14 | 224 | 209 |
| 1 | 4 | -14 | 100 | -75 |
| -2 | 4 | -14 | 150 | -133 |
| 3 | 4 | -14 | 87 | -83 |
| 4 | 4 | -14 | 48 | 54 |
| -4 | 4 | -14 | 87 | 88 |
| 5 | 4 | -14 | 55 | 48 |
| -7 | 4 | -14 | 68 | -56 |
|  | 4 | 15 | 70 | 73 |
| 1 | 4 | 15 | 52 | 81 |
| -1 | 4 | 15 | 156 | 199 |
| -2 | 4 | 15 | 121 | -153 |
| -4 | 4 | 15 | 103 | 89 |
|  | 4 | -15 | 291 | 315 |
| 1 | 4 | -15 | 93 | -104 |
| -1 | 4 | -15 | 110 | -89 |
| -2 | 4 | -15 | 90 | -85 |
| 3 | 4 | -15 | 59 | -65 |
| -4 | 4 | -15 | 99 | 94 |
| -6 | 4 | -15 | 36 | 39 |
| -7 | 4 | -15 | 112 | -85 |
| 1 | 4 | 16 | 148 | 206 |
| -1 | 4 | 16 | 150 | 201 |
| -2 | 4 | 16 | 137 | -158 |
|  | 4 | -16 | 197 | 216 |
| 1 | 4 | -16 | 79 | -101 |
| -1 | 4 | -16 | 114 | -103 |
| -2 | 4 | -16 | 34 | -31 |
| -3 | 4 | -16 | 41 | -44 |
| -4 | 4 | -16 | 86 | 74 |
| 1 | 4 | 17 | 131 | 174 |
| -1 | 4 | 17 | 86 | 122 |
| -2 | 4 | 17 | 95 | -122 |
|  | 4 | -17 | 194 | 209 |
| 1 | 4 | -17 | 50 | -61 |
| -1 | 4 | -17 | 106 | -109 |

| h | k | l | $F_o$ | $F_c$ |
|---|---|---|---|---|
| -2 | 4 | -17 | 40 | 42 |
| -3 | 4 | -17 | 95 | -82 |
| -4 | 4 | -17 | 87 | 60 |
| -6 | 4 | -17 | 45 | -44 |
| | 4 | -18 | 104 | 126 |
| -1 | 4 | -18 | 50 | -58 |
| 2 | 4 | -18 | 60 | -75 |
| -3 | 4 | -18 | 56 | -63 |
| -4 | 4 | -18 | 63 | 53 |
| -5 | 4 | -18 | 56 | 50 |
| -6 | 4 | -18 | 95 | -93 |
| | 4 | 19 | 60 | 89 |
| 1 | 4 | -19 | 47 | 62 |
| 2 | 4 | -19 | 68 | -89 |
| -2 | 4 | -19 | 48 | -52 |
| -4 | 4 | -19 | 31 | 38 |
| -5 | 4 | -19 | 55 | 56 |
| -1 | 4 | 20 | 75 | -79 |
| | 4 | -20 | 36 | -44 |
| 1 | 4 | -20 | 66 | 77 |
| -1 | 4 | -20 | 41 | 65 |
| -2 | 4 | -20 | 68 | -87 |
| -4 | 4 | -20 | 36 | 38 |
| | 4 | -21 | 34 | -46 |
| -1 | 4 | -21 | 69 | 80 |
| -2 | 4 | -21 | 70 | -91 |
| 1 | 5 | | 363 | -298 |
| -1 | 5 | | 41 | -48 |
| 2 | 5 | | 40 | -29 |
| -2 | 5 | | 322 | 286 |
| 3 | 5 | | 223 | 216 |
| -3 | 5 | | 468 | -455 |
| 4 | 5 | | 190 | 183 |
| -4 | 5 | | 119 | 96 |
| 5 | 5 | | 208 | -203 |
| -5 | 5 | | 150 | -129 |
| -7 | 5 | | 101 | -100 |
| 1 | 5 | | 58 | 55 |
| -1 | 5 | 1 | 21 | 19 |
| 2 | 5 | 1 | 154 | -164 |
| -2 | 5 | 1 | 328 | 289 |

| h | k | l | $F_o$ | $F_c$ |
|---|---|---|---|---|
| -3 | 5 | 1 | 310 | -272 |
| 5 | 5 | 1 | 97 | -75 |
| -5 | 5 | 1 | 245 | 236 |
| 6 | 5 | 1 | 60 | -61 |
| -7 | 5 | 1 | 86 | -71 |
| 1 | 5 | -1 | 112 | -70 |
| -1 | 5 | -1 | 285 | 282 |
| 2 | 5 | -1 | 120 | 98 |
| -2 | 5 | -1 | 168 | 149 |
| -3 | 5 | -1 | 486 | -513 |
| 4 | 5 | -1 | 298 | 289 |
| -4 | 5 | -1 | 216 | 208 |
| 5 | 5 | -1 | 229 | -214 |
| 6 | 5 | -1 | 100 | -98 |
| -7 | 5 | -1 | 112 | -111 |
| 1 | 5 | 2 | 59 | -29 |
| 2 | 5 | 2 | 302 | -260 |
| -2 | 5 | 2 | 60 | 48 |
| 3 | 5 | 2 | 433 | 492 |
| -3 | 5 | 2 | 117 | -104 |
| 4 | 5 | 2 | 191 | -178 |
| -4 | 5 | 2 | 258 | -224 |
| -5 | 5 | 2 | 173 | 156 |
| 6 | 5 | 2 | 119 | -104 |
| -7 | 5 | 2 | 96 | -82 |
| -8 | 5 | 2 | 36 | 30 |
| 1 | 5 | -2 | 66 | -49 |
| -1 | 5 | -2 | 101 | 74 |
| 2 | 5 | -2 | 211 | 206 |
| -2 | 5 | -2 | 60 | 33 |
| 3 | 5 | -2 | 194 | -163 |
| -3 | 5 | -2 | 447 | -472 |
| 4 | 5 | -2 | 343 | 365 |
| -4 | 5 | -2 | 216 | 192 |
| 5 | 5 | -2 | 109 | -93 |
| 6 | 5 | -2 | 52 | -53 |
| -6 | 5 | -2 | 75 | 74 |
| -8 | 5 | -2 | 54 | -47 |
| 1 | 5 | 3 | 432 | -396 |
| -1 | 5 | 3 | 328 | 329 |
| 2 | 5 | 3 | 290 | -269 |

| h | k | l | $F_o$ | $F_c$ |
|---|---|---|---|---|
| -2 | 5 | 3 | 183 | -147 |
| -3 | 5 | 3 | 154 | 132 |
| 4 | 5 | 3 | 191 | -212 |
| -4 | 5 | 3 | 271 | -259 |
| 5 | 5 | 3 | 46 | 51 |
| -5 | 5 | 3 | 131 | 109 |
| 6 | 5 | 3 | 147 | -117 |
| -7 | 5 | 3 | 50 | -51 |
| 1 | 5 | -3 | 108 | -88 |
| -1 | 5 | -3 | 77 | 55 |
| 2 | 5 | -3 | 229 | 219 |
| -2 | 5 | -3 | 128 | -118 |
| 3 | 5 | -3 | 217 | -221 |
| -3 | 5 | -3 | 239 | -229 |
| 4 | 5 | -3 | 194 | 192 |
| 5 | 5 | -3 | 54 | -65 |
| 6 | 5 | -3 | 36 | -36 |
| -6 | 5 | -3 | 127 | 118 |
| -8 | 5 | -3 | 95 | -84 |
| 1 | 5 | 4 | 262 | -308 |
| -1 | 5 | 4 | 444 | 438 |
| 2 | 5 | 4 | 49 | -51 |
| -2 | 5 | 4 | 291 | -252 |
| 3 | 5 | 4 | 254 | 256 |
| -3 | 5 | 4 | 210 | 193 |
| -4 | 5 | 4 | 104 | -92 |
| -4 | 5 | 4 | 104 | -72 |
| -5 | 5 | 4 | 201 | 204 |
| -6 | 5 | 4 | 94 | 78 |
| 1 | 5 | -4 | 216 | -218 |
| -1 | 5 | -4 | 101 | 86 |
| 2 | 5 | -4 | 157 | 153 |
| -2 | 5 | -4 | 217 | -225 |
| -4 | 5 | -4 | 190 | -189 |
| -5 | 5 | -4 | 100 | 89 |
| 6 | 5 | -4 | 68 | -60 |
| -6 | 5 | -4 | 123 | 108 |
| -8 | 5 | -4 | 103 | -100 |
| 1 | 5 | 5 | 372 | -449 |
| -1 | 5 | 5 | 380 | 425 |
| -2 | 5 | 5 | 326 | -290 |
| 3 | 5 | 5 | 101 | 101 |
| -3 | 5 | 5 | 173 | -175 |
| -4 | 5 | 5 | 151 | -146 |
| -5 | 5 | 5 | 104 | 84 |
| -6 | 5 | 5 | 137 | 115 |
| -7 | 5 | 5 | 43 | 29 |
| 1 | 5 | -5 | 189 | -200 |
| -1 | 5 | -5 | 201 | 234 |
| 2 | 5 | -5 | 34 | -58 |
| -2 | 5 | -5 | 235 | -216 |
| 3 | 5 | -5 | 184 | 193 |
| -3 | 5 | -5 | 200 | 183 |
| 4 | 5 | -5 | 96 | -104 |
| -4 | 5 | -5 | 309 | -306 |
| -5 | 5 | -5 | 210 | 200 |
| 6 | 5 | -5 | 48 | -51 |
| -6 | 5 | -5 | 54 | 60 |
| -8 | 5 | -5 | 75 | -70 |
| -1 | 5 | 6 | 166 | 177 |
| -2 | 5 | 6 | 70 | 4 |
| -3 | 5 | 6 | 255 | -247 |
| -4 | 5 | 6 | 101 | -61 |
| -5 | 5 | 6 | 58 | -48 |
| -6 | 5 | 6 | 117 | 97 |
| -7 | 5 | 6 | 66 | 39 |
| 1 | 5 | -6 | 122 | -154 |
| -1 | 5 | -6 | 185 | 208 |
| 2 | 5 | -6 | 137 | -115 |
| -2 | 5 | -6 | 149 | -152 |
| 3 | 5 | -6 | 216 | 182 |
| -3 | 5 | -6 | 218 | 217 |
| 4 | 5 | -6 | 65 | -65 |
| -4 | 5 | -6 | 339 | -389 |
| -5 | 5 | -6 | 227 | 222 |
| 1 | 5 | 7 | 157 | -160 |
| -1 | 5 | 7 | 41 | -39 |
| -2 | 5 | 7 | 157 | 148 |
| -3 | 5 | 7 | 221 | -212 |
| -6 | 5 | 7 | 69 | 68 |
| -7 | 5 | 7 | 43 | 22 |
| 1 | 5 | -7 | 69 | 83 |

| h | k | l | $F_o$ | $F_c$ |
|---|---|---|---|---|
| -1 | 5 | -7 | 117 | 150 |
| 2 | 5 | -7 | 303 | -345 |
| -2 | 5 | -7 | 41 | 62 |
| 3 | 5 | -7 | 266 | 262 |
| 4 | 5 | -7 | 39 | -30 |
| -4 | 5 | -7 | 195 | -197 |
| -5 | 5 | -7 | 104 | 102 |
| -6 | 5 | -7 | 103 | 98 |
| -7 | 5 | -7 | 55 | -50 |
| -8 | 5 | -7 | 27 | 33 |
| 1 | 5 | 8 | 40 | 51 |
| -1 | 5 | 8 | 123 | -126 |
| 2 | 5 | 8 | 55 | -22 |
| -2 | 5 | 8 | 178 | 191 |
| -3 | 5 | 8 | 272 | -298 |
| -4 | 5 | 8 | 100 | 80 |
| -6 | 5 | 8 | 65 | 56 |
| 1 | 5 | -8 | 106 | 81 |
| -1 | 5 | -8 | 67 | -86 |
| 2 | 5 | -8 | 256 | -276 |
| -2 | 5 | -8 | 142 | 136 |
| 3 | 5 | -8 | 212 | 260 |
| -3 | 5 | -8 | 173 | -191 |
| -5 | 5 | -8 | 54 | 60 |
| -6 | 5 | -8 | 74 | 64 |
| 1 | 5 | 9 | 112 | 132 |
| -1 | 5 | 9 | 79 | -84 |
| 2 | 5 | 9 | 144 | -145 |
| -3 | 5 | 9 | 190 | -192 |
| -6 | 5 | 9 | 60 | 52 |
| -7 | 5 | 9 | 48 | -30 |
| 1 | 5 | -9 | 158 | -162 |
| -1 | 5 | -9 | 108 | -92 |
| -2 | 5 | -9 | 295 | 361 |
| 3 | 5 | -9 | 86 | 104 |
| -3 | 5 | -9 | 209 | -196 |
| -4 | 5 | -9 | 103 | 111 |
| 5 | 5 | -9 | 54 | -84 |
| -6 | 5 | -9 | 46 | 44 |
| 1 | 5 | 10 | 85 | 99 |
| 2 | 5 | 10 | 162 | -194 |
| -3 | 5 | 10 | 49 | -45 |
| -4 | 5 | 10 | 95 | -113 |
| -5 | 5 | 10 | 94 | 88 |
| 1 | 5 | -10 | 169 | -169 |
| -1 | 5 | -10 | 148 | 152 |
| 2 | 5 | -10 | 73 | 67 |
| -2 | 5 | -10 | 231 | 278 |
| -3 | 5 | -10 | 256 | -276 |
| 4 | 5 | -10 | 55 | 109 |
| -4 | 5 | -10 | 87 | 81 |
| 5 | 5 | -10 | 77 | -104 |
| -5 | 5 | -10 | 60 | -59 |
| -6 | 5 | -10 | 88 | 73 |
| -1 | 5 | 11 | 48 | 50 |
| -4 | 5 | 11 | 120 | -130 |
| -5 | 5 | 11 | 103 | 95 |
| 1 | 5 | -11 | 149 | -176 |
| -1 | 5 | -11 | 168 | 169 |
| 2 | 5 | -11 | 92 | 116 |
| -3 | 5 | -11 | 225 | -266 |
| 4 | 5 | -11 | 49 | 103 |
| -4 | 5 | -11 | 59 | 35 |
| 5 | 5 | -11 | 87 | -112 |
| -6 | 5 | -11 | 77 | 59 |
| 1 | 5 | 12 | 59 | -72 |
| -1 | 5 | 12 | 93 | 125 |
| -3 | 5 | 12 | 60 | 55 |
| -4 | 5 | 12 | 114 | -104 |
| -5 | 5 | 12 | 97 | 85 |
| -6 | 5 | 12 | 39 | 29 |
| 1 | 5 | -12 | 144 | -153 |
| -1 | 5 | -12 | 158 | 179 |
| 2 | 5 | -12 | 77 | 118 |
| -2 | 5 | -12 | 74 | -75 |
| -3 | 5 | -12 | 109 | -109 |
| -4 | 5 | -12 | 38 | 46 |
| 5 | 5 | -12 | 47 | -70 |
| -6 | 5 | -12 | 47 | 48 |
| 1 | 5 | 13 | 90 | -129 |
| -1 | 5 | 13 | 76 | 87 |
| -4 | 5 | 13 | 50 | -48 |

| h | k | l | $F_o$ | $F_c$ |
|---|---|---|---|---|
| -5 | 5 | 13 | 68 | 57 |
| 1 | 5 | -13 | 103 | -158 |
| -1 | 5 | -13 | 167 | 165 |
| -2 | 5 | -13 | 115 | -123 |
| -4 | 5 | -13 | 61 | -71 |
| -5 | 5 | -13 | 63 | 70 |
| -6 | 5 | -13 | 40 | 35 |
| 1 | 5 | 14 | 63 | -96 |
| -1 | 5 | 14 | 86 | 121 |
| -2 | 5 | 14 | 79 | -86 |
| 1 | 5 | -14 | 43 | -72 |
| -1 | 5 | -14 | 144 | 172 |
| -2 | 5 | -14 | 120 | -134 |
| -4 | 5 | -14 | 121 | -119 |
| -5 | 5 | -14 | 110 | 96 |
| -6 | 5 | -14 | 28 | 33 |
| -7 | 5 | -14 | 60 | -41 |
| 1 | 5 | 15 | 82 | -133 |
| -1 | 5 | 15 | 130 | 187 |
| -3 | 5 | 15 | 50 | -80 |
| -1 | 5 | -15 | 58 | 78 |
| 3 | 5 | -15 | 38 | 93 |
| -4 | 5 | -15 | 102 | -113 |
| -5 | 5 | -15 | 109 | 110 |
| 1 | 5 | 16 | 115 | -176 |
| -1 | 5 | 16 | 58 | 87 |
| -3 | 5 | 16 | 103 | -118 |
| -1 | 5 | -16 | 66 | 60 |
| 3 | 5 | -16 | 46 | 89 |
| -3 | 5 | -16 | 32 | -52 |
| -4 | 5 | -16 | 90 | -89 |
| -5 | 5 | -16 | 122 | 113 |
| -3 | 5 | 17 | 137 | -141 |
| 3 | 5 | -17 | 43 | 70 |
| -3 | 5 | -17 | 60 | -82 |
| -5 | 5 | -17 | 79 | 71 |
| -3 | 5 | 18 | 108 | -112 |
| -2 | 5 | -18 | 59 | 80 |
| -3 | 5 | -18 | 81 | -102 |
| -4 | 5 | -18 | 38 | 37 |
| -3 | 5 | 19 | 68 | -57 |

| h | k | l | $F_o$ | $F_c$ |
|---|---|---|---|---|
| -2 | 5 | -19 | 68 | 79 |
| -3 | 5 | -19 | 70 | -94 |
| -4 | 5 | -19 | 29 | 29 |
| -2 | 5 | -20 | 22 | 40 |
| -3 | 5 | -20 | 59 | -71 |

# APPENDIX E

The simplified forms for calculation of electron densities

a. For three dimensions

$$\rho(x_1x_2x_3)=1/v\sum_{\bar{h}_3}^{h_3}\sum_{\bar{h}_2}^{h_2}\sum_{\bar{h}_1}^{h_1}(A_{h_1h_2h_3}\cos(h_1x_1+h_2x_2+h_3x_3)$$

$$+B_{h_1h_2h_3}\sin(h_1x_1+h_2x_2+h_3x_3))$$

b. For two dimensions

$$\rho(x_1x_2)=1/s\sum_{\bar{h}_2}^{h_2}\sum_{\bar{h}_1}^{h_1}(A_{h_1h_2}\cos(h_1x_1+h_2x_2)+B_{h_1h_2}\sin(h_1x_1+h_2x_2))$$

c. For one dimension

$$\rho(x_1)=1/l\sum_{\bar{h}_1}^{h_1}(A_{h_1}\cosh_1x_1+B_{h_1}\sinh_1x_1)$$

Because of the centrosymmetrical nature of the x-ray reflections (Friedel's law), which is due to the electron density being real, some simplification of the above Fourier equations can be done based on the following reasoning.

a. For three dimensions, instead of taking all the reflections from the whole sphere of reflection, twice of the half sphere of reflection may be taken.

b. For two dimensions, twice of the half circle of reflection may be taken.

Errors start when the halfs are being taken. Because some reflections show up at the common circle, line, or point, the whole reflections can not be divided exactly into two. Usually more than twice the half is taken. The common errors are as follows. (The following equations are correct, only when all unique reflections are included

using proper weighing).

a. For three dimensions

$$\rho(x_1x_2x_3)=2/v\sum_{0}^{h_3}\sum_{\bar{h}_2}^{h_2}\sum_{\bar{h}_1}^{h_1}(A_{h_1h_2h_3}\cos(h_1x_1+h_2x_2+h_3x_3)$$

$$+B_{h_1h_2h_3}\sin(h_1x_1+h_2x_2+h_3x_3))$$

b. For two dimensions

$$\rho(x_1x_2)=2/s\sum_{0}^{h_2}\sum_{\bar{h}_1}^{h_1}(A_{h_1h_2}\cos(h_1x_1+h_2x_2)+B_{h_1h_2}\sin(h_1x_1+h_2x_2))$$

c. For one dimension

$$\rho(x_1)=2/l\sum_{0}^{h_1}(A_{h_1}\cosh_1x_1+B_{h_1}\sinh_1x_1)$$

The physical meaning of these errors are that

a. for three dimensions

the common circle between the two half spheres has been used twice;

c. for two dimensions

the common line between the two half circles has been used twice;

c. for one dimensions

the common point between the two half lines has been used twice;

These errors in the Fourier equations are very significant, because it is be these simplified Fourier equations that most computer Fourier programs are written.

The correct forms of the simplified electron density are

a. For three dimensions

$$\rho(x_1x_2x_3)=1/v\sum_{\bar{h}_2}^{h_2}\sum_{\bar{h}_1}^{h_1}(A_{h_1h_20}\cos(h_1x_1+h_2x_2)+B_{h_1h_20}\sin(h_1x_1$$

$$+h_2x_2))+2/v\sum_{1}^{h_3}\sum_{\bar{h}_2}^{h_2}\sum_{\bar{h}_1}^{h_1}A_{h_1h_2h_3}\cos(h_1x_1+h_2x_2+h_3x_3)$$

$$+B_{h_1h_2h_3}\sin(h_1x_1+h_2x_2+h_3x_3))$$

b. For two dimensions

$$\rho(x_1x_2)=1/s\sum_{\bar{h}_1}^{h_1}(A_{h_10}\cosh_1x_1+B_{h_10}\sinh_1x_1)+2/s\sum_{\bar{1}}^{h_2}\sum_{\bar{h}_1}^{h_1}$$

$$(A_{h_1h_2}\cos(h_1x_1+h_2x_2)+B_{h_1h_2}\sin(h_1x_1+h_2x_2))$$

The first part represents the center line ($h_2$ being zero) in Fig. 22, while the second part represents twice the upper circle, which is equal to the whole circle except the center line.

c. For one dimension

$$\rho(x_1)=Ao/1+2/1\sum_{1}^{h_1}(A_{h_1}\cosh_1x_1+B_{h_1}\sinh_1x_1)$$

Derivation of the correct simplified equations

a. For one dimension

Given $\rho(x_1)=1/1\sum_{\bar{h}_1}^{h_1}(A_{h_1}\cosh_1x_1+B_{h_1}\sinh_1x_1)$

Left side$=1/1(\sum_{\bar{h}_1}^{-1}+h_1=o+\sum_{1}^{h_1})(A_{h_1}\cosh_1x_1+B_{h_1}\sinh_1x_1)$

$$=Ao/1+1/1(\sum_{\bar{h}_1}^{-1}+\sum_{1}^{h_1})(A_{h_1}\cosh_1x_1+B_{h_1}\sinh_1x_1)$$

Since $\sum_{\bar{h}_1}^{-1}(A_{h_1}\cosh_1x_1+B_{h_1}\sinh_1x_1)=\sum_{-1}^{\bar{h}_1}(A_{h_1}\cosh_1x_1+B_{h_1}\sinh_1x_1)$

$$=\sum_{1}^{h_1}(A_{\bar{h}_1}\cosh\bar{h}_1x_1+B_{\bar{h}_1}\sinh\bar{h}_1x_1)$$

$$=\sum_{1}^{h_1}(A_{\bar{h}_1}\cosh_1x_1-B_{\bar{h}_1}\sinh_1x_1)$$

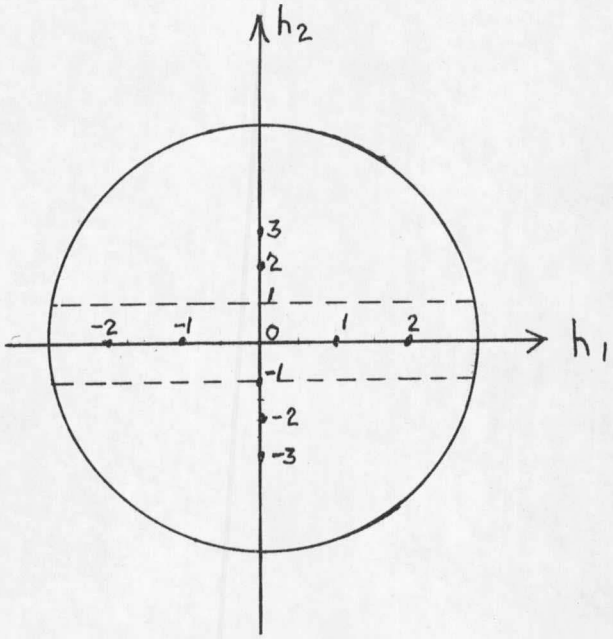



Figure 22 Physical meaning of the two dimensional simplified Electron Density

Thus, Left side $=Ao/_1+1/1\sum_{1}^{h_1}(A_{h_1}\cosh_1 x_1+A_{\bar{h}_1}\cosh_1 x_1$

$+B_{h_1}\sinh_1 x_1-B_{\bar{h}_1}\sinh_1 x_1)$

From Friedel's law

$A_{h_1}=A_{\bar{h}_1}$

$B_{h_1}=-B_{\bar{h}_1}$

Left side $=Ao/1+1/1\sum_{1}^{h_1}(A_{h_1}\cosh_1 x_1+A_{h_1}\cosh_1 x_1+B_{h_1}\sinh_1 x_1$

$+B_{h_1}\sinh_1 x_1)$

$=Ao/1+2/1\sum_{1}^{h_1}(A_{h_1}\cosh_1 x_1+B_{h_1}\sinh_1 x_1)$

Therefore,

$\rho(x)=Ao/1+2/1\sum^{h_1}(A_{h_1}\cosh_1 x_1+B_{h_1}\sinh_1 x_1)$

b. For two dimensions

Given

$$\rho(x_1x_2)=1/s\sum_{\bar{h}_2}^{h_2}\sum_{\bar{h}_1}^{h_1}(A_{h_1h_2}\cos(h_1x_1+h_2x_2)+B_{h_1h_2}\sin(h_1x_1+h_2x_2))$$

Left side $=1/s(\sum_{\bar{h}_2}^{-1}+\sum_{1}^{h_2})\sum_{\bar{h}_1}^{h_1}(A_{h_1h_2}\cos(h_1x_1+h_2x_2)$

$+B_{h_1h_2}\sin(h_1x_1+h_2x_2))$

$=1/s\sum_{\bar{h}_1}^{h_1}(A_{h_1 0}\cosh_1 x_1+B_{h_1 0}\sinh_1 x_1)+1/s(\sum_{\bar{h}_2}^{-1}+\sum_{1}^{h_2})\sum_{\bar{h}_1}^{h_1}$

$(A_{h_1h_2}\cos(h_1x_1+h_2x_2)+B_{h_1h_2}\sin(h_1x_1+h_2x_2))$

Since $\sum_{\bar{h}_2}^{-1}\sum_{\bar{h}_1}^{h_1}(A_{h_1h_2}\cos(h_1x_1+h_2x_2)+B_{h_1h_2}\sin(h_1x_1+h_2x_2))$

$=\sum_{-1}^{\bar{h}_2}\sum_{\bar{h}_1}^{h_1}(A_{h_1h_2}\cos(h_1x_1+h_2x_2)+B_{h_1h_2}\sin(h_1x_1+h_2x_2))$

$=\sum_{1}^{h_2}\sum_{\bar{h}_1}^{h_1}(A_{h_1h_2}\cos(h_1x_1+\bar{h}_2x_2)+B_{h_1h_2}\sin(h_1x_1+\bar{h}_2x_2))$

Then,

Left side $=1/s\sum_{\bar{h}_1}^{h_1}(A_{h_1 0}\cosh_1 x_1+B_{h_1 0}\sinh_1 x_1)+1/s\sum_{1}^{h_2}\sum_{\bar{h}_1}^{h_1}(A_{h_1h_2}$

$$\cos(h_1x_2+h_2x_2)+B_{h_1h_2}\sin(h_1x_1+h_2x_2)+A_{h_1\bar{h}_2}\cos$$

$$(h_1x_1+\bar{h}_2x_2)+B_{h_1\bar{h}_2}\sin(h_1x_1+\bar{h}_2x_2))$$

Let $R = \sum_{1}^{h_2}\sum_{\bar{h}_1}^{h_1}(A_{h_1h_2}\cos(h_1x_1+h_2x_2)+B_{h_1h_2}\sin(h_1x_1+h_2x_2)+$

$$A_{h_1\bar{h}_2}\cos(h_1x_1+\bar{h}_2x_2)+B_{h_1\bar{h}_2}\sin(h_1x_1+\bar{h}_2x_2))$$

Since $R=(\sum_{\bar{h}_1}^{\bar{1}}+h_1=0+\sum_{1}^{h_1})\sum_{1}^{h_2}($ " $)$

$$=\sum_{1}^{h_2}(A_{Oh_2}\cosh_2x_2+B_{Oh_2}\sinh_2x_2+A_{O\bar{h}_2}\cos\bar{h}_2x_2+B_{O\bar{h}_2}\sin\bar{h}_2x_2)$$

$$+\sum_{1}^{h_1}\sum_{1}^{h_2}(A_{h_1h_2}\cosh(h_1x_1+h_2x_2)+B_{h_1h_2}\sin(h_1x_1+h_2x_2)$$

$$+A_{h_1\bar{h}_2}\cos(h_1x_1+\bar{h}_2x_2)+B_{h_1\bar{h}_2}\sin(h_1x_1+\bar{h}_2x_2)+A_{\bar{h}_1h_2}\cos(\bar{h}_1x_1+h_2x_2)$$

$$+Bx_{h_1h_2}\sin(\bar{h}_1x_1+h_2x_2)+A_{\bar{h}_1\bar{h}_2}\cos(\bar{h}_1x_1+\bar{h}_2x_2)+B_{\bar{h}_1\bar{h}_2}\sin(\bar{h}_1x_1+\bar{h}_2x_2)$$

From Friedel's law

$$A_{h_1h_2}=A_{\bar{h}_1\bar{h}_2}, \qquad A_{\bar{h}_1h_2}=A_{h_1\bar{h}_2}$$

$$B_{h_1h_2}=-B_{\bar{h}_1\bar{h}_2}, \qquad B_{\bar{h}_1h_2}=-B_{h_1\bar{h}_2}$$

Then, $R=2\sum_{1}^{h_2}(A_{Oh_2}\cosh_2x_2+B_{Oh}\sinh_2x_2)+2\sum_{1}^{h_2}\sum_{1}^{h_1}(A_{h_1h_2}\cos(h_1x_1+h_2x_2)$

$$+B_{h_1h_2}\sin(h_1x_1+h_2x_2)+A_{\bar{h}_1h_2}\cos(\bar{h}_1x_1+h_2x_2)+B_{\bar{h}_1h_2}\sin$$

$$(\bar{h}_1x_1+h_2x_2))$$

$$=2\sum_{1}^{h_2}(A_{Oh_2}\cosh_2x_2+B_{Oh_2}\sinh_2x_2)+2\sum_{1}^{h_2}\sum_{1}^{h_1}(A_{h_1h_2}\cos(h_1x_1+h_2x_2)$$

$$+B_{h_1h_2}\sin(h_1x_1+h_2x_2))+2\sum_{1}^{h_2}\sum_{1}^{h_1}(A_{\bar{h}_1h_2}\cos(\bar{h}_1x_1+h_2x_2)$$

$$+B_{\bar{h}_1h_2}\sin(\bar{h}_1x_1+h_2x_2))$$

$$=2\sum_{1}^{h_2}(A_{Oh_2}\cosh_2x_2+B_{Oh_2}\sinh_2x_2)+2\sum_{1}^{h_2}\sum_{1}^{h_1}(A_{h_1h_2}\cos(h_1x_1+h_2x_2)$$

$$+B_{h_1h_2}\sin(h_1x_1+h_2x_2)+2\sum_{1}^{h_2}\sum_{-1}^{\bar{h}_1}(A_{h_1h_2}\cos(h_1x_1+h_2x_2)$$

$$+B_{h_1h_2}\sin(h_1x_1+h_2x_2))$$

$$=2(\sum_{\bar{h}_1}^{-1}+h_1=0+\sum_{1}^{h_1})\sum_{1}^{h_2}(A_{h_1h_2}\cos(h_1x_1+h_2x_2)+B_{h_1h_2}\sin(h_1x_1+h_2x_2))$$

$$=2\sum_{\bar{h}_1}^{h_1}\sum_{1}^{h_2}(A_{h_1h_2}\cos(h_1x_1+h_2x_2)+B_{h_1h_2}\sin(h_1x_1+h_2x_2))$$

Therefore,

$$\rho(x_1x_2)=1/s\sum_{\bar{h}_1}^{h_1}(A_{h_10}\cosh_1x_1+B_{h_10}\sinh_1x_1)+2/s\sum_{1}^{h_2}\sum_{\bar{h}_1}^{h_1}(A_{h_1h_2}\cos$$

$$(h_1x_1+h_2x_2)+B_{h_1h_2}\sin(h_1x_1+h_2x_2))$$

c. For three dimensions

Given

$$\rho(x_1x_2x_3)=1/v\sum_{\bar{h}_3}^{h_3}\sum_{\bar{h}_2}^{h_2}\sum_{\bar{h}_1}^{h_1}(A_{h\ h\ h}\cos(h_1x_1+h_2x_2+h_3x_3)+$$

$$B_{h_1h_2h_3}\sin(h_1x_1+h_2x_2+h_3x_3))$$

Show

$$\rho(x_1x_2x_3)=1/v\sum_{\bar{h}_2\bar{h}_1}^{h_2h_1}(A_{h_1h_20}\cos(h_1x_1+h_2x_2)+B_{h_1h_20}\sin$$

$$(h_1x_1+h_2x_2))+2/v\sum_{1\,\bar{h}_2\bar{h}_1}^{h_3h_2h_1}(A_{h_1h_2h_3}\cos(h_1x_1+h_2x_2+h_3x_3)$$

$$+B_{h_1h_2h_3}\sin(h_1x_1+h_2x_2+h_3x_3))$$

The proof is proceeded as follows.

$$\rho(x_1x_2x_3)=1/v(\sum_{-h_3}^{-1}+h_3=0+\sum_{1}^{h_3})\sum_{\bar{h}_2\bar{h}_1}^{h_2h_1}(A_{h_1h_2h_3}\cos(h_1x_1+h_2x_2+h_3x_3)$$

$$+B_{h_1h_2h_3}\sin(h_1x_1+h_2x_2+h_3x_3))$$

$$=1/v\sum_{\bar{h}_2\bar{h}_1}^{h_2h_1}(A_{h_1h_20}\cos(h_1x_1+h_2x_2)+B_{h_1h_20}\sin(h_1x_1+h_2x_2)$$

$$+1/v\sum_{1\,\bar{h}_2\bar{h}_1}^{h_3h_2h_1}(A_{h_1h_2h_3}\cos(h_1x_1+h_2x_2+h_3x_3)+B_{h_1h_2h_3}\sin$$

$$(h_1x_1+h_2x_2+h_3x_3)+A_{h_1h_2\bar{h}_3}\cos(h_1x_1+h_2x_2+\bar{h}_3x_3)$$

$$+B_{h_1h_2\bar{h}_3}\sin(h_1x_1+h_2x_2+\bar{h}_3x_3))$$

Now, we just have to show

$$\sum_{1\,\bar{h}_2\bar{h}_1}^{h_3h_2h_1}(A_{h_1h_2h_3}\cos(h_1x_1+h_2x_2+h_3x_3)+B_{h_1h_2h_3}\sin(h_1x_1+h_2x_2+h_3x_3)$$

$$+A_{h_1h_2\bar{h}_3}\cos(h_1x_1+h_2x_2+\bar{h}_3x_3)+B_{h_1h_2\bar{h}_3}\sin(h_1x_1+h_2x_2+\bar{h}_3x_3))$$

$$=2\sum_{1\,\bar{h}_2\bar{h}_1}^{h_3h_2h_1}(A_{h_1h_2h_3}\cos(h_1x_1+h_2x_2+h_3x_3)+B_{h_1h_2h_3}\sin(h_1x_1+h_2x_2+h_3x_3))$$

Let us work on $h_2$ first

$$\text{Left side}=\sum_{1\,\bar{h}_1}^{h_3h_1}(A_{h_1Oh_3}\cos(h_1x_1+h_3x_3)+B_{h_1Oh_3}\sin(h_1x_1+h_3x_3)$$

$$+A_{h_1 0\bar{h}_3}\cos(h_1x_1+\bar{h}_3x_3)+B_{h_1 0\bar{h}_3}\sin(h_1x_1+\bar{h}_3x_3))$$

$$+\sum_{1}^{h_3}\sum_{1}^{h_2}\sum_{\bar{h}_1}^{h_1}(A_{h_1h_2h_3}\cos(h_1x_1+h_2x_2+h_3x_3)+B_{h_1h_2h_3}\sin$$

$$(h_1x_1+h_2x_2+h_3x_3)+A_{h_1h_2\bar{h}_3}\cos(h_1x_1+h_2x_2+\bar{h}_3x_3)$$

$$+B_{h_1h_2\bar{h}_3}\sin(h_1x_1+h_2x_2+\bar{h}_3x_3)+A_{h_1\bar{h}_2h_3}\cos(h_1x_1+\bar{h}_2x_2+h_3x_3)$$

$$+B_{h_1\bar{h}_2h_3}\sin(h_1x_1+\bar{h}_2x_2+h_3x_3)+A_{h_1\bar{h}_2\bar{h}_3}\cos(h_1x_1+\bar{h}_2x_2+\bar{h}_3x_3)$$

$$+B_{h_1\bar{h}_2\bar{h}_3}\sin(h_1x_1+\bar{h}_2x_2+\bar{h}_3x_3))$$

Let $$I=\sum_{1}^{h_3}\sum_{\bar{h}_1}^{h_1}(A_{h_1 0h_3}\cos(h_1x_1+h_3x_3)+B_{h_1 0h_3}(h_1x_1+h_3x_3)$$

$$+A_{h_1 0\bar{h}_3}\cos(h_1x_1+\bar{h}_3x_3)+B_{h_1 0\bar{h}_3}\sin(h_1x_1+\bar{h}_3x_3))$$

$$II=\sum_{1}^{h_3}\sum_{1}^{h_2}\sum_{\bar{h}_1}^{h_1}(A_{h_1h_2h_3}\cos(h_1x_1+h_2x_2+h_3x_3)+B_{h_1h_2h_3}\sin(h_1x_1$$

$$+h_2x_2+h_3x_3)+A_{h_1h_2\bar{h}_3}\cos(h_1x_1+h_2x_2+\bar{h}_3x_3)+B_{h_1h_2\bar{h}_3}$$

$$\sin(h_1x_1+h_2x_2+\bar{h}_3x_3)+A_{h_1\bar{h}_2h_3}\cos(h_1x_1+\bar{h}_2x_2+h_3x_3)$$

$$+B_{h_1\bar{h}_2h_3}\sin(h_1x_1+\bar{h}_2x_2+h_3x_3)+A_{h_1\bar{h}_2\bar{h}_3}\cos(h_1x_1+\bar{h}_2x_2+\bar{h}_3x_3)$$

$$+B_{h_1\bar{h}_2\bar{h}_3}\sin(h_1x_1+\bar{h}_2x_2+\bar{h}_3x_3))$$

Let us, then, work on $h_1$

$$I=\sum_{1}^{h_3}(A_{00h_3}\cosh_3x_3+B_{00h_3}\sinh_3x_3+A_{00\bar{h}_3}\cos\bar{h}_3x_3+B_{00\bar{h}_3}\sin\bar{h}_3x_3)$$

$$+\sum_{1}^{h_3}\sum_{1}^{h_1}(A_{h_1 0h_3}\cos(h_1x_1+h_3x_3)+B_{h_1 0h_3}\sin(h_1x_1+h_3x_3)+A_{h_1 0\bar{h}_3}$$

$$\cos(h_1x_1+\bar{h}_3x_3)+B_{h_1Oh_3}\sin(h_1x_1+\bar{h}_3x_3)+A_{\bar{h}_1Oh_3}\cos(\bar{h}_1x_1+h_3x_3)$$

$$B_{\bar{h}_1Oh_3}\sin(\bar{h}_1x_1+h_3x_3)+A_{\bar{h}_1O\bar{h}_3}\cos(\bar{h}_1x_1+\bar{h}_3x_3)+B_{\bar{h}_1O\bar{h}_3}\sin$$

$$(\bar{h}_1x_1+\bar{h}_3x_3))$$

From Friedel's Law

$$A_{OOh_3}=A_{OO\bar{h}_3}, \qquad B_{OOh_3}=-B_{OO\bar{h}_3}$$

$$A_{h_1Oh_3}=A_{\bar{h}_1O\bar{h}_3}, \qquad B_{h_1Oh_3}=-B_{\bar{h}_1O\bar{h}_3}$$

$$A_{\bar{h}_1Oh_3}=A_{h_1O\bar{h}_3}, \qquad B_{\bar{h}_1Oh_3}=-B_{h_1O\bar{h}_3}$$

Then,

$$I=2\sum_{1}^{h_3}(A_{OOh_3}\cosh_3x_3+B_{OOh_3}\sinh_3x_3)+2\sum_{1}^{h_3}\sum_{1}^{h_1}(A_{h_1Oh_3}\cos(h_1x_1+h_3x_3)$$

$$+B_{h_1Oh_3}\sin(h_1x_1+h_3x_3))+2\sum_{1}^{h_3}\sum_{1}^{h_1}(A_{\bar{h}_1Oh_3}\cos(\bar{h}_1x_1+h_3x_3)+B_{\bar{h}_1Oh_3}$$

$$\sin(\bar{h}_1x_1+h_3x_3))$$

since

$$\sum_{1}^{h_3}\sum_{1}^{h_1}(A_{\bar{h}_1Oh_3}\cos(\bar{h}_1x_1+h_3x_3)+B_{\bar{h}_1Oh_3}\sin(\bar{h}_1x_1+h_3x_3)$$

$$=\sum_{1}^{h_3-1}\sum_{\bar{h}_1}^{-1}(A_{h_1Oh_3}\cos(h_1x_1+h_3x_3)+B_{h_1Oh_3}\sin(h_1x_1+h_3x_3))$$

Thus,

$$I=2(\sum_{\bar{h}_1}^{-1}+h_1=0+\sum_{1}^{h_1})\sum_{1}^{h_3}(A_{h_1Oh_3}\cos(h_1x_1+h_3x_3)+B_{h_1Oh_3}\sin(h_1x_1+h_3x_3)$$

$$=2\sum_{1}^{h_3}\sum_{\bar{h}_1}^{h_1}(A_{h_1Oh_3}\cos(h_1x_1+h_3x_3)+B_{h_1Oh_3}\sin(h_1x_1+h_3x_3))$$

$$II=\sum_{1}^{h_3}\sum_{1}^{h_2}(A_{Oh_2h_3}\cos(h_2x_2+h_3x_3)+B_{Oh_2h_3}\sin(h_2x_2+h_3x_3)$$

$$+A_{Oh_2\bar{h}_3}\cos(h_2x_2+\bar{h}_3x_3)+B_{Oh_2\bar{h}_3}\sin(h_2x_2+\bar{h}_3x_3)+A_{O\bar{h}_2h_2}\cos$$

$$(\bar{h}_2x_2+h_3x_3)+B_{O\bar{h}_2h_3}\sin(\bar{h}_2x_2+h_3x_3)+A_{O\bar{h}_2\bar{h}_3}\cos(\bar{h}_2x_2+\bar{h}_3x_3)$$

$$+B_{O\bar{h}_2\bar{h}_3}\sin(\bar{h}_2x_2+\bar{h}_3x_3)+\sum_{h_3}\sum_{h_2}\sum_{h_1}(A_{h_1h_2h_3}\cos(h_1x_1+h_2x_2+h_3x_3)$$

$$+B_{h_1h_2h_3}\sin(h_1x_1+h_2x_2+h_3x_3)+A_{h_1h_2\bar{h}_3}\cos(h_1x_1+h_2x_2+\bar{h}_3x_3)$$

$$+B_{h_1h_2\bar{h}_3}\sin(h_1x_1+h_2x_2+\bar{h}_3x_3)+A_{h_1\bar{h}_2h_3}\cos(h_1x_1+\bar{h}_2x_2+h_3x_3)$$

$$+B_{h_1\bar{h}_2h_3}\sin(h_1x_1+\bar{h}_2x_2+h_3x_3)+A_{h_1\bar{h}_2\bar{h}_3}\cos(h_1x_1+\bar{h}_2x_2+\bar{h}_3x_3)+B_{h_1\bar{h}_2\bar{h}_3}$$

$$\sin(h_1x_1+\bar{h}_2x_2+\bar{h}_3x_3)+A_{\bar{h}_1h_2h_3}\cos(\bar{h}_1x_1+h_2x_2+h_3x_3)+B_{\bar{h}_1h_2h_3}\sin(\bar{h}_1x_1$$

$$+h_2x_2+h_3x_3)+A_{\bar{h}_1h_2\bar{h}_3}\cos(\bar{h}_1x_1+h_2x_2+\bar{h}_3x_3)+B_{\bar{h}_1h_2\bar{h}_3}\sin(\bar{h}_1x_1+h_2x_2+\bar{h}_3x_3)$$

$$+A_{\bar{h}_1\bar{h}_2h_3}\cos(\bar{h}_1x_1+\bar{h}_2x_2+h_3x_3)+B_{\bar{h}_1\bar{h}_2h_3}\sin(\bar{h}_1x_1+\bar{h}_2x_2+h_3x_3)+A_{\bar{h}_1\bar{h}_2\bar{h}_3}$$

$$\cos(\bar{h}_1x_1+\bar{h}_2x_2+\bar{h}_3x_3)+B_{\bar{h}_1\bar{h}_2\bar{h}_3}\sin(\bar{h}_1x_1+\bar{h}_2x_2+\bar{h}_3x_3)$$

From Friedel's law

$A_{Oh_2h_3}=A_{O\bar{h}_2\bar{h}_3}$, $B_{Oh_2h_3}=-B_{O\bar{h}_2\bar{h}_3}$, $A_{h_1\bar{h}_2h_3}=A_{\bar{h}_1h_2\bar{h}_3}$, $B_{h_1\bar{h}_2h_3}=-B_{\bar{h}_1h_2\bar{h}_3}$

$A_{O\bar{h}_2h_3}=A_{Oh_2\bar{h}_3}$, $B_{O\bar{h}_2h_3}=-B_{Oh_2\bar{h}_3}$ $A_{\bar{h}_1\bar{h}_2h_3}=A_{h_1h_2\bar{h}_3}$, $B_{\bar{h}_1\bar{h}_2h_3}=-B_{h_1h_2\bar{h}_3}$

$A_{h_1h_2h_3}=A_{\bar{h}_1\bar{h}_2\bar{h}_3}$, $B_{h_1h_2h_3}=-B_{\bar{h}_1\bar{h}_2\bar{h}_3}$ $A_{\bar{h}_1h_2h_3}=A_{h_1\bar{h}_2\bar{h}_3}$, $B_{\bar{h}_1h_2h_3}=-B_{h_1\bar{h}_2h_3}$

Then,

$$II=2\sum_{h_3}\sum_{h_2}(A_{Oh_2h_3}\cos(h_2x_2+h_3x_3)+B_{Oh_2h_3}\sin(h_2x_2+h_3x_3)+A_{O\bar{h}_2h_3}\cos$$

$$(\bar{h}_2x_2+h_3x_3)+B_{O\bar{h}_2h_3}\sin(\bar{h}_2x_2+h_3x_3))+2\sum_{h_3}\sum_{h_2}\sum_{h_1}(A_{h_1h_2h_3}\cos(h_1x_1+$$

$$h_2x_2+h_3x_3)+B_{h_1h_2h_3}\sin(h_1x_1+h_2x_2+h_3x_3)+A_{h_1\bar{h}_2h_3}\cos(h_1x_1+\bar{h}_2x_2+h_3x_3)$$

$$+B_{h_1\bar{h}_2h_3}\sin(h_1x_1+\bar{h}_2x_2+h_3x_3)+A_{\bar{h}_1\bar{h}_2h_3}\cos(\bar{h}_1x_1+\bar{h}_2x_2+h_3x_3)+B_{\bar{h}_1\bar{h}_2h_3}$$

$$\sin(\bar{h}_1x_1+\bar{h}_2x_2+h_3x_3)+A_{\bar{h}_1h_2h_3}\cos(\bar{h}_1x_1+h_2x_2+h_3x_3)+B_{\bar{h}_1h_2h_3}$$

$$\sin(\bar{h}_1x_1+h_2x_2+h_3x_3))$$

$$II=2\sum_{1}^{h_3}\sum_{1}^{h_2}(A_{Oh_2h_3}\cos(h_2x_2+h_3x_3)+B_{Oh_2h_3}\sin(h_2x_2+h_3x_3)+A_{O\bar{h}_2h_3}\cos$$

$$(\bar{h}_2x_2+h_3x_3)+B_{O\bar{h}_2h_3}\sin(\bar{h}_2x_2+h_3x_3))+2\sum_{1}^{h_3}\sum_{1}^{h_2}\sum_{1}^{h_1}(A_{h_1h_2h_3}\cos(h_1x_1+h_2x_2+$$

$$h_3x_3)+B_{h_1h_2h_3}\sin(h_1x_1+h_2x_2+h_3x_3)+A_{h_1\bar{h}_2h_3}\cos(h_1x_1+\bar{h}_2x_2+h_3x_3)$$

$$+B_{h_1\bar{h}_2h_3}\sin(h_1x_1+\bar{h}_2x_2+h_3x_3))+2\sum_{1}^{h_3}\sum_{1}^{h_2}\sum_{1}^{h_1}(A_{\bar{h}_1h_2h_3}\cos(\bar{h}_1x_1+h_2x_2+h_3x_3)$$

$$+B_{\bar{h}_1h_2h_3}\sin(\bar{h}_1x_1+h_2x_2+h_3x_3)+A_{\bar{h}_1\bar{h}_2h_3}\cos(\bar{h}_1x_1+\bar{h}_2x_2+h_3x_3)$$

$$+B_{\bar{h}_1\bar{h}_2h_3}\sin(\bar{h}_1x_1+\bar{h}_2x_2+h_3x_3))$$

Since $\sum_{1}^{h_3}\sum_{1}^{h_2}\sum_{1}^{h_1}(A_{\bar{h}_1h_2h_3}\cos(\bar{h}_1x_1+h_2x_2+h_3x_3)+B_{\bar{h}_1h_2h_3}\sin(\bar{h}_1x_1$

$$+h_2x_2+h_3x_3)+A_{\bar{h}_1\bar{h}_2h_3}\cos(\bar{h}_1x_1+\bar{h}_2x_2+h_3x_3)+B_{\bar{h}_1\bar{h}_2h_3}\sin(\bar{h}_1x_1+\bar{h}_2x_2+h_3x_3))$$

$$=\sum_{1}^{h_3}\sum_{1}^{h_2-1}\sum_{\bar{h}_1}(A_{h_1h_2h_3}\cos(h_1x_1+h_2x_2+h_3x_3)+B_{h_1h_2h_3}\sin(h_1x_1+h_2x_2+h_3x_3)+$$

$$+A_{h_1\bar{h}_2h_3}\cos(h_1x_1+\bar{h}_2x_2+h_3x_3)+B_{h_1\bar{h}_2h_3}\sin(h_1x_1+\bar{h}_2x_2+h_3x_3)$$

Thus,

$$II=2(\sum_{\bar{h}_1}^{-1}+\sum_{1}^{h_1}+h_1=0)\sum_{1}^{h_3}\sum_{1}^{h_2}(A_{h_1h_2h_3}\cos(h_1x_1+h_2x_2+h_3x_3)+B_{h_1h_2h_3}$$

$$\sin(h_1x_1+h_2x_2+h_3x_3)+A_{h_1\bar{h}_2h_3}\cos(h_1x_1+\bar{h}_2x_2+h_3x_3)+B_{h_1\bar{h}_2h_3}$$

$$\sin(h_1x_1+\bar{h}_2x_2+h_3x_3))$$

$$II=2\sum_{1}^{h_3}\sum_{1}^{h_2}\sum_{\bar{h}_1}^{h_1}(A_{h_1h_2h_3}\cos(h_1x_1+h_2x_2+h_3x_3)+B_{h_1h_2h_3}\sin(h_1x_1+h_2x_2+h_3x_3)$$

$$+A_{h_1\bar{h}_2h_3}\cos(h_1x_1+\bar{h}_2x_2+h_3x_3)+B_{h_1\bar{h}_2h_3}\sin(h_1x_1+\bar{h}_2x_2+h_3x_3))$$

$$II=2\sum_{1}^{h_3}\sum_{1}^{h_2}\sum_{\bar{h}_1}^{h_1}(A_{h_1h_2h_3}\cos(h_1x_1+h_2x_2+h_3x_3)+B_{h_1h_2h_3}\sin(h_1x_1+h_2x_2+h_3x_3)$$

$$+2\sum_{1}^{h_3-1}\sum_{\bar{h}_2}^{h_1}\sum_{\bar{h}_1}(A_{h_1h_2h_3}\cos(h_1x_1+h_2x_2+h_3x_3)+B_{h_1h_2h_3}\sin(h_1x_1+h_2x_2+h_3x_3))$$

Hence

Left side=I+II

$$=2\sum_{1}^{h_3}\sum_{\bar{h}_1}^{h_1}(A_{h_1Oh_3}\cos(h_1x_1+h_3x_3)+B_{h_1Oh_3}\sin(h_1x_1+h_3x_3))$$

$$+2\sum_{1}^{h_3}\sum_{1}^{h_2}\sum_{\bar{h}_1}^{h_1}(A_{h_1h_2h_3}\cos(h_1x_1+h_2x_2+h_3x_3)+B_{h_1h_2h_3}\sin(h_1x_1+$$

$$h_2x_2+h_3x_3))+2\sum_{1}^{h_3-1}\sum_{\bar{h}_2}^{h_1}\sum_{\bar{h}_1}(A_{h_1h_2h_3}\cos(h_1x_1+h_2x_2+h_3x_3)+B_{h_1h_2h_3}$$

$$\sin(h_1x_1+h_2x_2+h_3x_3))$$

$$\text{Left side}=2\Big(\sum_{\bar{h}_2}^{-1}+h_2=0+\sum_{1}^{h_2}\Big)\sum_{1}^{h_3}\sum_{\bar{h}_1}^{h_1}(A_{h_1h_2h_3}\cos(h_1x_1+h_2x_2+h_3x_3)$$

$$+B_{h_1h_2h_3}\sin(h_1x_1+h_2x_2+h_3x_3))$$

$$=2\sum_{1}^{h_3}\sum_{\bar{h}_2}^{h_2}\sum_{\bar{h}_1}^{h_1}(A_{h_1h_2h_3}\cos(h_1x_1+h_2x_2+h_3x_3)+B_{h_1h_2h_3}\sin$$

$$(h_1x_1+h_2x_2+h_3x_3)$$

Therefore,

$$\rho(x_1x_2x_3)=1/v\sum_{\bar{h}_2}^{h_2}\sum_{\bar{h}_1}^{h_1}(A_{h_1h_20}\cos(h_1x_1+h_2x_2)+B_{h_1h_20}\sin(h_1x_1$$

$$+h_2x_2))+2/v\sum_{1}^{h_3}\sum_{\bar{h}_2}^{h_2}\sum_{\bar{h}_1}^{h_1}(A_{h_1h_2h_3}\cos(h_1x_1+h_2x_2+h_3x_3)$$

$$+B_{h_1h_2h_3}\sin(h_1x_1+h_2x_2+h_3x_3))$$

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