THE STRUCTURES AND CRYSTAL CHEMISTRY OF BUSTAMITE AND RHODONITE

BY

DONALD RALPH PEACOR

S.B., Tufts University

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S.M., Massachusetts Institute of Technology

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Signature of Author. . . . . .
Department of Geology, August 20, 1962

Certified by . . . . . .
Thesis Supervisor

Accepted by. . . . . .
Chairman, Departmental Committee
on Graduate Students

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Donald R. Peacor

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ABSTRACT

Bustamite ($CaMnSi_2O_6$) has space group $P\bar{1}$ and unit cell parameters a = 15.412Å, b = 7.157Å, c = 13.824Å, α = 89°29', β = 94°51', γ = 102°56', with Z = 12. Three-dimensional intensity data were gathered with the single-crystal, Geiger-counter diffractometer. Application of the minimum function to P(xz) and comparison of the unit cells of bustamite and wollastonite ($CaSiO_3$) yielded a trial structure which was refined with least-squares.

Rhodonite ($Mn_4CaSi_5O_{15}$) has space group $P\bar{1}$ and unit cell parameters a = 7.682Å, b = 11.818Å, c = 6.707Å, α = 92°21', β = 93°57', γ = 105°40', with Z = 2. Interpretation of the three-dimensional Patterson function led to the identification of (Mn,Ca) inversion peaks which were used to form the minimum function. Interpretation of this function resulted in a trial structure which was refined by means of least-squares.

The structures of bustamite and rhodonite are similar to those of other metasilicates having chains of silica tetrahedra. Oxygen atoms are arranged approximately in close-packing. Planes of Mn and Ca ions occupying octahedral interstices alternate with planes of tetrahedrally coordinated Si ions, between oxygen sheets. Silica tetrahedra each share two vertices to form chains with a repeat unit of three tetrahedra in bustamite and five in rhodonite.

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Part I

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Part I-A

Determination and refinement of the crystal structure of bustamite, $CaMnSi_2O_6$

By Donald R. Peacor and M.J. Buerger
Massachusetts Institute of Technology
Cambridge, Massachusetts

Abstract

Bustamite is triclinic, space group $\underline{P}\bar{1}$, with cell dimensions $\underline{a}$ = 15.412 Å, $\underline{b}$ = 7.157 Å, $\underline{c}$ = 13.824 Å, α = 89°29', β = 94°51', γ = 102°56'. The unit cell ideally contains 12($CaMnSi_2O_6$). Three-dimensional intensity data were gathered with the single-crystal Geiger-counter diffractometer. Application of the minimum function to $\underline{P}(\underline{xz})$, and comparison of the unit cells of bustamite and wollastonite yielded a trial structure which was refined with least-squares.

Planes of approximately close-packed oxygen atoms are oriented parallel to (101). Planes containing Ca and Mn atoms in octahedral coordination alternate with planes of Si

atoms in tetrahedral coordination between oxygen planes. Ca and Mn are ordered. Si tetrahedra are linked to form chains parallel to b with a repeat unit of three tetrahedra.

Introduction

Several authors have noted the similarity of the properties of bustamite, $CaMnSi_2O_6$, to that of wollastonite, $CaSiO_3$. On the basis of a similarity of optical properties of the two minerals, Sundius[1] and Schaller[2,3] proposed that bustamite is Mn-rich wollastonite. Berman and Gonyer[4] accepted this view when they determined the unit cell of bustamite and noted its correspondence to that of wollastonite (Table A1). Buerger[5] and Liebau *et al.*[6] found, however, that the unit cells are different although closely related (Table A1).

Because of the recent interest in the structures of the minerals of the wollastonite family, it is important to understand the relation of bustamite to other triclinic metasilicates. In this paper the results of an investigation of the structure are given.

Unit cell and space group

Specimens of bustamite from Franklin, N.J., were kindly provided by Professor C. Frondel of Harvard University. The unit cell obtained by Buerger was confirmed with zero, first, second, and third-level *b* axis Weissenberg photographs.

Table A1

Symmetry and unit cell data for bustamite and wollastonite.

Wollastonite (Buerger[5])	Bustamite (Berman and Gonyer[4])	Bustamite (Buerger[5])	β-$Mn_{0.8}Ca_{0.2}SiO_3$ (Liebau et al.)	Bu (I Bu
$P\bar{1}$	P1 or $P\bar{1}$	$F\bar{1}$	F1 or $F\bar{1}$	
7.94 Å	7.64 Å	2x7.73 Å	2x8.03 Å	1
7.32	7.16	7.18	7.11	
7.07	6.87	2x6.92	2x6.84	1
90°02'	92°08'	89°34'	-	8
95°22'	94°54½'	94°53'	-	9
103°26'	101°35'	102°47'	-	10

Final cell parameters (Table A1) were obtained by least-squares refinement of data from a, b, and c-axis zero-level back-reflection precision Weissenberg photographs. Refinement was carried out using an IBM 709 program written by C. W. Burnham.[7] Although it is usual to choose a reduced, primitive triclinic unit cell, the face-centered cell was retained because of its close correspondence to that of wollastonite.[5]

Using the refined cell parameters and an analysis of Franklin, N.J., bustamite,[8] the unit-cell contents were found to correspond to the following formula:

$$\begin{array}{llll} Ca_{13.37} & & & \\ Mn_{10.57} & & & \\ Mg_{\ 0.48} & & Si_{24.00} & O_{72.68} \\ Zn_{\ 0.20} & & & \\ Fe_{\ \underline{0.11}} & & & \\ \quad 24.73 & & & \end{array}$$

Since a precise value for the specific gravity was not available, this distribution was obtained by normalizing the formula to 24.00 Si atoms per cell. The excess of Ca, Mn, etc., relative to Si (24.73 : 24.00) is attributed to a slight error in the analysis.

The above formula corresponds ideally to $12(CaMnSi_2O_6)$ per face-centered cell, or $3(CaMnSi_2O_6)$ per

primitive cell. Space group $\underline{P}\bar{1}$ contains only equipoints of rank 1 and 2. Three Ca and three Mn atoms can all occupy general equipoints of rank 2 only if there is disorder between at least one Ca and one Mn. Complete order of Ca and Mn requires that at least one Ca and one Mn be on inversion centers of rank 1. The grouping of analyses of natural material about the ideal composition suggested the latter. Since no Ca atoms occupy inversion centers in wollastonite, there was a strong possibility that this constituted a major difference between the structures.

Intensity data

The specimen used for the intensity measurement was a prism bounded by (100) and (001) cleavages, 0.233 mm long and 0.030 x 0.048 mm in cross section. The crystal was mounted on the single-crystal diffractometer with the $\underline{b}$-axis as rotation axis. Intensities of the reflections with $\underline{\text{CuK}}\alpha$ radiation were measured with an argon-filled Geiger counter. Care was taken not to exceed the linearity range of the Geiger counter; counting rates were maintained below

500 c.p.s. by using aluminum absorption foils. Intensities were measured by direct counting. Background was measured on each side of a peak and the average background subtracted from the value of background plus integrated intensity obtained by scanning through the peak. Of approximately 1650 non-equivalent reflections in the Cu sphere, 1212 were recorded. These were corrected for the Lorentz and polarization factors using an IBM 709 program written by C. T. Prewitt,[9] and for absorption using an IBM 709 program written by C. W. Burnham.[10]

Structure determination

Determination of x and z coordinates. Comparison of h0l reflections of bustamite and wollastonite showed that the distribution and intensities of each were similar. This suggested that the projections of the structures along b are the same. The Patterson projection P(xz) of bustamite was therefore prepared. Its similarity to that of P(xz) of wollastonite confirmed that the structures are very probably the same in projection.

The structure of the wollastonite[11] projected along $\underline{b}$ is shown in Fig. A1. Ca_1 and Ca_2 are superimposed in projection. On the assumption that Ca and Mn atoms in bustamite have a similar arrangement, a minimum function $\underline{M}_2(\underline{xz})$ was prepared for bustamite using the equivalent of the superimposed $Ca_1 + Ca_2$ inversion peaks of wollastonite. In wollastonite, the Patterson projection $\underline{P}(\underline{xz})$ contains an image of the structure as seen from Ca_3. The Patterson projection and $\underline{M}_2(\underline{xz})$ were therefore superimposed to obtain the minimum function $\underline{M}_4(\underline{xz})$ shown in Fig. A2.

Note that for each atom of $\rho\,(\underline{xz})$ there is a corresponding peak of the correct relative weight in $\underline{M}_4(\underline{xz})$ of bustamite. There are four extra peaks, labelled $\underline{A}$, $\underline{B}$, $\underline{C}$, and $\underline{D}$, in $\underline{M}_4(\underline{xz})$. Three of these, $\underline{A}$, $\underline{B}$ and $\underline{C}$, are near the peaks corresponding to O_7, O_8 and Si_3 of wollastonite. Structure factors $\underline{F}_{\underline{h}0\underline{l}}$, calculated omitting these atoms, gave a discrepancy factor $\underline{R}$ = 31%. Using these structure factors the electron-density projections $\rho\,(\underline{xz})$, Fig. A3, and $\Delta\rho(\underline{xz})$ were then calculated. As can be seen from a comparison of Figs. A1 and A3, these confirmed that the projections $\rho\,(\underline{xz})$ of bustamite and wollastonite are essentially the same. None of the false peaks, $\underline{A}$, $\underline{B}$, $\underline{C}$ and $\underline{D}$ of $\underline{M}_4(\underline{xz})$ appeared in $\rho(\underline{xz})$, while peaks corresponding to O_7, O_8 and Si_3 do occur. A second structure factor calculation based on coordinates from $\rho\,(\underline{xz})$ and $\Delta\rho\,(\underline{xz})$ yielded an $\underline{R}$ of 21% for all $\underline{F}_{\underline{h}0\underline{l}}$.

Figure 1, Part IA

Projection along b of the structure of wollastonite. Oxygen atoms are represented by large circles, Ca atoms by circles of intermediate size, and Si atoms by small circles.

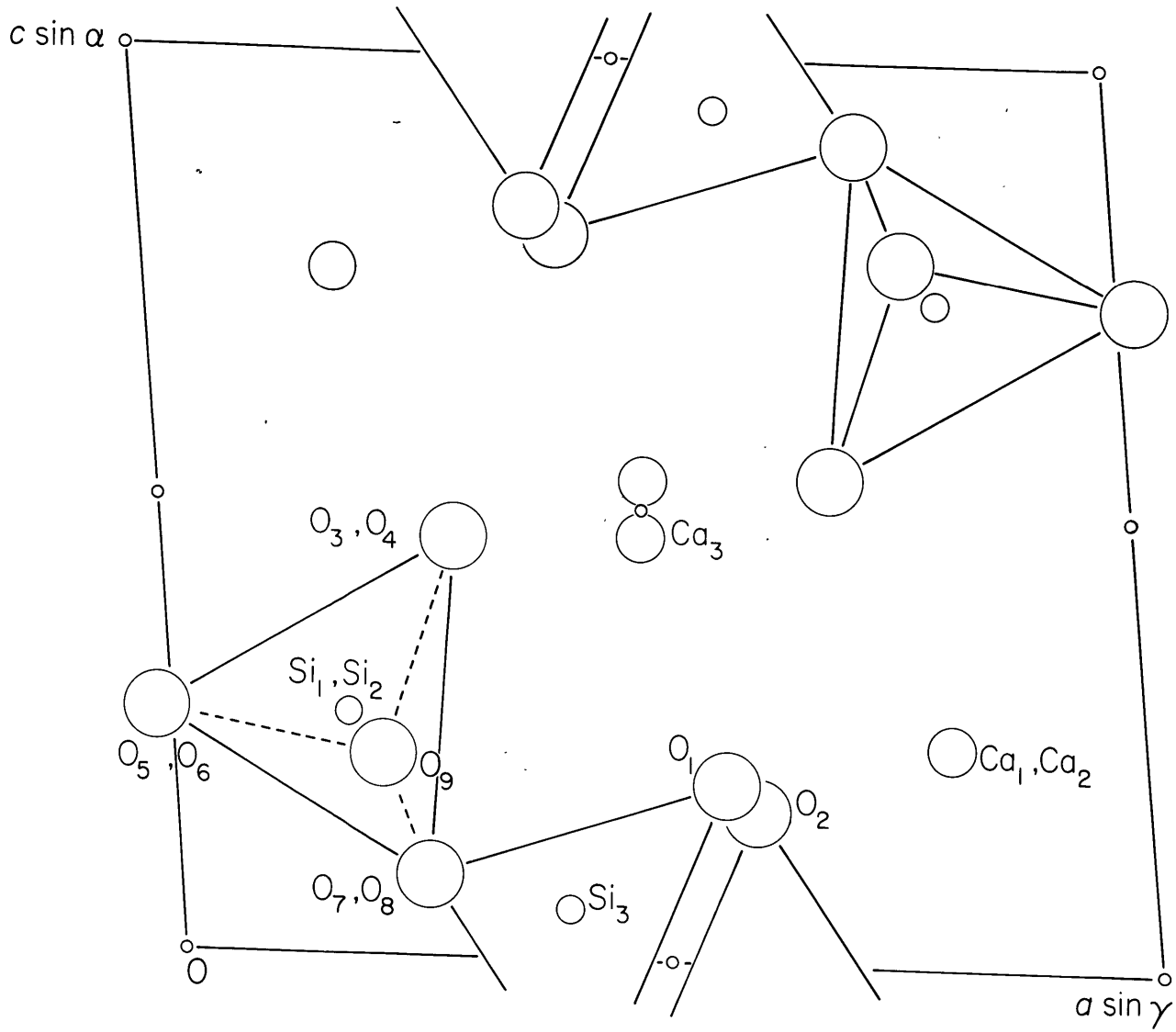

c sin α
O3 , O4
Ca3
Si1 , Si2
O5 , O6
O9
O1
O2
Ca1 , Ca2
O7 , O8
Si3
O
a sin γ

Figure 2, Part IA

Bustamite, $M_4(xz)$. The high (Ca + Mn) peak is shaded in. Peaks which do not correspond to atoms are labelled A, B, C and D.

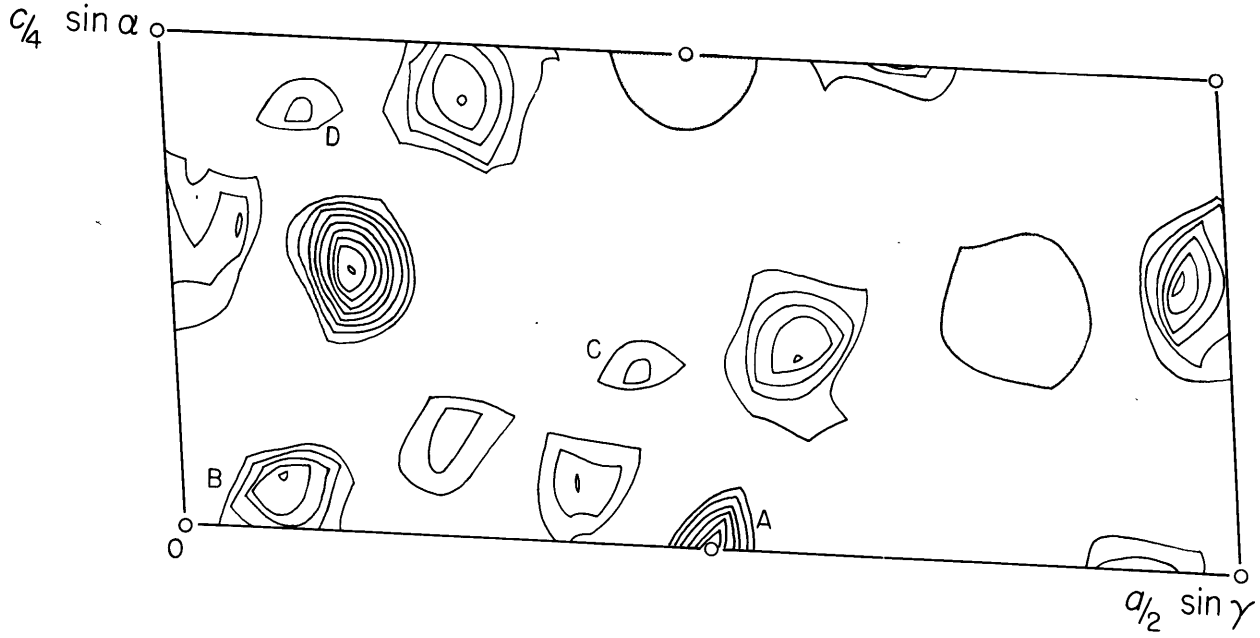
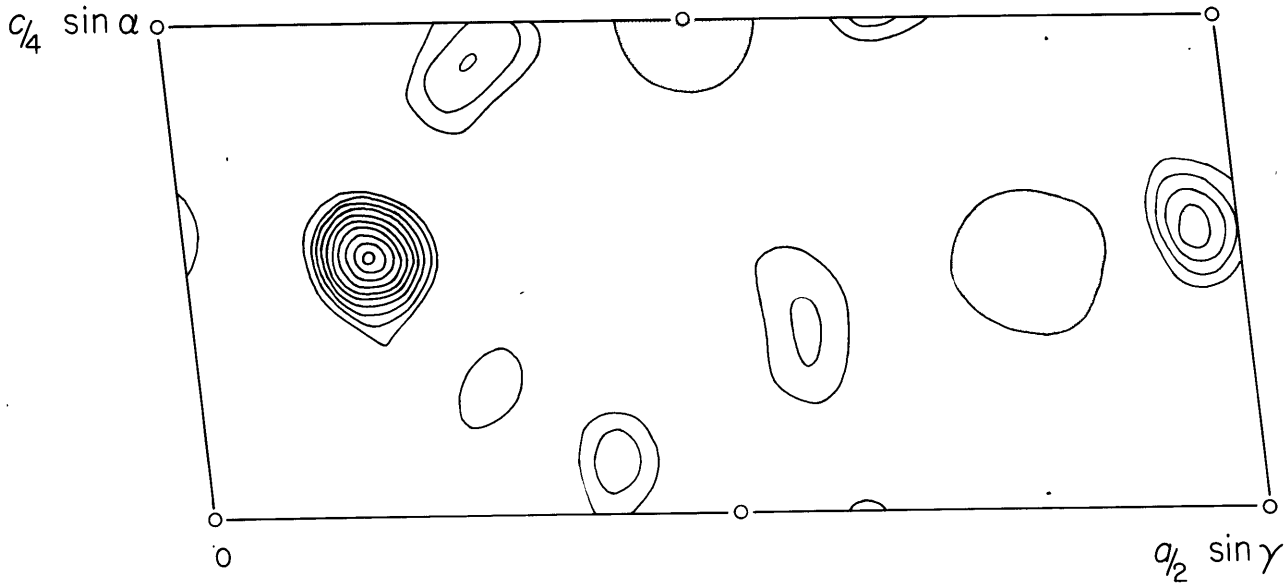

c/4 sin α
D
C
B
A
0
a/2 sin γ

Figure 3, Part IA

Bustamite, $\rho(x,z)$. (Ca + Mn) peaks are shaded in.


$c/4 \sin\alpha$
0
$a/2 \sin\gamma$

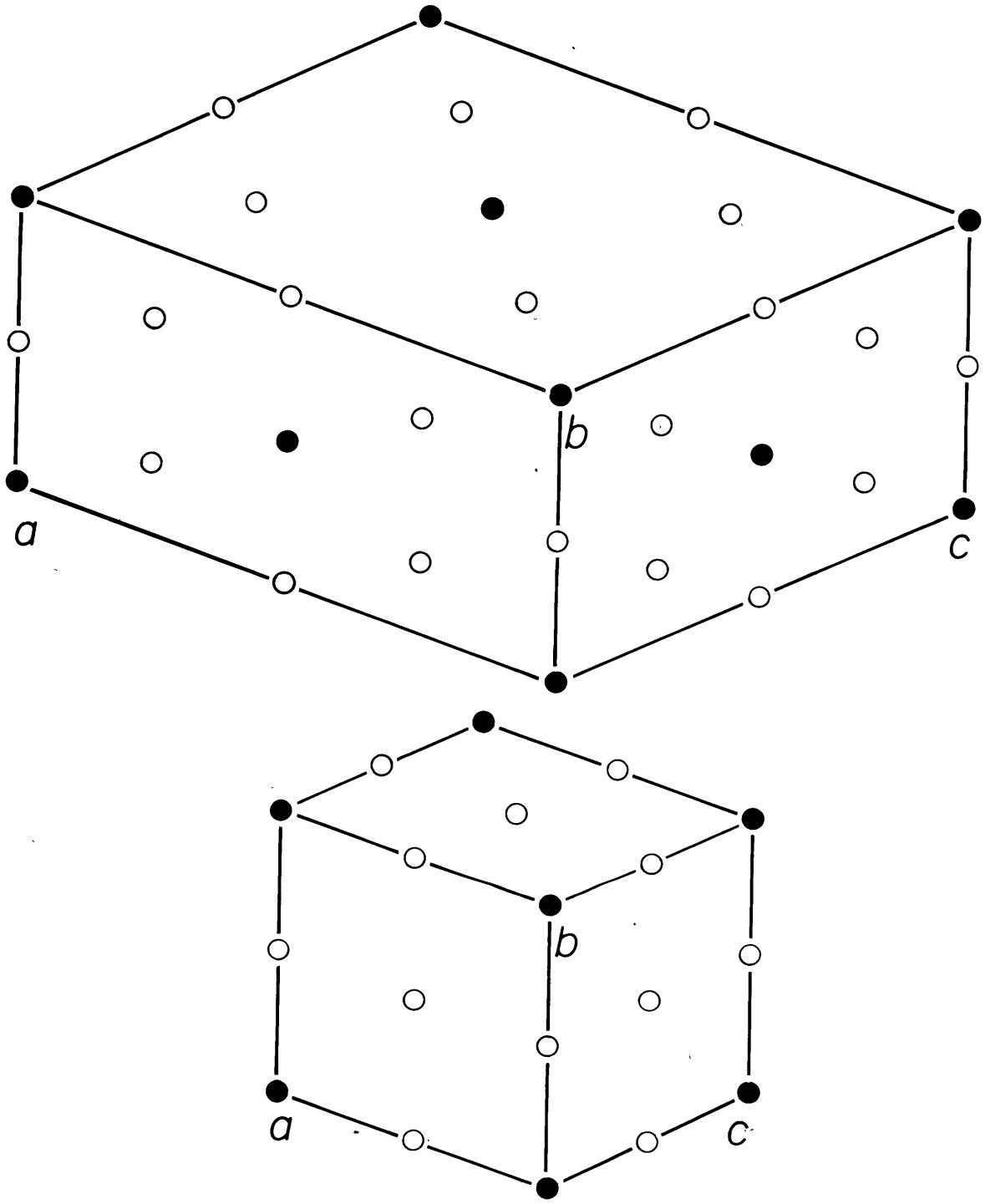
Determination of y coordinates. The lower part of Fig. A4 shows the primitive triclinic unit cell of wollastonite and the upper part shows the face-centered bustamite cell in corresponding orientation. Inversion centers coinciding with lattice points are shown as solid circles and all other inversion centers as open circles. All inversion centers lie on (101) planes which intersect $\underline{a}$ and $\underline{c}$ at 0 and $\frac{1}{2}$ in wollastonite and at 0, $\frac{1}{4}$, $\frac{1}{2}$ and $\frac{3}{4}$ in bustamite. The distribution of inversion centers is the same in both structures, except that those centers on planes parallel to (101) in bustamite intersecting $\underline{a}$ and $\underline{c}$ at $\frac{1}{4}$ and $\underline{a}$ and $\underline{c}$ at $\frac{3}{4}$ are shifted by $\frac{b}{4}$ relative to those in wollastonite.

Figures A1 and A3 show that Si and (Ca, Mn) atoms lie approximately on planes parallel to (101) which contain the inversion centers in both structures. Planes containing Si atoms alternate with those containing (Ca, Mn).

Figure A1 shows that in wollastonite there are inversion centers in the (101) planes at $\underline{y} = 0$ and $\frac{1}{2}$. Because the sub-structure has period $\frac{b}{2}$, there are also pseudocenters for the Ca atoms and their coordinating oxygen atoms, which project at the same $\underline{xz}$ coordinate, at $\underline{y} = \frac{1}{4}$ and $\frac{3}{4}$. Since the Si atoms are not in the substructure these pseudocenters do not apply to them.

Figure 4, Part IA

Comparison of unit cells of bustamite (above) and wollastonite (below). Lattice points (which are coincident with inversion centers) are shown as solid circles. Other inversion centers are shown as open circles.


a
b
c
a
b
c

A reasonable model for the structure of bustamite results from combining the above information with the fact that wollastonite and bustamite are similiar in projection. Coordinates of Ca and Mn atoms and their coordinating oxygen atoms in bustamite differ from those in wollastonite in the following ways:

1. The pseudoinversion centers in wollastonite at $y = \frac{1}{4}, \frac{3}{4}$ in (101) planes containing Ca become true inversion centers in bustamite.

2. The inversion centers at $y = 0, \frac{1}{2}$ in wollastonite become pseudoinversion centers in bustamite.

The relative arrangement of silica tetrahedra is the same in both structures except that tetrahedra in alternating sheets are displaced by $\frac{b}{2}$ by the face-centering translation in bustamite.

The above arrangement of inversion centers requires that the (Ca, Mn) of bustamite, equivalent to Ca_3 of wollastonite, be located on inversion centers; that is, four (Ca, Mn) atoms are still in two general positions of rank 2, and two (Ca, Mn) atoms are on centers with rank 1. This is just the distribution required for ordering of Ca and Mn atoms which was noted in the section on unit cell and space group.

Structure factors were calculated for all 1212 observed reflections using x and z parameters derived from the projection, and y parameters of wollastonite adjusted as required above. Ca and Mn atoms were assumed to be completely disordered, since at this point there was still no direct evidence for ordering. The discrepancy factor, R, was only 31%, suggesting that the proposed structure was probably correct.

Refinement

Refinement was carried out using SFLSQ2, a least-squares IBM 709 program using the full matrix[12]. For the initial refinement, form-factor curves were used for Ca and Mn assuming complete disorder, and a correction made for the average real component of anomalous dispersion. All atoms were assumed to be half ionized. All 1212 reflections were used as input to each cycle of refinement, but those reflections with $(F_o-F_c)/F_c > 0.5$ were rejected by the program. The weighting scheme recommended by Hughes[13] was used throughout. Isotropic temperature factors for all atoms were initially

set at 0.5, a value consistent with temperature factors of other silicate structures refined in this laboratory.

The discrepancy factor R decreased to 12.3% after only three cycles, confirming the correctness of the proposed structure. For these cycles, only the scale factor and coordinates were allowed to vary. Using structure factors calculated from coordinates of cycle 3, a three-dimensional difference Fourier synthesis $\Delta\rho(xyz)$ was computed. (All three-dimensional Fourier syntheses were computed using the IBM 709/7090 program ERFR$_2$.[14]) The only major discontinuities in the synthesis were negative or positive peaks at the positions of (Ca + Mn) atoms. The peak heights are listed in Table A2. Interatomic distances, also shown in Table A2, were calculated using ORXFE, an IBM 704 program.[15]

Mn has five more electrons than Ca, assuming equal ionization of Mn and Ca. Thus the positive peaks at the positions of cations 1 and 3 clearly indicate that Mn atoms are located there, while the negative peaks of cations 2 and 4 suggest that Ca occupies those positions. The radius of Mn^{+2} (0.91 Å) is less than that of Ca^{+2} (1.06 Å). The smaller average cation-oxygen distances of cations 1 and 3 and the larger distances of cations 2 and 4 therefore confirm the ordering indicated by the peaks of $\Delta\rho(xyz)$.

Table A2

Interatomic distances and cation peak heights after cycle 3 of refinement.

Cation number	Equipoint rank	Average cation-oxygen interatomic distance	Peak height in $\Delta\rho$ (xyz)	Interpretation of ordering
1	2	2.25 Å	377	Mn, excess Ca
2	2	2.38	-1170	Ca
3	1	2.21	642	Mn
4	1	2.39	-1250	Ca

It was noted above that there is an excess of Ca over Mn in the material used for this study. The peak at the position of cation 1 in $\Delta\rho$ (xyz) is slightly lower than that for cation 3. In addition, the average cation-oxygen distance is slightly larger for cation 1 than for cation 3. This indicates that the excess Ca substitutes for Mn preferentially in the site labelled cation 1.

Three structure-factor computations were made (taking account of both the real and imaginary components of anomalous dispersion of Mn and Ca) for the following distributions of the excess Ca:

1. all excess Ca assigned to cation 1;
2. $\frac{1}{3}$ excess Ca assigned to cation 1, $\frac{2}{3}$ to cation 3;
3. all excess Ca assigned to cation 3.

The R value was essentially equal for all three distributions ($\sim$9.5%) but the comparison of F_{obs} and F_{cal} was slightly better with the excess Ca substituting for the Mn of cation 1. Since this confirmed the conclusion reached on the basis of the peaks of $\Delta\rho$ (xyz) and the interatomic distances, this distribution of the excess Ca was accepted as being correct.

Refinement was continued with the Ca and Mn distribution determined above, taking full account of anomalous dispersion. The Zn, Fe and Mg reported in the analysis were considered to

substitute for Mn, since these atoms are smaller than Mn.

Two more cycles (4 and 5) were executed varying only coordinates and the scale factor. The coordinates were essentially unchanged in cycle 5. Individual isotropic temperature factors were varied in cycles 6 and 7. Refinement was concluded with two cycles in the first of which the coordinates and the scale factor were permitted to vary, and another cycle in which isotropic temperature factors were refined. Final parameters and their errors are listed in Table 3.

Description of the bustamite structure

The electron density $\rho(\underline{xyz})$ was computed using the signs of the structure factors of the final cycle of refinement. The peaks of this three-dimensional function are shown projected parallel to b in Fig. A5. Figure A6 is an interpretation of the same projection. The similarity of the structures of bustamite and wollastonite (Fig. A1) has been noted above several times. The relations between these structures is discussed in another place.[16]

Table A3

Coordinates and isotropic temperature factors for atoms of bustamite.

	x	σ(x)	y	σ(y)	z	σ(z)	B	σ(B)
Mn_1	.1009	.0001	.6725	.0003	.3733	.0001	.56	.03
Ca_1	.0994	.0001	.1583	.0004	.3785	.0001	.69	.03
Mn_2	$\frac{1}{4}$	0	0	0	$\frac{1}{4}$	0	.56	.04
Ca_2	$\frac{1}{4}$	0	$\frac{1}{2}$	0	$\frac{1}{4}$	0	.73	.05
Si_1	.0884	.0002	.2003	.0005	.1343	.0002	.34	.04
Si_2	.0888	.0002	.6454	.0005	.1325	.0002	.32	.04
Si_3	.1975	.0002	.9805	.0005	.0218	.0002	.16	.04
O_1	.2158	.0005	.9758	.0014	.4027	.0005	.68	.12
O_2	.2018	.0005	.4840	.0014	.4069	.0005	.57	.12
O_3	.1563	.0005	.1838	.0014	.2293	.0005	.48	.12
O_4	.1509	.0005	.7206	.0014	.2315	.0005	.50	.12
O_5	.0131	.0005	.3964	.0014	.3549	.0005	.64	.12
O_6	.0140	.0005	.8513	.0014	.3717	.0005	.66	.12
O_7	.1287	.0005	.1240	.0014	.0393	.0005	.57	.12
O_8	.1364	.0005	.7625	.0013	.0411	.0005	.29	.11
O_9	.0926	.0006	.4250	.0016	.1147	.0006	1.34	.14

Figure 5, Part IA

Projection along b of the peaks of $\rho(xyz)$.

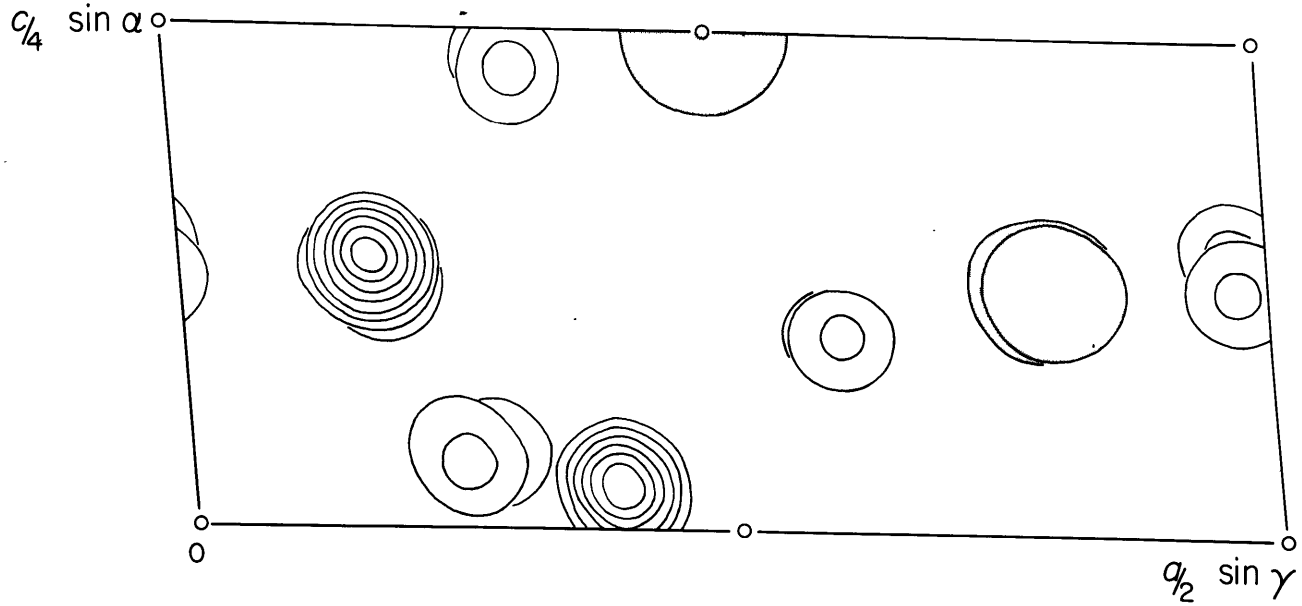
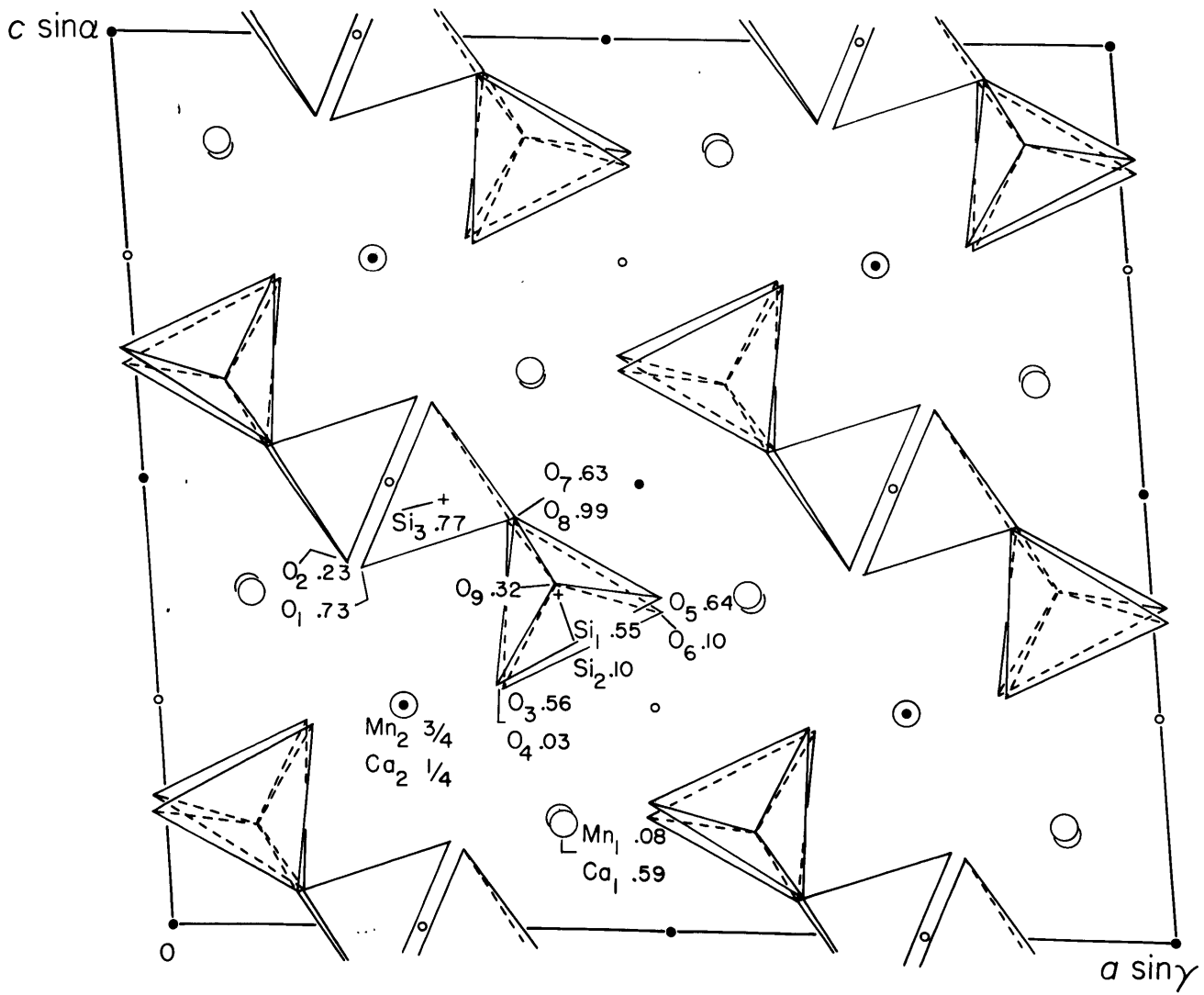

$c/_4$ sin α
0
$a/_2$ sin γ

Figure 6, Part IA

Interpretation of $\rho(xyz)$. Inversion centers at $y = 0, \frac{1}{2}$ shown as solid circles and inversion centers at $y = \frac{1}{4}, \frac{3}{4}$ as open circles.


c sinα
O7 .63
O8 .99
Si3 .77
O2 .23
O1 .73
O9 .32
O5 .64
Si1 .55
O6 .10
Si2 .10
O3 .56
O4 .03
Mn2 3/4
Ca2 1/4
Mn1 .08
Ca1 .59
0
a sinγ

In Fig. A6 the arrangement of oxygen atoms crudely approximates close packing, all oxygen atoms except O_9 lying in sheets which are parallel to (101). Ca and Mn atoms and Si atoms alternate in layers between sheets of oxygen atoms, with Ca and Mn in octahedral coordination and Si in tetrahedral coordination. SiO_4 tetrahedra all share two oxygen atoms with other tetrahedra to form a chain whose repeat unit is three tetrahedra and which is oriented parallel to the b axis. The nature of the arrangement of tetrahedra is best shown in Figs. A7 and A8. Fig. A7 is a projection of the structure parallel to a while Fig. A8 is a projection along c.

The sheet of Ca and Mn octahedra can be compared to the sheet of Mg octahedra in brucite. Octahedra share edges to form a continuous two-dimensional sheet in brucite. The wollastonite arrangement may be interpreted in terms of ideal close packing of the oxygen atoms in sheets coordinating Ca atoms. As shown in Figs. A7 and A8, octahedra share edges to form a band three octahedra wide, extending infinitely parallel to b. Individual bands are separated by a column of unoccupied octahedrally coordinated voids. There is actually considerable distortion of the close-packed oxygen layers, however, particularly around the column of vacant octahedra.

Figure 7, Part IA

Structure of bustamite from $x = \frac{1}{4}$ to $\frac{1}{4}$ projected onto a plane defined by the axes b and c sin β.

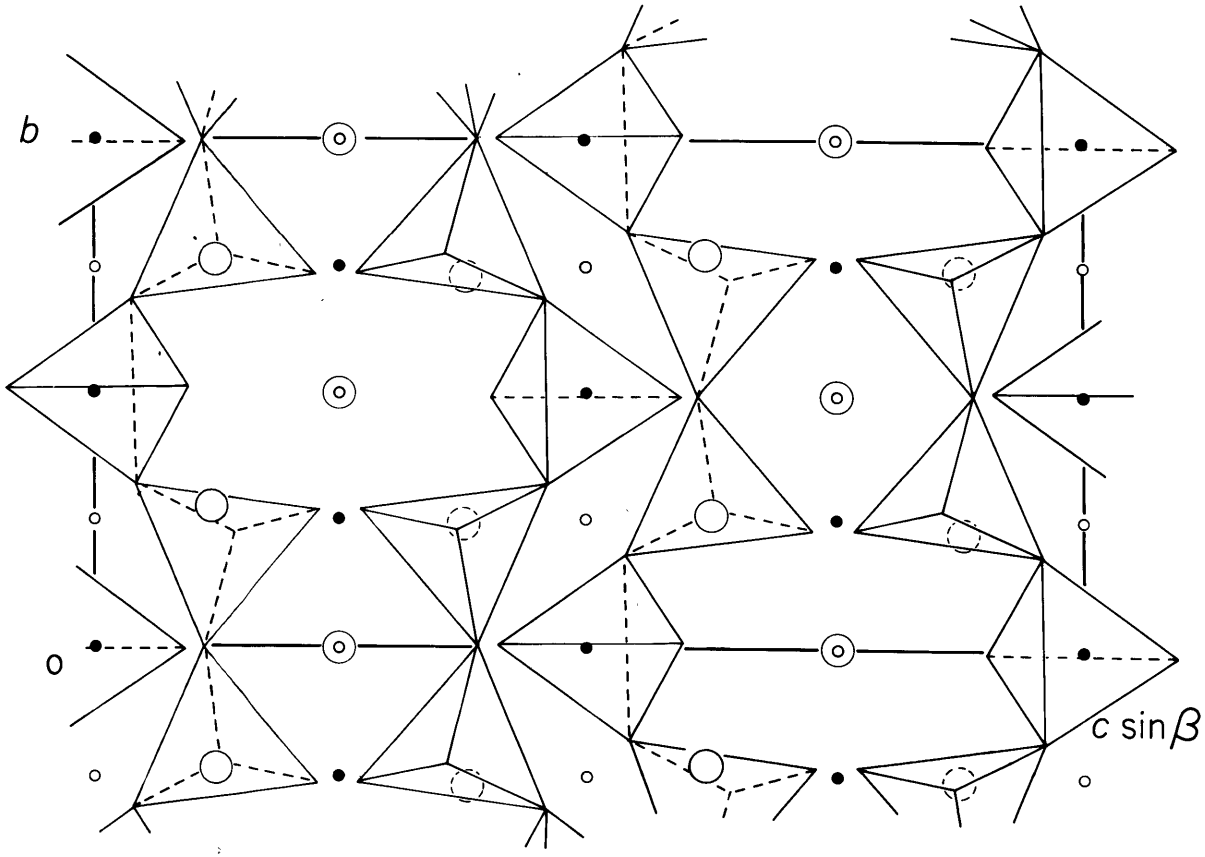
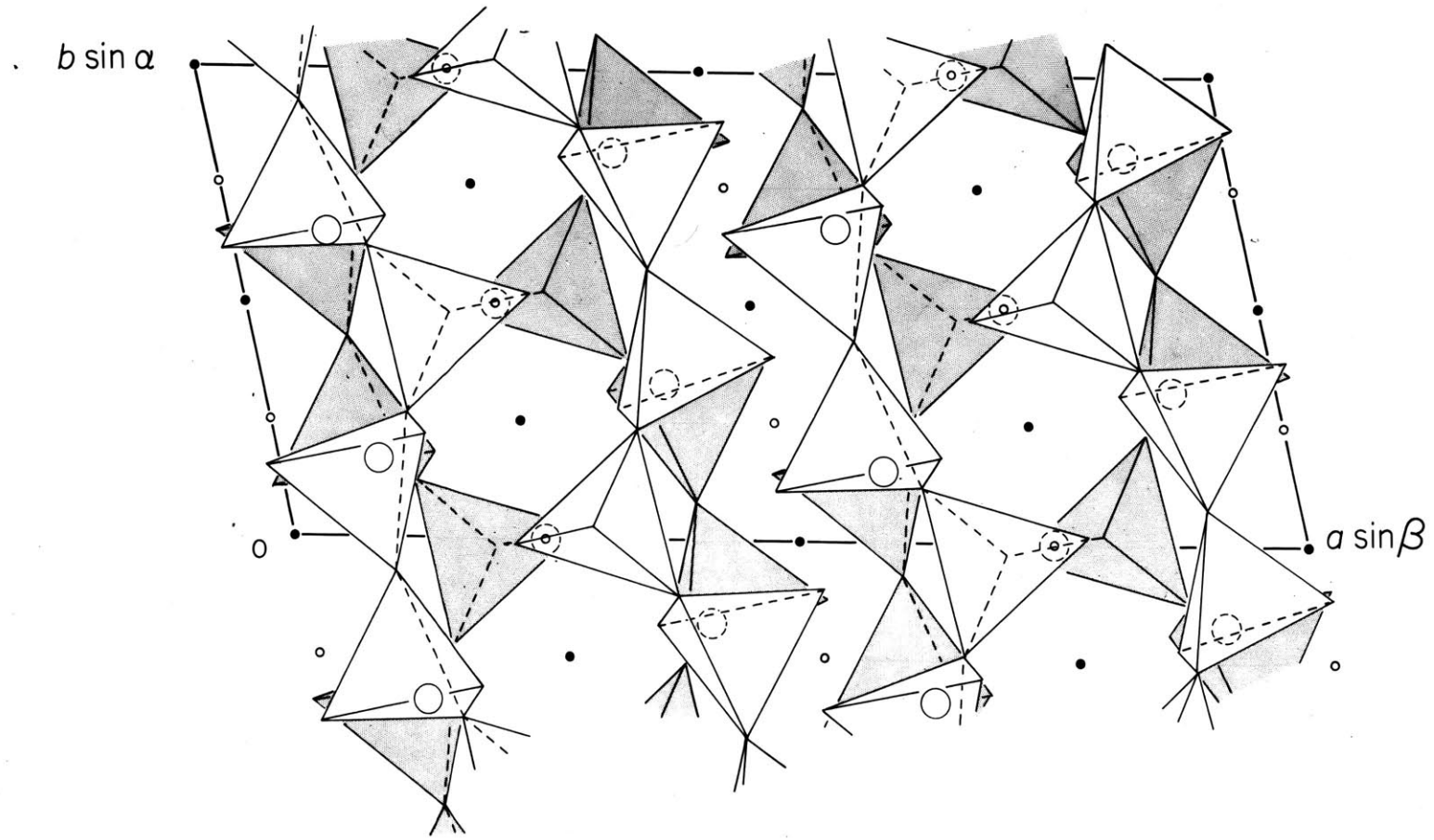

b
0
c sin β

Figure 8, Part IA

Projection along c of the structure of bustamite.


b sin α
0
a sinβ

Interatomic distances are listed in Table A4. These are discussed in detail elsewhere.[16] All distances are close to accepted values. The average Si-O distance is 1.623 Å. Smith and Bailey[17] state that the average Si-O distance of a silicate is a function of the extent of tetrahedral linkage. The distance 1.623 Å falls exactly at the value predicted by them for metasilicates.

There are three non-equivalent Si-O-Si angles in bustamite, which are:

$$Si_1 - O_9 - Si_2,\ 161°,$$
$$Si_1 - O_7 - Si_4,\ 135°,$$
$$Si_2 - O_8 - Si_4,\ 137°.$$

Corresponding angles in wollastonite are 149°, 139° and 140° respectively.[18] In a survey of Si-O-Si angles, Liebau[19] found that the average for well-determined structures is about 140°. Angles greater than 150° are uncommon and, under normal conditions, represent a relatively unstable condition. The angle Si_1-O_9-Si_2 is large in both bustamite and wollastonite, but unusually so in bustamite. In addition, the isotropic temperature factor for O_9 of bustamite is considerably larger (1.34) than all other temperature factors of the structure (see Table A3). In wollastonite, this temperature factor (0.68) is only slightly above the average for the entire structure.

Table A4

Interatomic distances in bustamite

Si_1 - O_3	1.628 Å	Ca_1 - O_1	2.437 Å
O_5	1.587	O_2	2.531
O_7	1.645	O_3	2.298
O_9	1.616	O_5	2.382
Av.	1.619	O_6	2.302
		O_8	2.358
Si_2 - O_4	1.626	O_9	2.899
O_6	1.585	Av.	2.384 (excluding O_9)
O_8	1.647		
O_9	1.613	Mn_2 - $2O_1$	2.215
Av.	1.618	$2O_3$	2.154
		$2O_4$	2.241
Si_3 - O_1	1.600	Av.	2.203
O_2	1.595		
O_7	1.660	Ca_2 - $2O_2$	2.344
O_8	1.671	$2O_3$	2.412
Av.	1.632	$2O_4$	2.421
		$2O_9$	2.891
		Av.	2.392 (excluding O_9)

Table A4 (Conti.)

Interatomic distances in bustamite

Mn_1 -	O_1	2.499
	O_2	2.286
	O_4	2.163
	O_5	2.144
	O_6	2.041
	O_7	2.335
	Av.	2.245

Acknowledgements

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Part I-B

Comparison of the crystal structures of bustamite and wollastonite

Donald R. Peacor

Massachusetts Institute of Technology
Cambridge 39, Massachusetts, U.S.A.

Abstract

The structures of bustamite and wollastonite differ principally only in arrangement of the chains of tetrahedra. Chains in alternating sheets may be described by the sequence AAA.... in wollastonite and ABAB.... in bustamite. Both structures have a pseudomonoclinic cell, this unit having space group $P2_1/m$ in wollastonite and A2/m in bustamite.

Introduction

On the basis of a comparison of optical properties, Sundius (1931) postulated that bustamite ($CaMnSi_2O_6$) is Mn-rich wollastonite ($CaSiO_3$). Schaller (1938, 1955) also concluded that bustamite had the wollastonite structure because of a close relationship between the optical properties of the two minerals. Berman and Gonyer (1937), using rotating-crystal photographs, found that their unit cells were similar (Table 1B) and concluded that they were related only by solid solution. Buerger, however (1956) found that the unit cell of bustamite (Table 1B) is closely related to , but different from the cell of wollastonite. He noted that there is a sort of superstructure relation between the two minerals. Liebau et al. (1958) confirmed Buerger's unit cell and guessed that the difference in structures is based only on a different ordering of chains and cations.

The structure of bustamite has recently been determined and refined (D.R. Peacor and M.J. Buerger, 1962). The structure of wollastonite was determined by Mamedov and Belov (1956) and refined by Buerger and Prewitt (1961). These structures are different but bear a very close relationship to one another.

Table 1B

Symmetry and unit-cell data for bustamite and wollastonite

	wollastonite Buerger	bustamite Berman and Gonyer	bustamite Buerger	β-$Mn_{0.8}Ca_{0.2}SiO_3$ Liebau et al.	bustamite Peacor and Buerger	bustamite Peacor
a	7.94 Å	7.64 Å	2 x 7.73 Å	2 x 8.03 Å	15.412 Å	7.736 Å
b	7.32	7.16	7.18	7.11	7.157	7.157
c	7.07	6.87	2 x 6.92	2 x 6.84	13.824	13.824
α	90°02'	92°08'	89°34'	-	89°29'	90°31'
β	95°22'	94°54½'	94°53'	-	94°51'	94°35'
γ	103°26'	101°35'	102°47'	-	102°56'	103°52'
Space group	$P\bar{1}$	P1 or $P\bar{1}$	$F\bar{1}$	F1 or $F\bar{1}$	$F\bar{1}$	$A\bar{1}$

Description of structures

The face-centered unit cell of bustamite may be transformed to an A-centered cell with the following transformation matrix:

$$\begin{matrix} -\frac{1}{2} & -\frac{1}{2} & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{matrix}$$

The A-centered cell bears a close relationship to the wollastonite cell, as does the face-centered cell (Table 1B). Since the relation between the structures of wollastonite and bustamite is clearer if bustamite is described in terms of the A-centered cell, all description of bustamite is referred to it in this paper.

Atomic coordinates for both bustamite and wollastonite are listed in Table 2B. The similarity shows that the asymmetric units of each structure are essentially the same. The structures are shown projected along b in Figs. 1A and 1B . Four wollastonite unit cells and two bustamite unit cells are shown. Ca or Mn atoms are shown as large open circles, inversion centers at $y = \frac{1}{4}, \frac{3}{4}$ as small open circles, and inversion centers at $y = 0, \frac{1}{2}$ as small solid circles. The structures are the same in projection except for minor coordinates shifts. The arrangement of the oxygen

Table 2B

Coordinates and isotropic temperature factors of atoms in wollastonite (upper values) and bustamite (lower values). For comparison , bustamite z coordinates are multiplied by 2. Coordinates of atoms in bustamite are given relative to the A-centered unit cell.

Atom	x	y	z	B
Ca_1	.1985	.4228	.7608	.41
Mn_1	.2018	.4284	.7466	.56
Ca_2	.2027	.9293	.7640	.45
Ca_1	.1988	.9411	.7570	.69
Ca_3	.4966	.2495	.4720	.37
Mn_2	1/2	1/4	1/2	.56
Ca_3	.5034	.7505	.5280	.37
Ca_2	1/2	3/4	1/2	.73
Si_1	.1852	.3870	.2687	.24
	.1768	.3881	.2686	.34
Si_2	.1849	.9545	.2692	.24
	.1775	.9434	.2650	.32
Si_3	.3970	.7235	.0560	.22
	.3950	.7171	.0436	.16
O_1	.4291	.2314	.8019	.48
	.4316	.2400	.8054	.68

Atom	x	y	z	B
O_2	.4008	.7259	.8302	.37
	.4036	.7178	.8138	.57
O_3	.3037	.4635	.4641	.60
	.3126	.4725	.4586	.48
O_4	.3017	.9374	.4655	.64
	.3017	.9302	.4630	.50
O_5	.0154	.6254	.7343	.63
	.0261	.6167	.7098	.64
O_6	.0175	.1319	.7353	.71
	.0280	.1627	.7434	.66
O_7	.2732	.5118	.0919	.37
	.2574	.5047	.0786	.57
O_8	.2713	.8717	.0940	.51
	.2729	.8739	.0822	.29
O_9	.2188	.1784	.2228	.68
	.1851	.1676	.2294	1.34

Figure 1A, Part IB

Projection along b of the structure of wollastonite (space group $P\bar{1}$). Four unit cells are shown.

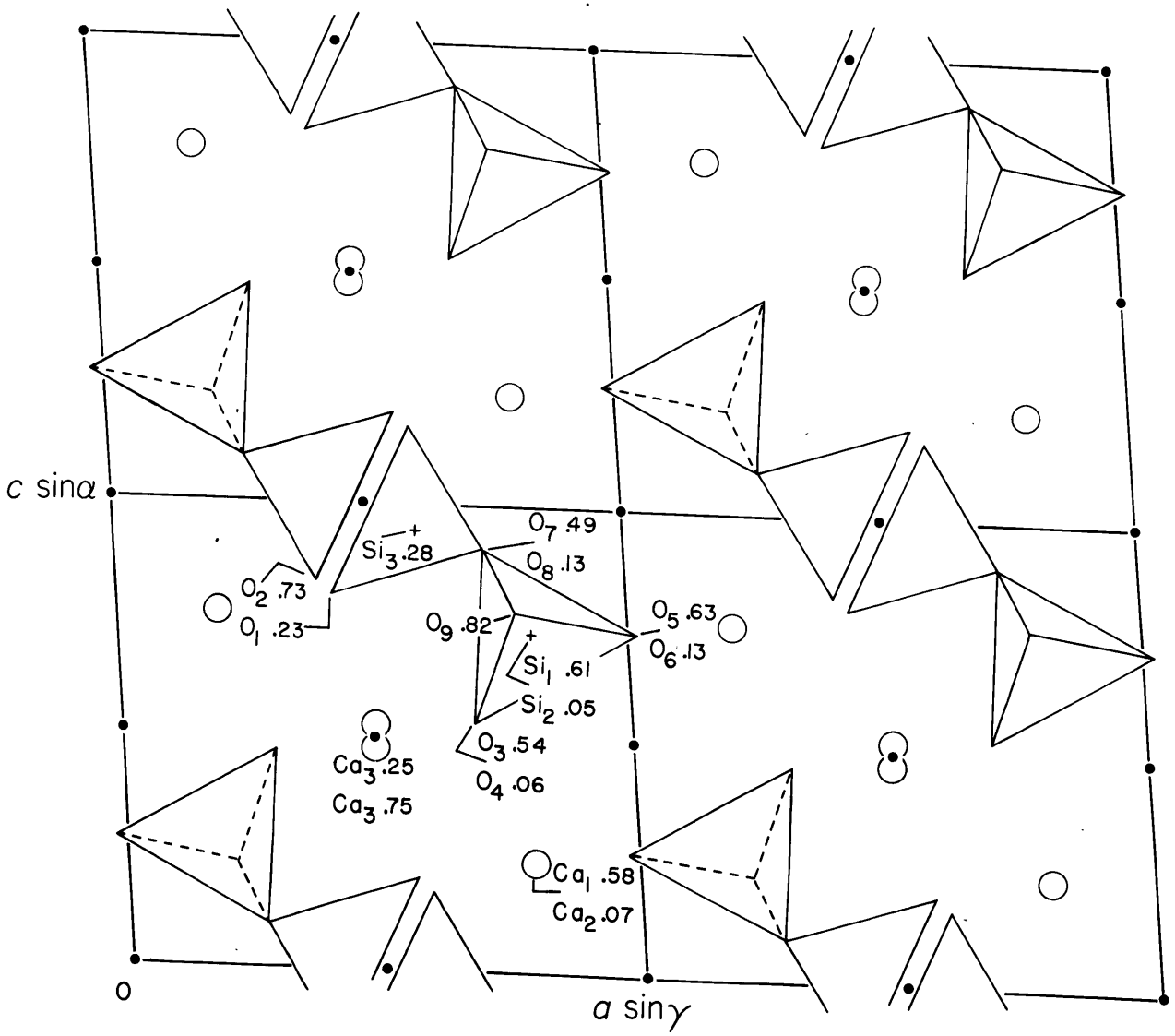
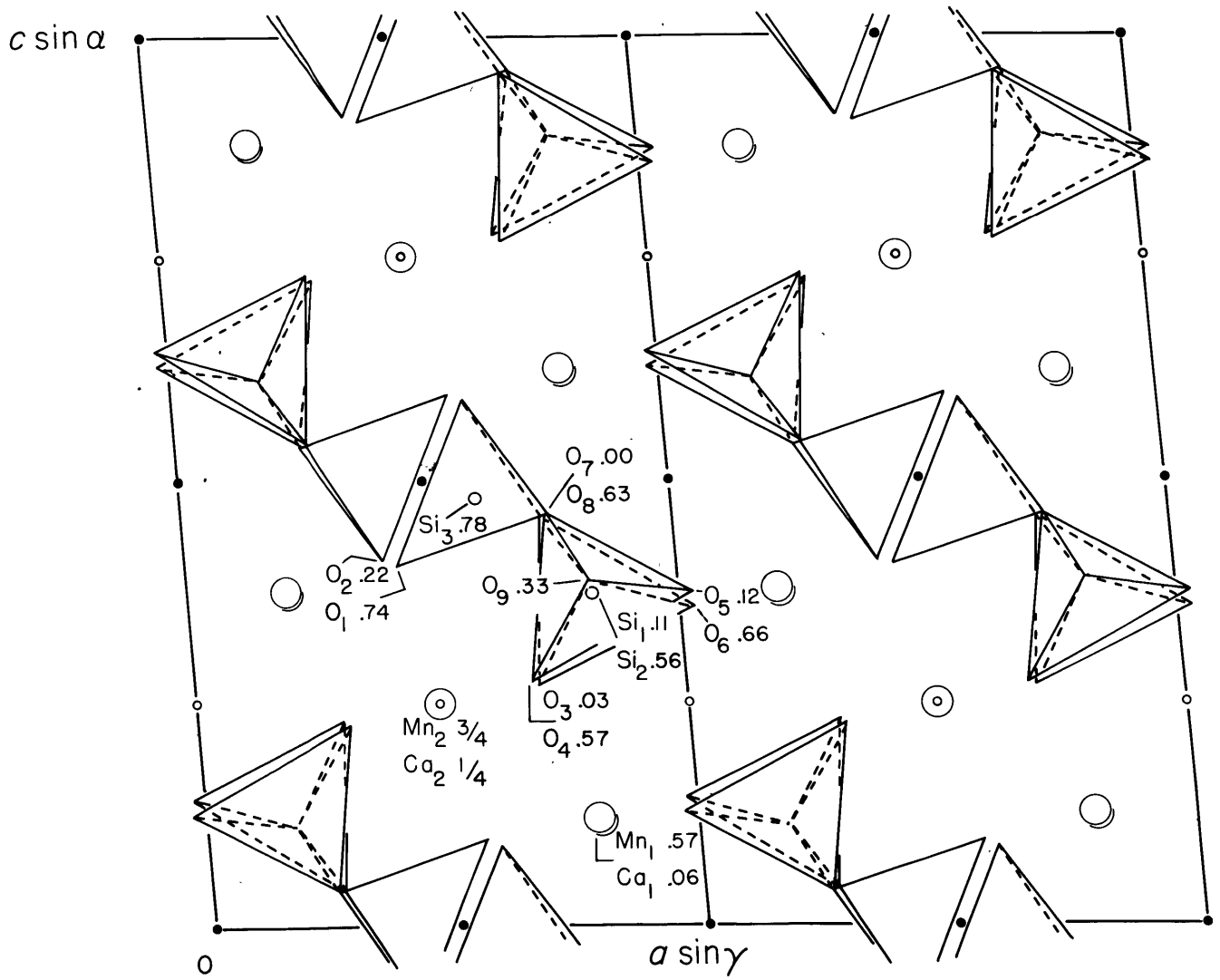

c sinα
0
a sinγ
Si3 .28
O7 .49
O8 .13
O2 .73
O1 .23
O9 .82
O5 .63
O6 .13
Si1 .61
Si2 .05
O3 .54
O4 .06
Ca3 .25
Ca3 .75
Ca1 .58
Ca2 .07

Figure 1B, Part IB

Projection along b of the structure of bustamite (space group $A\bar{1}$) Two unit cells are shown.


c sin α
O7 .00
O8 .63
Si3 .78
O2 .22
O1 .74
O9 .33
O5 .12
Si1 .11
O6 .66
Si2 .56
O3 .03
O4 .57
Mn2 3/4
Ca2 1/4
Mn1 .57
Ca1 .06
0
a sinγ

atoms of both structures approximates close packing in a crude way with an obvious layering parallel to (101). Layers consisting of Ca (wollastonite) or Ca and Mn (bustamite) atoms in octahedral coordination alternate with layers composed of Si atoms between the sheets of oxygen atoms. The SiO_4 tetrahedra are arranged in chains whose repeat unit is three tetrahedra and which are oriented parallel to the b axis (Figs. 2 and 3).

Arrangement of SiO_3 chains

The primary difference in the structures of bustamite and wollastonite lies in the arrangement of the SiO_3 chains. Note first that the arrangement of Mn and Ca atoms is approximately the same in both structures over all space. This is most easily seen in Figs. 2A and 2B. This relation also holds true for all oxygen atoms which coordinate Ca or Mn atoms. (This relation will be discussed in more detail in the section on substructure.) The difference in the structures then lies principally in the location of O_9 and the silicon atoms. In successive layers in wollastonite these atoms are related by the translation 001, and in bustamite by the

Figure 2A, Part IB

Projection along a of the structure of wollastonite. Only Ca atoms and translation-related chains are shown.

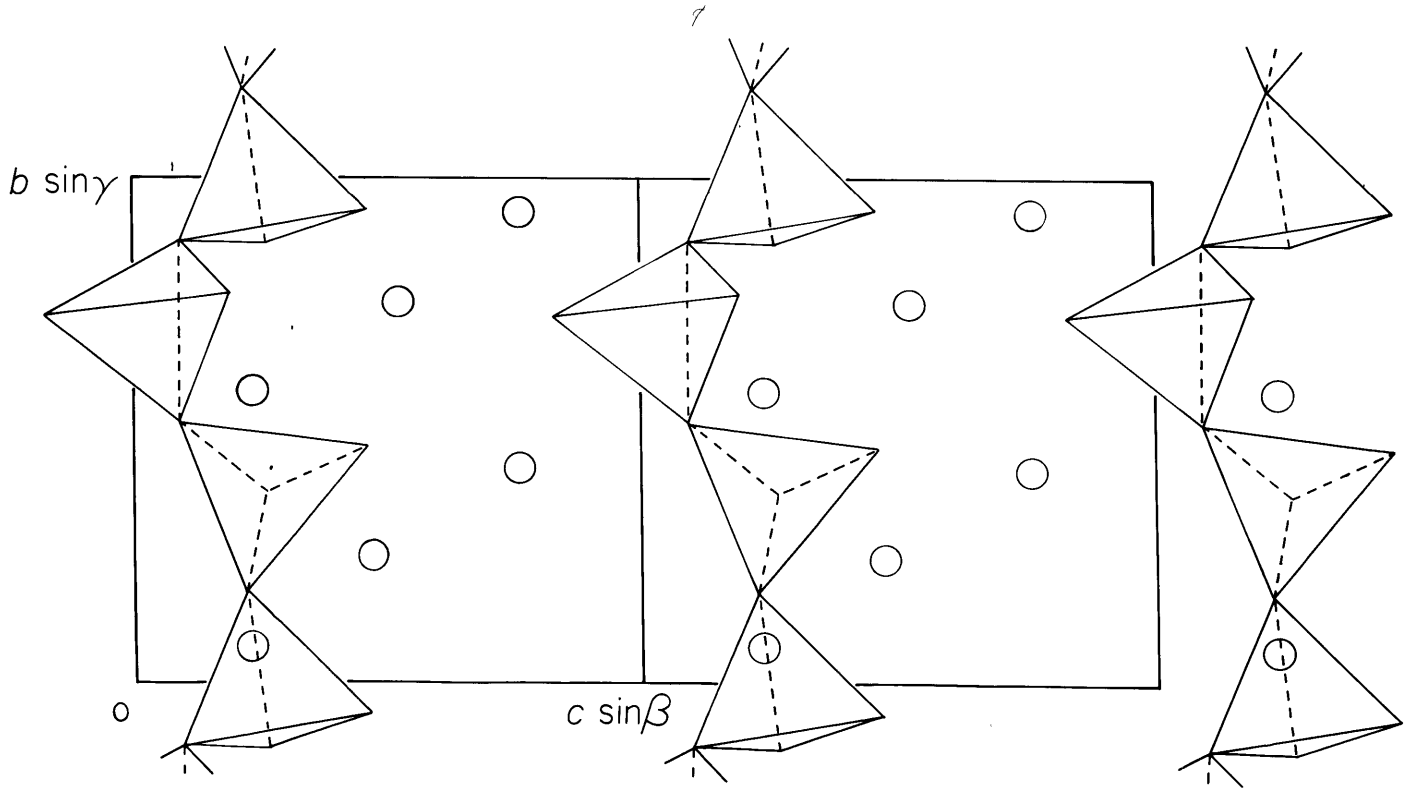

b sinγ
o
c sinβ

Figure 2B, Part IB

Projection along a of the structure of bustamite. Only Ca and Mn atoms and translation-related chains are shown.

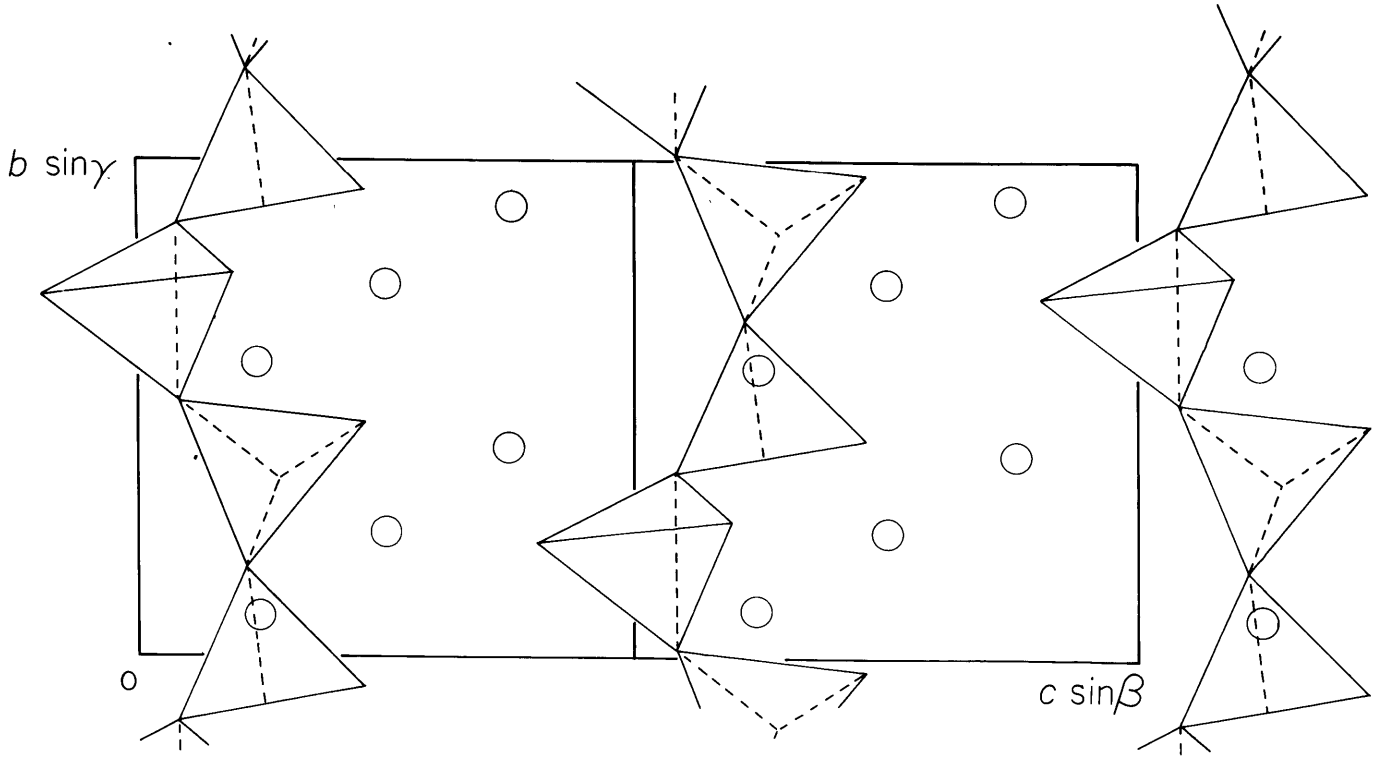

b sinγ
o
c sinβ

Figure 3A, Part IB

Projection along c of the structure of wollastonite. The primitive triclinic cell is outlined with a light line. The pseudomonoclinic cell (space group $P2_1/m$) is partially outlined with a dotted line, and mirror planes are indicated with a heavy line.

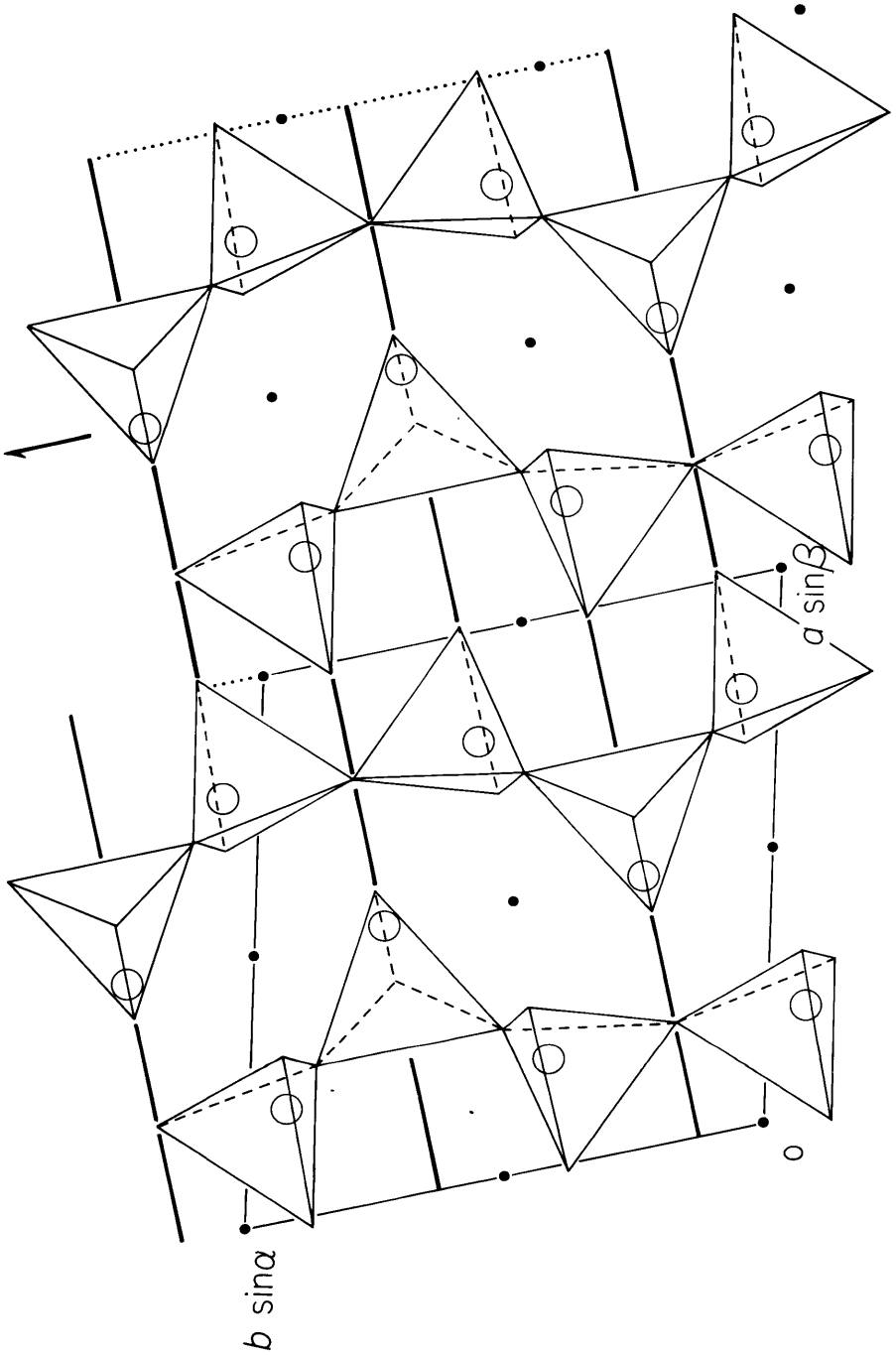
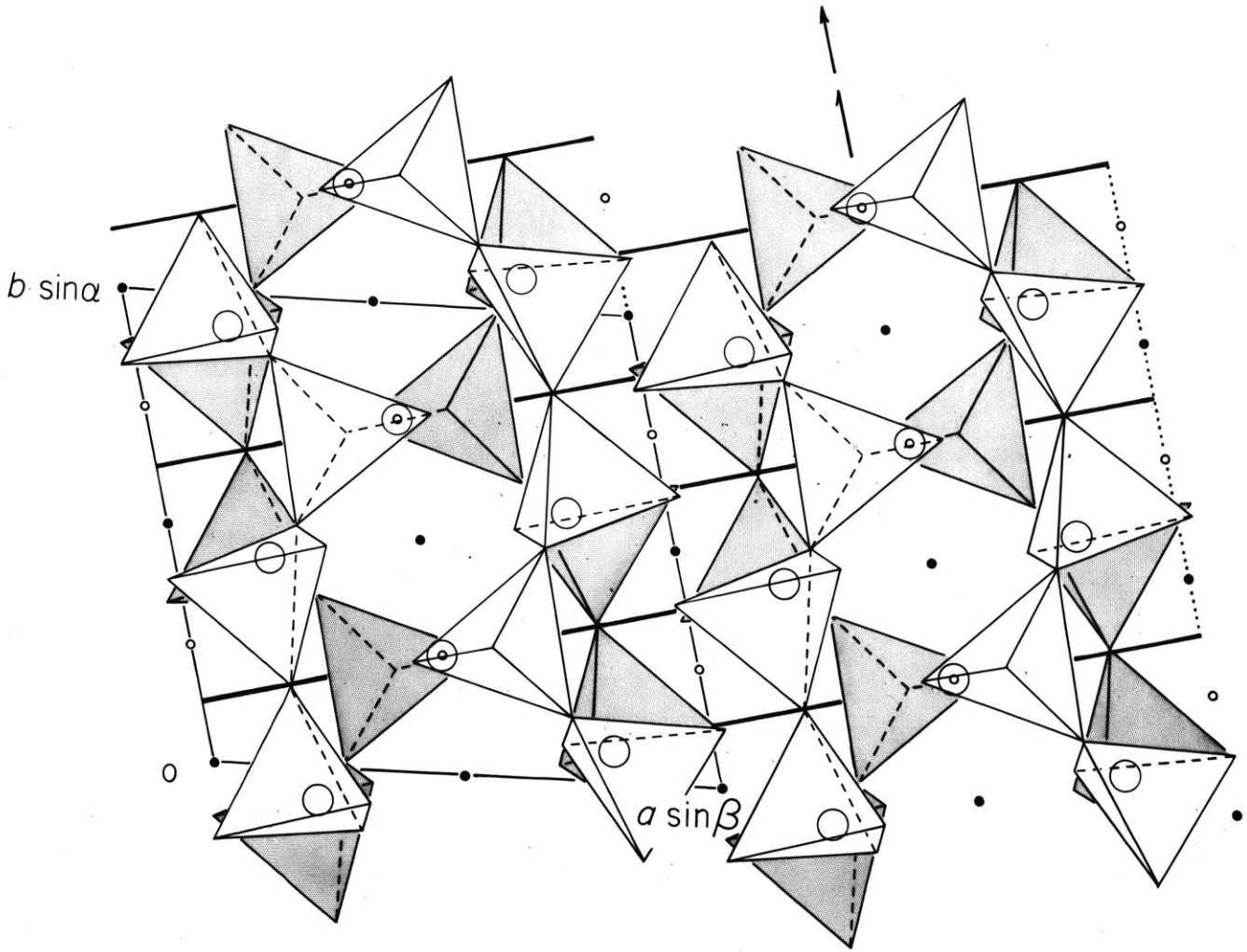

a sinβ
o
b sinα

Figure 3B, Part IB

Projection along a of the structure of **busta-**mite. The A-centered triclinic cell is out-lined with a light line. **The pseudomonoclinic cell (space group A2/m) is partially outlined with a dotted line, and mirror planes are indicated with a heavy line.**


b sinα
0
a sinβ

translation $0\frac{1}{2}\frac{1}{2}$. This merely means that SiO_3 chains in successive layers are shifted by y/2 in bustamite but not in wollastonite. The arrangement is illustrated in Figs. 2A and 2B, where the related structures are shown projected along a. Only translation-related chains and Ca and Mn atoms are shown. The arrangement of the SiO_3 chains may be represented by the notation AAA...., in wollastonite, and by ABAB.... in bustamite. Here A symbolizes a shift of 0 and B a shift of $\frac{1}{2}$ in the b direction for SiO_3 chains of successive layers.

It is interesting to compare this with the polymorphism of $MgSiO_3$ described by Brown et al. (1961). Here the layers of Mg and Si atoms also alternate between layers of oxygen atoms arranged approximately in close packing. SiO_3 chains in successive layers may be displaced by c/2 (the axis c is parallel to the chains of tetrahedra) giving rise to stacking relations analogous to those between bustamite and wollastonite. In the polymorphs of $MgSiO_3$, however, the relative positions of the Mg polyhedra may differ from level to level.

Substructure relations

Both bustamite and wollastonite are characterized by a prominent substructure with period b/2 (Fig. B1). All atoms except Si_3 and O_9 are related to a second atom by a shift of about b/2. Note, for example, in Fig. B1A, that Ca_1 and Ca_2 fall almost exactly over each other, and differ in y by 0.51. The relation is imperfect in some cases, as with O_1 and O_2 of wollastonite, where the shift (Δ x, Δ y, Δ z) is 0.03, -0.49, -0.03. Nevertheless, it is approximately true. The coordinates of the substructure atoms are very similar in the two structures. Thus, with the exception of Si_3 and O_9, the structures of wollastonite and bustamite are approximately the same.

Cation ordering

Schaller (1938) states that minerals in this group have been found with "MnO ranging from a few per cent...to a maximum of 33 per cent." No Mn was reported in the wollastonite refined by Buerger and Prewitt (1961). The bustamite (ideally $CaMnSi_2O_6$) whose structure was refined by Peacor and Buerger contained a slight excess of Ca relative to Mn.

In wollastonite the Ca atoms are distributed over three general positions. The Ca and Mn are ordered in bustamite, with one Ca and one Mn inversion centers and two Ca and two Mn in general positions. In addition, evidence strongly suggested that the "excess" Ca of bustamite replaces Mn at the position Mn_1 rather than the special position Mn_2.

Although all Ca or Mn atoms of each structure have approximately the same coordinates, there is not complete equivalence of positions. The Ca_2 and Mn_2 atoms of bustamite on inversion centers are equivalent to the Ca_3 atom in a general position in wollastonite. The Mn_1 and Ca_1 atoms in general positions of bustamite, however, are not equivalent to Ca_1 and Ca_2 of wollastonite. Half of the Mn_1 atoms of bustamite occupy positions in the structure similar to those of Ca_1 of wollastonite, and half occupy positions similar to Ca_2. The same is true of Ca_1 of bustamite. This is reflected in the difference in distribution of inversion centers in (101) layers containing Ca and Mn atoms, as can be seen in Figs. B1A and B1B. Compounds whose compositions are intermediate between bustamite and wollastonite still must be investigated to determine the limits and mechanism of solid solution in each. It is possible, if not probably, that metastable intermediate compounds exist which have partial or complete

disorder both in Ca and Mn and in SiO_3 chain distributions.

Interatomic distances

All average Ca-O distances are remarkably similar (2.388 $\pm$ .004 Å) in both structures as shown in Table 3B, except for that of Ca_1 of wollastonite. The comparison of Si-O distances is particularly interesting. The average of all Si-O distances is 1.623 Å in bustamite and 1.626 Å in wollastonite, the difference being well within the standard deviation. All average Si-O distances for Si_1 and Si_2 are almost exactly equal, and Si_3-O distances are uniformly larger than Si_1-O and Si_2-O distances in both structures.

There is an excellent correlation of individual Si-O distances with coordination of oxygen. For instance, all Si-O_7 and Si-O_8 distances are greater than 1.64 Å, 1.673 Å being the largest. Both O_7 and O_8 are coordinated to two Si atoms, from which they receive a total bond strength of 2, and to one Ca or Mn atom, from which they receive a bond strength of $\frac{1}{3}$. The excess of bond strength ($\frac{1}{3}$) is thus compensated by unusually large Si-O distances. All Si-O_5 and Si-O_6 distances are less than 1.59 Å, 1.572 Å being the

Table 38

Cation-oxygen interatomic distances

Bustamite			Wollastonite		
Mn_1 -	O_1	2.499 Å	Ca_1 -	O_1	2.302 Å
	O_2	2.286		O_2	2.272
	O_4	2.163		O_3	2.324
	O_5	2.144		O_5	2.302
	O_6	2.041		O_6	2.272
	O_7	2.335		O_7	2.412
	Av.	2.245		Av.	2.314
Ca_1 -	O_1	2.437	Ca_2 -	O_1	2.316
	O_2	2.531		O_2	2.369
	O_3	2.298		O_4	2.421
	O_5	2.382		O_5	2.501
	O_6	2.302		O_6	2.316
	O_8	2.358		O_8	2.406
	O_9	2.899		Av.	2.388
	Av.	2.384 (excluding O_9)			

Bustamite		Wollastonite	
Mn_2 -$2O_1$	2.215	Ca_3 - O_1	2.439
$2O_3$	2.154	O_2	2.349
$2O_4$	2.241	O_3	2.429
Av.	2.203	O_3'	2.335
		O_4	2.441
		$O_{4'}$	2.349
		O_9	2.642
		Av.	2.390(excluding O_9)
Ca_2 -$2O_2$	2.344	Ca_3 - O_1	2.439
$2O_3$	2.412	O_2	2.349
$2O_4$	2.421	O_3	2.429
$2O_9$	2.891	$O_{3'}$	2.335
Av.	2.392(excluding O_9)	O_4	2.441
		$O_{4'}$	2.349
		O_9	2.642
		Av.	2.390
Si_1 - O_3	1.628	Si_1 - O_3	1.618
O_5	1.587	O_5	1.572
O_7	1.645	O_7	1.659
O_9	1.616	O_9	1.647
Av.	1.619	Av.	1.624

Bustamite		Wollastonite	
$Si_2 - O_4$	1.626	$Si_2 - O_4$	1.617
O_6	1.585	O_6	1.581
O_8	1.647	O_8	1.650
O_9	1.613	O_9	1.637
Av.	1.618	Av.	1.621
$Si_3 - O_1$	1.600	$Si_3 - O_1$	1.599
O_2	1.595	O_2	1.599
O_7	1.660	O_7	1.665
O_8	1.671	O_8	1.673
Av.	1.632	Av.	1.634

smallest. These oxygen atoms are coordinated to one Si atom from which they receive a bond of strength 1 and to two Ca or Mn atoms from which they receive a bond of strength $\frac{2}{3}$. Thus there is a bond deficiency $\frac{1}{3}$, which results in unusually short Si-O distances.

The only major differences in coordination between the two structures involve O_9. This is coordinated to Si_1 and Si_2 in both structures, but Si-O distances are larger in wollastonite. In addition, O_9 is coordinated to both Ca atoms in bustamite, but with very large Ca-O distances, and to only one Ca in wollastonite, at a shorter distance.

Pseudomonoclinic cells

Ito (1950) noted that the angle α of the wollastonite unit cell is very nearly 90° and that (140), which is normal to (100), approximates a mirror plane. From these data he suggested that the triclinic wollastonite cell is made up of "twinned or otherwise juxtaposed" monoclinic cells. Individual monoclinic units are related by the glide b/4 or -b/4. He noted that the monoclinic unit, which he called protowollastonite, must have either of the space groups P2/m or $P2_1/m$.

Figures 3A and 3B are projections along c of the structures of wollastonite and bustamite respectively. Prewitt and Buerger (in press) noted that wollastonite has a pseudomonoclinic cell with space group $P2_1/m$. This cell is partially outlined on the right side of Fig. B3A with a dotted line, while the mirror planes are indicated by doubly heavy lines. The triclinic cell is outlined on the left with a lighter line. Fig. B3B is an equivalent diagram of bustamite. The basic repeat unit is the same in bustamite as in wollastonite; i.e., two chains related by a 2_1 axis. The bustamite pseudomonoclinic cell is A-centered however, with space group A2/m. In wollastonite 2_1 axes are aligned along c. In bustamite there is a similar relation except that 2_1 and 2-fold axes alternate along c.

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Part II

Thesis content not specifically prepared for publication.

Chapter 1

Review of Literature on Phase Relations and Crystal Structures in the System $CaSiO_3$ - $MnSiO_3$

Phase-relations. The following naturally occurring and synthetic compounds have been described in that part of the system $CaSiO_3$ - $MnSiO_3$ which may be considered to be binary: wollastonite ($CaSiO_3$), parawollastonite ($CaSiO_3$), pseudowollastonite ($CaSiO_3$), johannsenite ($CaMnSi_2O_6$), bustamite ($CaMnSi_2O_6$), rhodonite ($MnSiO_3$), κ-$MnSiO_3$, β-$MnSiO_3$. Solid solution limits are not given in the above formulas since they are imperfectly known. These relations are discussed in detail in the following sections.

Wollastonite is the stable low temperature polymorph of $CaSiO_3$ and is the form commonly found in contact metamorphosed, Ca-rich rocks. Wollastonite inverts at approximately 1125°C. (Glasser and Glasser, 1960) to pseudowollastonite, which is the form usually found in slags, but rarely in nature. Parawollastonite is known only from natural occurrences. Its stability range, if any, relative to those of pseudowollastonite and wollastonite is unknown.

Bustamite is the high-temperature form of $CaMnSi_2O_6$. Johannsenite, the low-temperature form, inverts to bustamite

at approximately 830°C. (Schallyer, 1938 and Schiavinato, 1953).

The relations between the polymorphs of $MnSiO_3$ are less well known. Liebau et al. (1958). in an investigation of the system $CaMnSi_2O_6$ - $MnSiO_3$, found three forms, which they named κ-, β- and γ-$MnSiO_3$. γ-$MnSiO_3$ is equivalent to rhodonite and is stable at low temperatures. It inverts at approximately 650°C. to β-$MnSiO_3$, which has the bustamite structure. The third form, α-$MnSiO_3$ us metastable at all temperatures and is produced only as an intermediate form.

Phase relations in the subsolidus region of the system $CaSiO_3$ - $MnSiO_3$ are poorly known. The most reliable information is derived in many cases from surveys of mineralogical compositions and relations. Sundius (1931) surveyed pyroxenoid analyses for those minerals in the ternary system $Fe(Mg)SiO_3$ - $CaSiO_3$ - $MnSiO_3$. Wollastonite, bustamite and rhodonite were included in this survey. The compositions of the natural wollastonites are all very close to $CaSiO_3$, with no more than 8 mol. per cent $(Fe,Mg)SiO_3$ and less than about 3 mol. per cent $MnSiO_3$ in solid solution. Bustamite compositions range from 32 to 57 mol. per cent $CaSiO_3$ and rhodonite compositions 0 to 22 mol. per cent

$CaSiO_3$. There is thus no mineral representative in the range 22-32 mol. per cent $CaSiO_3$ between bustamite and wollastonite. This indicates that the formulas for these minerals should be written as follows:

wollastonite $CaSiO_3$

bustamite $Ca_{1+x}Mn_{1-x}(SiO_3)_2$, x=.07 to -.18

rhodonite $Mn_{4+x}Ca_{1-x}(SiO_3)_5$, x=0.0 to 1.0

One sample investigated by Sundius contained coexisting bustamite with 33 mol. per cent $CaSiO_3$ and rhodonite with 20 mol. per cent, strongly supporting other evidence for an immiscibility gap between rhodonite and bustamite. Because of the similarity in the optics and physical properties of bustamite and rhodonite, Sundius concluded that there is a complete series of solid solutions between them at low temperatures, despite the wide range in intermediate compositions not represented.

Schaller (1938) reported that he had examined samples of bustamite or wollastonite "with percentages of MnO ranging from a few per cent to a maximum of 33 per cent MnO, or 61 per cent of $MnO \cdot SiO_2$". He concluded from this, and a similarity of optical properties of the two minerals, that they "are a homogeneous solid solution of $CaO \cdot SiO_2$ (wollastonite) with $MnO \cdot SiO_2$".

Voos (1935) investigated the system $CaSiO_3$ - $MnSiO_3$ at temperatures above 1200°C. He recognized only two phases, pseudowollastonite and a material he called β-solid solution. The latter material has the wollastonite structure and is represented by a complete series of solid solutions between $CaSiO_3$ and $MnSiO_3$. Pseudowollastonite was found to be stable only at very high temperatures in the Ca-rich portion of the system. The results of Voos are seemingly at variance with those of Sundius, but on closer examination they are seen to be compatible. Voos used the powder x-ray photographic technique to identify phases. Buerger (1956) has shown that the diffraction patterns of bustamite and wollastonite are very similar, except in the case of weak super structure reflections. The powder technique would therefore not be adequate to show the minor differences in the diffraction patterns of these two minerals.

Liebau, Sprung and Thilo (1958) investigated phase relations in the system $CaMnSi_2O_6$ - $MnSiO_3$. As noted above they found, three $MnSiO_3$ polymorphs: γ-$MnSiO_3$ (rhodonite), β-$MnSiO_3$ (bustamite structure), α-$MnSiO_3$ (pseudowollastonite structure, metastable). They agreed with Sundius that rhodonite may contain only up to 20 mol. per cent $CaSiO_3$. They found, further, that the temperature

of the rhodonite - bustamite inversion decreases with rising Ca content. The occurrence of the bustamite structure at high temperatures throughout this system confirms the work of Voos.

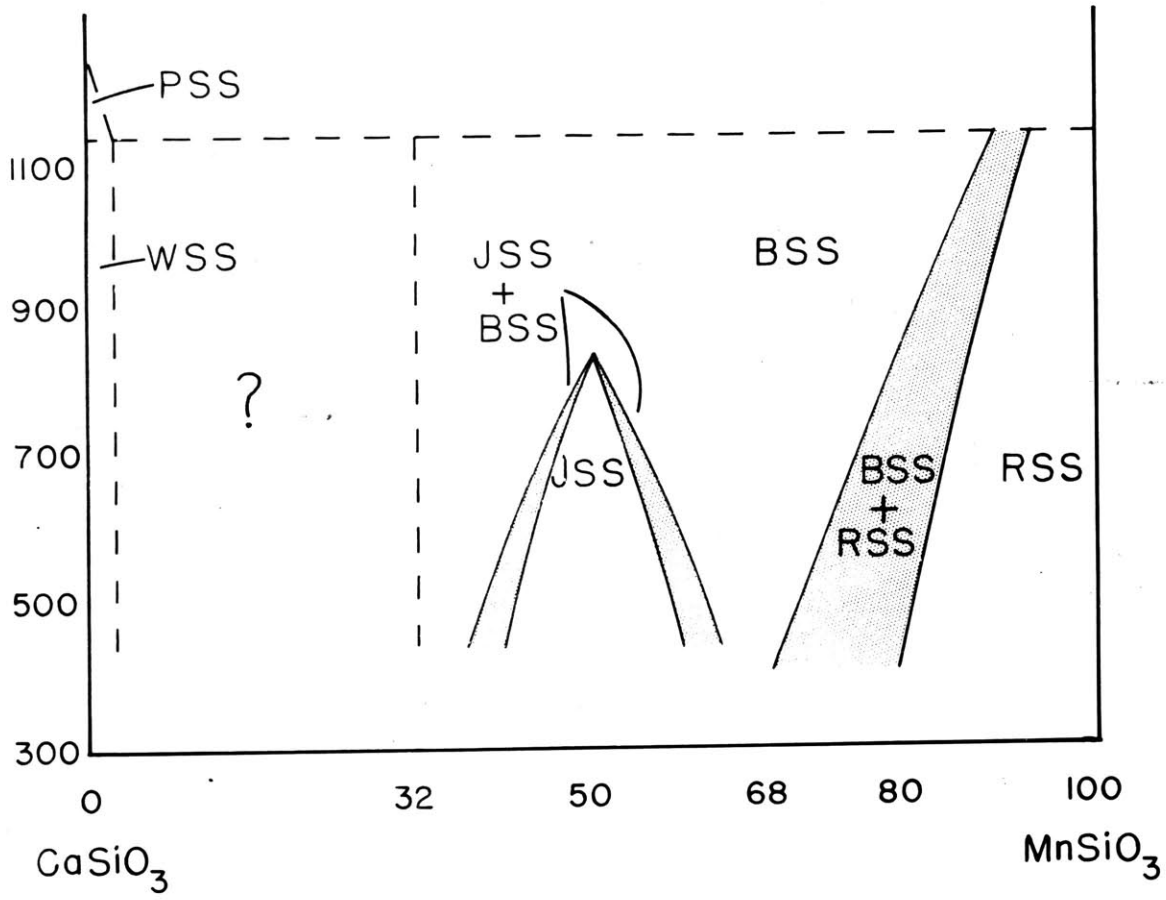
Glaser (1926) noted a single transition in $MnSiO_3$ and Jaeger and van Klooster (1916) noted two transitions at 1120° and 1208°C. This confirms the work of Liebau with respect to the rhodonite $-\beta$-$MnSiO_3$ transition. One of the three forms found by Jaeger and van Klooster may actually be the metastable α-$MnSiO_3$.

Glasser and Glasser (1960) and Glasser (1958) concluded that rhodonite is the only stable form of $MnSiO_3$ at all temperatures up to the melting point, in a study of synthetic phases in the system MnO-SiO_2. Glasser noted that $MnSiO_3$ synthesized at high temperatures and quenched exhibits diffuse x-ray reflections similar to those of heated natural rhodonite. He suggested that there may be some disorder at high temperatures and/or a rapid unquenchable inversion.

Fig. 11 is a diagrammatic representation of the probable subsolidus phase relations, taken in part from several of the above references. It is intended to show only relative features.

Figure 1.1

Phase relations in the subsolidus region of the system $CaSiO_3$-$MnSiO_3$ as a function of temperature and composition.



JSS = Johannsenite solid solution
BSS = Bustamite " "
WSS = Wollastonite " "
RSS = Rhodonite " "
PSS = Pseudowollastonite " "

X-ray crystallography. Wollastonite is triclinic, with space group $P\bar{1}$, and unit cell parameters (Buerger, 1956) as listed in table 1.1. Parawollastonite is monoclinic, with a unit cell (table 1.1) very closely related to that of wollastonite (Tolliday, 1958). Barnick (1935) proposed a structure for parawollastonite which contains three-membered rings of silica tetrahedra similar to those found in benitoite. Ito (1950) seeingly confirmed a similar structure for wollastonite. Buerger (1956) showed, however, that the structures of pectolite, bustamite and wollastonite are closely related, and that the structure of pectolite is based on a chain of silica tetrahedra with a repeat unit of three tetrahedra. Mamedov and Belov (1956) solved the structure of wollastonite and confirmed that it contains a chain of tetrahedra similar to that found in pectolite, $Ca_2NaH(SiO_3)_3$. Buerger and Prewitt (1961) subsequently refined the structure of wollastonite. Tolliday (1958) has shown that the structure of parawollastonite is based on a similar chain, and is closely related to the structure of wollastonite. A structure containing three-membered rings of silica tetrahedra has been proposed by Boll-Dornberger (1961) for pseudowollastonite. Lattice constants are shown

Table 1.1

Unit cells and space groups of Ca, Mn metasilicates

Mineral	Author	Space group	a (Å)	b (Å)	c (Å)	α	β	γ
Wollastonite	Buerger (1956)	$P\bar{1}$	7.94	7.32	7.07	90°02'	95°22'	103°26'
Parawollastonite	Tolliday (1958)	$P2_1$	15.42	7.32	7.07	-	95°24'	-
Pseudowollastonite	Jeffrey and Heller (1953)	$P1$ or $P\bar{1}$	6.82	6.82	19.65	90°24'	90°24'	119°18'
Bustamite	Bergman and Gonyer (1937)	$P1$ or $P\bar{1}$	7.64	7.16	6.87	92°08'	94°54'	101°35'
Bustamite	Buerger (1956)	$F\bar{1}$	15.46	7.18	13.84	89°34'	94°53'	102°47'
β-$Mn_{0.8}Ca_{0.2}Si_2O_6$	Liebau et al. (1958)	$F1$ or $F\bar{1}$	16.06	7.11	13.68	-	-	-
Johannsenite	Schiavinato (1953)	$C\frac{2}{c}$	9.81	9.02	5.26	-	105°	-
Rhodonite	Hilmer et al. (1956)	$P\bar{1}$	6.68	7.66	12.20	111.1°	86.0°	93.2°

in table 1.1. The relations between the structures of the polymorphs of $CaSiO_3$ have been discussed in detail by Prewitt (1962).

Berman and Gonyer (1937) investigated the unit cell of bustamite by means of rotating crystal photographs, and found it to be similar to that of wollastonite (table 1.1). Buerger (1956) found, however, that the a and c axes of bustamite are doubled relative to those of wollastonite (table 1.1). The unit cell, in an orientation similar to that of wollastonite, is face-centered. Buerger suggested that "Bustamite evidently bears a kind of superstructure relation to wollastonite, and it may be regarded as a double salt, $CaSiO_3 \cdot MnSiO_3$". Liebau et al. (1958) confirmed Buerger's unit cell determination with synthetic material with the composition $Ca_{0.2}Mn_{0.8}Si_2O_6$ (table 1.1). Liebau et al. also concluded that the structures of bustamite and wollastonite are different, but closely related. They proposed that the difference is based on a mutual ordering of chains and/or cations. Layarev and Tenisheva (1960), in a study of the infrared absorption spectra of the pyroxenoids, concluded that the structure of bustamite is based on chains of silica tetrahedra with a repeat unit of three tetrahedra, as in wollastonite. They concluded, however, that there are

"substantial differences between the crystal structures of wollastonite and bustamite".

Schiavinato (1953) determined the unit cell and space group of johannsenite (table 1.1) and found that they are equivalent to those of diopside, $CaMgSi_2O_6$. He concluded that johannsenite is isotypic with diopside.

Two schools have proposed different, but very similar, structures for rhodonite. Hilmer, Liebau, Thilo and Dornberger-Schiff (1956) and Liebau, Hilmer and Lindemann (1958) proposed a structure based on chains of silica tetrahedra with a repeat unit of five tetrahedra. This structure is very similar to those of other known pyroxenes and pyroxenoids. Oxygen atoms are arranged approximately in close packing. Planes of cations in octahedral coordination alternate with planes of Si atoms in tetrahedral coordination. Silica tetrahedra all share two vertices with other tetrahedra to form infinite chains. This structure may be incorrectly determined, or at best atom coordinates are only very approximately known, as can be seen in the following: 1. The discrepancy factor, R, was reported for only one of the two projections, (h01), for which data was available. The R-factor is extremely high, being 37% for the 58 strongest reflections, and 51% for all observed reflections. 2. No y coordinates are

reported for the oxygen atoms. 3. The structure was solved only with two projections. The final Fourier projections show the undulating contours expected of data with a high R-factor. Some oxygen coordinates appear to have been completely guessed. 4. The ordering of the Ca relative to Mn was guessed merely by analogy with the structure of $NaAsO_3$. Although the R-factor was higher with Ca in its assigned position, this position was still accepted as being correct.

Mamedov (1958) proposed a second structure for rhodonite. It may be described in the same general terms as the "Liebau-type". Only two projections were used for this structure also, despite the fact that the structure solution is one of at least moderate difficulty. The following points show that this structure is also subject to question. 1. Coordinates of Mn atoms were determined from two Patterson projections. Attempts to locate Si and O atoms with Harker-Kasper inequalities and Zachariasen statistical methods failed. 2. All Si and O coordinates were guessed on the basis of the predetermined Mn positions. 3. No refinement was attempted. 4. No. R-factor is given. Mamedov merely states that there is "good" agreement between observed and calculated structure factors.

Chapter 2

The Determination and Refinement of the Crystal Structure of Rhodonite

Introduction. Preparations were made to solve the crystal structure of rhodonite in the crystallographic laboratory several years ago. Specimens of rhodonite from Pajsberg, Sweden were kindly provided by Professor C. Frondel of Harvard University. Buerger determined that rhodonite is triclinic with the reduced unit cell whose dimensions are listed in table 2.1. Intensities were measured by Dr. N. Niizeki using a cleavage fragment mounted on the single-crystal, Geiger-counter diffractometer. The diffractometer settings Υ and φ were graphically determined. Intensities were obtained by integrating recorded peaks with a planimeter. All reflections were corrected for the Lorentz, and polarization factors. The corrected values of F^2 were then used to compute the three-dimensional Patterson function, P(xyz), in sections normal to c, and the Patterson projection P(x,y). These functions were computed using the Whirlwind computer in intervals of 1/50 along a and b, and 1/20 along c for the three-dimensional function.

All of the data described above, including all preliminary notes, were turned over to the author by M.J.Buerger.

Table 2.1

Lattice constants of rhodonite

Author	Specimen source	a (Å)	b (Å)	c (Å)	α	β	γ
Mamedov (1958)	Switzerland	7.77	12.20	6.70	85°15'	94°00'	111°29'
Hilmer et al. (1956)	Franklin, N.J.	6.68	7.66	12.20	111.1°	86.0°	93.2°
This thesis "Buerger cell"	Pajsberg, Sweden	7.682	11.818	6.707	92.355°	93.948°	105.665°
This thesis "Hilmer cell"	Pajsberg, Sweden	6.707	7.682	12.234	111.538°	85.247°	93.948°
Buerger personal communication	Pajsberg, Sweden	7.78	11.66	6.60	92°25'	93°50'	102°54'

Unit cell and space group. The unit cell obtained by Buerger (Table 2.1) was confirmed with a series of c-axis Weissenberg, photographs, except that minor changes were found in the magnitudes of the translations. This unit cell is the reduced cell, but is different from the cell obtained by Hilmer et al. (1956) and Mamedov (1958) (Table 2.1). The cells differ only in the choice of axis of length ~ 12 Å. Buerger chose this axis in order to obtain the reduced cell. The other axis was probably chosen because the two most prominent cleavages are parallel to it. Since it had been proposed that rhodonite contains chains of silica tetrahedra, and since cleavages usually parallel the tetrahedral "unit", this was a natural choice. The matrix of the transformation from the Hilmer cell to the Buerger cell is

$$\begin{matrix} 0 & -1 & 0 \\ 0 & 1 & 1 \\ -1 & 0 & 0 \end{matrix}$$

A specimen bounded by 100, 010, and 001 cleavages (relative to the Hilmer cell) was selected since it could be easily oriented with three principal axes as rotation axes with the optical goniometer. Back-reflection, 0-level precision-Weissenberg photographs were obtained with each of the three principal axes as rotation axes. Data obtained

from these films was used in conjunction with the IBM 709/7090 program LCLSQ3 (Burnham, unpublished) to obtain refined lattice parameters (Table 2.1). An IBM 709/7090 program (described in Appendix 2) was then used to obtain lattice parameters corresponding to the Buerger cell (Table 2.1).

Five analyses of Pajsberg rhodonite are tabulated by Doelter (1897). An average of these five analyses follows.

SiO_2	46.34%
MnO	43.97
FeO	1.61
CaO	7.03
MgO	1.00
Al_2O_3	0.11
Total	100.06%

This data was used to compute the unit cell contents in the following way. Since a precise value of the specific gravity was not available, the cell contents were normalized to 10.00 Si + Al atoms per unit cell. From this a specific gravity of 3.84 g/cc was calculated. This value was used to compute the unit cell formula, which follows.

$$\left|\begin{array}{ll} Mn & 8.01 \\ Ca & 1.62 \\ Mg & 0.32 \\ \underline{Fe} & \underline{0.29} \\ & 10.24 \end{array}\right| \quad \left|\begin{array}{ll} Si & 9.97 \\ \underline{Al} & \underline{0.03} \\ & 10.00 \end{array}\right| \quad O_{30.24}$$

In Chapter 1 it was noted that Sundius (1931) concluded that the formula of rhodonite should be written $Mn_{4+x}\ Ca_{1-x}\ Si_5O_{15}$; x = 0 - 1. Liebau et al. (1958) came to a similar conclusion in another review of rhodonite analyses.

It is interesting to compare the unit cell contents listed above with the results of Sundius and Liebau et al. Assuming that the space group is $P\bar{1}$ (and not P1) and that all cations occupy general positions, there are five cation positions of rank 2. The analysis is in good agreement with this, indicating that 8.01 Mn atoms may occupy four positions, and that Ca + Mg + Fe (2.23 per cell) occupy one position. The departure of the total cation content (10.24) from 10.00 is due to errors in chemical analyses or to an incorrect assumption in calculation of the specific gravity. This distribution assumes substitution of Mg and Fe for Ca. Since Mg and Fe ions are smaller than Mn ions, which are in turn smaller than Ca ions, this conclusion is questionable. The only conclusion that can be reached is that Ca may occupy only one position of the five positions which the large cations may occupy. The distribution of Mg and Fe cannot be ascertained.

Preliminary considerations. Liebau (1956) has shown that the unit cells of those metasilicates having structures

shown or proposed to be based on chains of silica tetrahedra are related. The chains have repeat units of two, three, five or seven tetrahedra (zwier-, drier-, funfer- and siebenketten). The translation parallel to the chains in pyroxenes (zwierketten) is about 5.2 Å and in bustamite (drierketten) 7.16 Å. Rhodonite has a translation of 12.23 Å and pyroxmangite a translation of 17.45 Å (Liebau, 1957). Thus, if a period of approximately 5 Å is assumed to be associated with two linked tetrahedra, as indicated by pyroxenes, rhodonite and pyroxmangite may be assumed to have five and seven tetrahedra respectively as repeat units. Structures supposedly confirming this have been proposed by Hilmer et al. (1956) and Liebau et al. (1958), and Mamedov (1958) for rhodonite and Liebau (1957, 1959) for pyroxmangite. There is a further relation among the unit-cell parameters of the metasilicates, however. All pyroxenes and pyroxenoids have two perfect cleavages parallel to the chains, as noted above. If two axes are chosen similarly with respect to these cleavages (other than the axes parallel to them) a close correspondence in their magnitudes is found. These relations are shown in Table 2.2, the two translations being chosen so that they are approximately normal to the cleavages. In those minerals whose structures are well known the cause of

Table 2.2

Comparison of unit cells of some pyroxenes and pyroxenoids

Mineral	Author	Translation approximately normal to chains		Translation along chain
Protoenstatite $MgSiO_3$	Smith (1959)	2 x 6.36 Å	2 x 6.36 Å	5.32 Å
Johannsenite $CaMnSi_2O_6$	Schiavinato (1953)	6.67	6.67	5.26
Bustamite $CaMnSi_2O_6$	This thesis	2 x 6.91	2 x 7.71	7.16
Pectolite $Ca_2NaH(SiO_3)_3$	Buerger (1956)	7.02	7.99	7.04
Rhodonite $(Mn,Ca)SiO_3$	This thesis	6.71	7.68	12.23
Pyroxmangite $(Fe,Mn,Ca,Mg)SiO_3$	Liebau (1957)	6.77	7.56	17.45

the similarity is easily seen. Each structure contains sheets of approximately close-packed oxygen atoms with Si atoms and octahedrally coordinated cations alternating in planes between them. The two axes described above intersect the close-packed sheets at angles of about 45°.

From the above discussion it can be inferred that the structure of rhodonite may be described as follows: 1. It contains sheets of approximately close-packed oxygen atoms. 2. Silica tetrahedra are arranged in a chain parallel to /$\bar{1}$10/. The chain has a repeat unit of five tetrahedra. 3. Mn atoms are arranged in sheets of edge-sharing octahedra.

Further evidence pointing to the above conclusions is found in a comparison of optical properties of rhodonite and bustamite. At the time of this investigation the structure of bustamite was not determined. As discussed in Chapter 1, Buerger (1956) and Liebau et al. (1958) had shown that it was closely related to that of wollastonite, and that it very probably was based on drier_ketten. Hey (1929) showed that the optical properties of rhodonite and bustamite are very similar. On the basis of optical properties of intermediate solid solution members, he incorrectly concluded that there is an isomorphous series between rhodonite and bustamite. This indicates that the structures may be very closely related.

The structures proposed by Hilmer et al. (1956) and Liebau et al. (1958) and Mamedov (1958) are both consistent with the above description. Since these are different, and both very poorly determined, it must be concluded that little more is definitely known about the structure of rhodonite than can be tentatively inferred from an elementary consideration of physical properties and unit cell relations.

Comparison of wollastonite and rhodonite. The discussion of the last section was based only on a comparison of the unit cell and physical properties of rhodonite with those of other pyroxenes and pyroxenoids. The conclusions reached can therefore be considered to be tentative at best. There are relations between the intensities of reflections of rhodonite and wollastonite which confirm these results, however.

Comparison of c-axis, o-level Weissenberg photographs of wollastonite and rhodonite shows that both have a substructure of approximately equal dimensions. This correspondence is of course also apparent in a comparison of the Patterson projections, P(x,y), of each. This sublattice, in projection at least, has the following translations relative to the rhodonite unit cell given above:

$$A^* = \frac{1}{5}\,a + \frac{2}{5}\,b$$

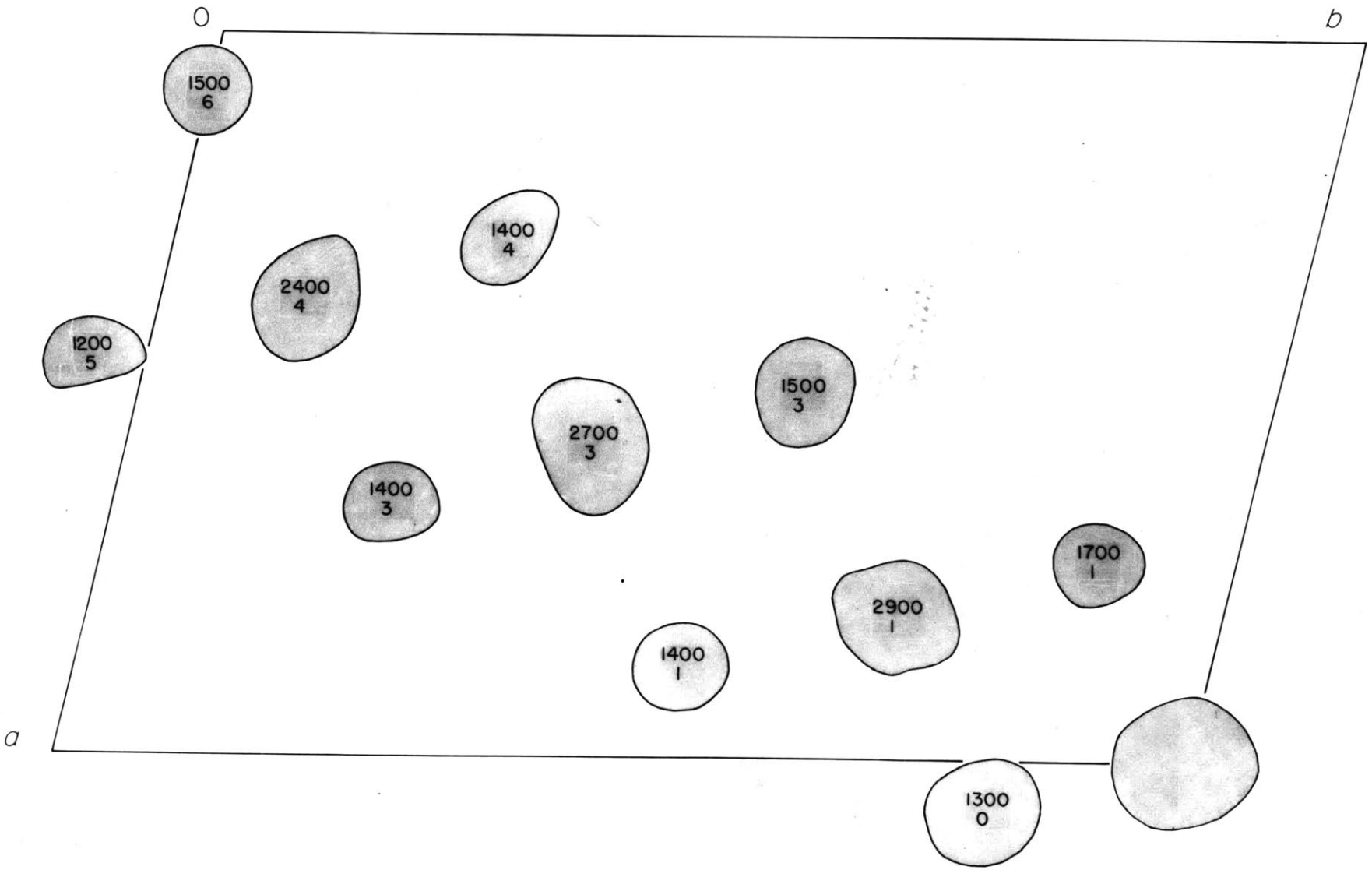
$$B^* = \frac{1}{5}\,a + \frac{3}{10}\,b$$

There are many substructure relations in wollastonite. The most important involves pairs of atoms related by the subperiod b/2. This is chiefly caused by chains of octahedra parallel to b sharing edges, the subperiod b/2 corresponding to an octahedron edge. The magnitude of b/2 in wollastonite is approximately equal to the magnitude of B in rhodonite. Thus there may also be a chain of edge-sharing octahedra in rhodonite, oriented parallel to B.

Interpretation of the Patterson function, P(xyz). Fig. 2.1 is a projection on (001) of some of the highest peaks of P(xyz). It is clear that this resembles a diagram of a chain of octahedra in which each octahedron shares an edge with each of two adjacent octahedra. For simplicity, peaks corresponding to the upper and lower vertices of each octahedra are not shown, although they are present. In each octahedron the relative peak heights correspond to weighting expected for an octahedron composed of oxygen atoms coordinating Mn; that is, the central peak is much higher than the four coordinating peaks. That these peaks correspond to a chain of Mn octahedra is further shown by distances between peaks, which correspond closely to values predicted from Mn and O radii. When all such peaks in the full cell are considered it is clear that the octahedra define a plane parallel to ($\bar{1}11$).

Figure 2.1

Selected peaks of P(xyz) projected onto (001). Each peak is labelled with its approximate height and the level, in 20ths, on which it appears.


0
b
a
1500
6
1400
4
2400
4
1200
5
1500
3
2700
3
1400
3
1700
1
2900
1
1400
1
1300
0

This is further evidence for the conclusions reached in the two preceeding sections.

The structures of other pyroxenes and pyroxenoids have a similar "octahedral sheet", as discussed above. In each of these the sheets are parallel to planes of inversion centers. The plane of central cations, in fact, coincides with the plane of inversion centers. If a brucite-like octahedral sheet is oriented similarly in rhodonite, such that chains of edge-sharing octahedra are oriented as in P(xyz), it is seen that the period between inversion centers is approximately the same as the period between centers in the "ideal" sheet. It was therefore assumed that such an arrangement exists in rhodonite.

Examination of a brucite-like sheet of edge-sharing octahedra shows that there are only two kinds of positions in the Mn plane where centers may be placed. These correspond to the center of a shared edge and to the center of an octahedron at a cation position. Examination of the structures proposed by Hilmer et al. and Liebau et al., and Mamedov shows that these structures differ principally in having each of these two arrangements respectively.

The Mamedov structure was thought most likely to be incorrect, since this required two Mn atoms to be on inversion centers. The structure is based on a chain of nine

edge-sharing octahedra with the central Mn atom on an inversion center at 000. The remaining Mn atom is on the center at $00\frac{1}{2}$. Peaks supposedly corresponding to Mn-Mn inversion peaks were easily located in the Patterson function. Peaks corresponding to nine of the ten Mn atoms in the unit cell were found in each minimum function formed. A suitable peak was not found at $00\frac{1}{2}$, or at any other center, which might correspond to the remaining Mn atom, however. This indicated that the structure was incorrect.

A second attempt was later made to verify this structure. Structure factors were calculated for all reflections, using only the Mn atoms in general positions and one Mn at 000 (after correcting two Mn coordinates for incorrectly published values) the R-factor was high (60%) but there was fair agreement between F_o and F_c for substructure reflections. An electron density function P(xyz) was then computed using only those reflections showing reasonable agreement between F_o and F_c and having large values of F. (The IBM 709/7090 program ERFR2 (Sly, Shoemaker and Van der Hende, 1962) was used to compute all Fourier syntheses in this investigation). Although peaks apparently corresponding to Si and O atoms were present, there was no peak representing the remaining Mn atom at $00\frac{1}{2}$, or on any other center. This was conclusive proof that the structure is incorrect.

The second possible arrangement of Mn octahedra was investigated in the following way. Inversion peaks corresponding to each of four Mn atoms were located in the Patterson function, P(xyz), and the minimum functions $M_2(xyz)$ contoured. Two of these were combined to form the function $M_4(xyz)$, the peaks of which are shown projected onto (001) in Fig. 2.2. Each peak is labelled with the level, in 20ths, on which it appeared. Fig. 2.3 is an interpretation of this figure, showing coordination polyhedra. The peak heights and positions of the remaining two minimum functions closely resemble those shown in Fig. 2.2. Six peaks labelled as Mn atoms are shown in Fig. 2.2. This nomenclature is used merely because six peaks appeared in the Mn chain, although there are only five Mn atoms in the structure. One of these is obviously a false peak, caused by superposition in P(xyz) of substructure vectors. Since the peak labelled Mn_6 was the smallest of the six in all minimum functions, this was considered to be a false peak.

From a consideration of interpeak distances and peak heights, peaks of $M_4(xyz)$ were correlated with all oxygen atoms with the exception of O_9, O_{13}, O_{14}, O_{15}. The resulting Mn coordination octahedra are shown in Fig. 2.3.

Figure 2.2

Peaks of $M_4(xyz)$ projected onto (00l). Each peak is labelled with the name of the atom which it represents and with the heights, in 20ths, on which it appears. Peaks corresponding to O_9, O_{13}, O_{14} and O_{15} are not present.

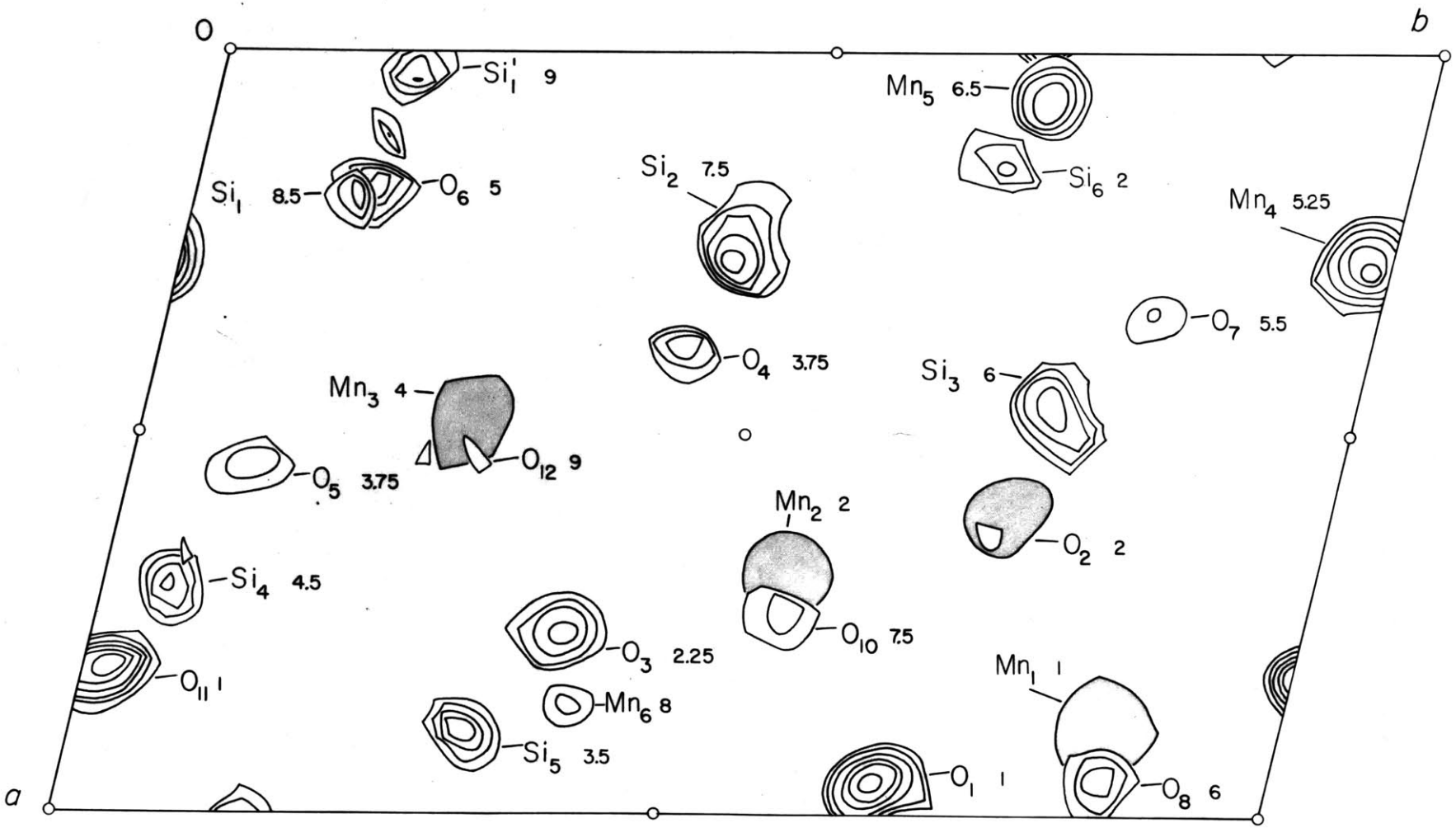
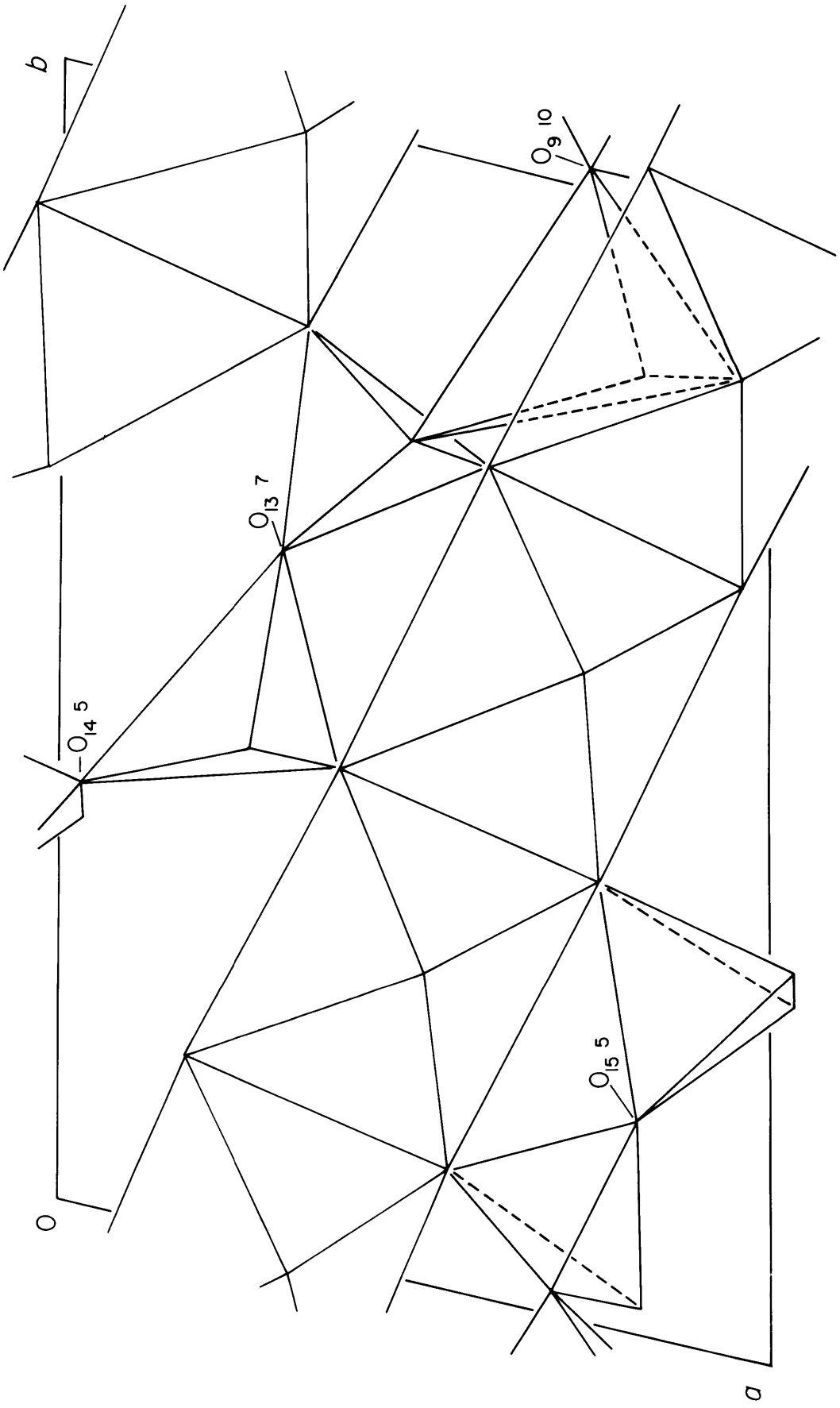

0
b
a
Si'1 9
Mn5 6.5
Si1 8.5
O6 5
Si2 7.5
Si6 2
Mn4 5.25
O7 5.5
O4 3.75
Mn3 4
Si3 6
O5 3.75
O12 9
Mn2 2
O2 2
Si4 4.5
O3 2.25
O10 7.5
Mn1 1
O11 1
Mn6 8
Si5 3.5
O1 1
O8 6

Figure 2.3

Coordination polyhedra (octahedra and tetrahedra) projected onto (001), obtained from an interpretation of Fig. 2.2. The positions of atoms O_9, O_{13}, O_{14} and O_{15} were predicted from an interpretation of the minimum function. They are labelled with the level, in 20ths, on which they occur.


b
O
a
O_{9}^{10}
O_{13}^{7}
O_{14}^{5}
O_{15}^{5}

Note that the coordination of Mn_5 is not completely octahedral. Peaks corresponding to Si_{2-5} were easily identified. The location of Si_1 was uncertain, however. There are two peaks, labelled Si_1 and Si_1^1, one of which corresponds to Si_1.

The positions of four oxygen atoms remained undetermined. Assuming that Si is tetrahedrally coordinated, and that these tetrahedra are linked in a chain, these positions (Fig. 2.3) were easily predicted. The validity of this proposed structure was checked by a consideration of Pauling bond strengths, all of which were reasonable. Coordinates are tabulated in Table 2.3. The peak labelled Si_1^1 was initially assigned to Si_1.

Refinement. The intensity data were first corrected for absorption in the following way. The crystal used in the measurement of intensities was a triangular prism approximately 0.1 mm long with triangular face edges of lengths 0.12, 0.13 and 0.10 mm. The mass absorption coefficient, μ, is 489 cm^{-1} and the average value of μr 2.5. All reflections were corrected for absorption using an IBM 709/7090 program written by C.W. Burnham (1962).

Structure factors calculated for hko reflections were in reasonable agreement with observed structure factors. Those reflections showing the best agreement were used in

Table 2.3

Atom coordinates obtained from the minimum function above, coordinates and isotropic temperature factors, and standard deviations after refinement below.

Atom	x	$\sigma(x)$	y	$\sigma(y)$	z**	$\sigma(Z)$	B	$\sigma(B)$
O_1	.970		.680		.950			
	.9544	.0011	.6772	.0007	.9628	.0014	.60	.19
O_2	.610		.720		.900			
	.6011	.0011	.7212	.0007	.8955	.0015	.49	.19
O_3	.761		.393		.887			
	.7485	.0011	.3895	.0007	.8858	.0015	.74	.20
O_4	.378		.434		.812			
	.3981	.0011	.4375	.0007	.8074	.0015	.65	.19
O_5	.545		.097		.812			
	.5485	.0011	.0975	.0007	.8053	.0015	.86	.20
O_6	.177		.150		.750			
	.1970	.0010	.1318	.0007	.7374	.0014	.36	.18
O_7	.340		.802		.725			
	.3218	.0011	.8149	.0007	.7438	.0015	.65	.19
O_8	.960		.852		.700			
	.9337	.0010	.8524	.0006	.6591	.0014	.33	.19

Table 2.3 cont.

O_9*	.320 .2560	.0010	.980 .9962	.0006	.500 .4459	.0013	.17	.17
O_{10}	.737 .7457	.0012	.572 .5871	.0008	.625 .5846	.0016	1.16	.21
O_{11}	.820 .8430	.0011	.026 .0414	.0007	.950 .9433	.0015	.53	.19
O_{12}	.550 .4181	.0010	.185 .2210	.0006	.550 .4846	.0014	.25	.18
O_{13}*	.320 .3191	.0010	.600 .6142	.0006	.650 .6300	.0014	.37	.18
O_{14}*	.020 .0546	.0011	.380 .4360	.0007	.750 .7006	.0014	.45	.18
O_{15}*	.810 .8607	.0010	.190 .2221	.0007	.750 .7024	.0014	.33	.18
Si_1	.200 .2191	.0004	.117 .1246	.0003	.500 .4956	.0006	.24	.07
Si_2	.248 .2667	.0004	.453 .4701	.0003	.625 .6375	.0006	.29	.07

Table 2.3 cont.

Si_3	.481 .4610	.0004	.757 .7393	.0002	.700 .7092	.0005	.12	.07
Si_4	.683 .7446	.0004	.044 .0891	.0003	.775 .7538	.0006	.32	.07
Si_5	.904 .9263	.0004	.355 .3466	.0002	.825 .8450	.0005	.19	.07
$Si_1{}^{1***}$	.020		.163		.575			
Mn_1	.897 .8819	.0002	.853 .8517	.0002	.950 .9697	.0003	.68	.05
Mn_2	.684 .6827	.0002	.563 .5548	.0002	.900 .8748	.0003	.75	.05
Mn_3	.478 .4916	.0002	.267 .2700	.0002	.800 .8109	.0003	.64	.05
Mn_4	.262 .3018	.0003	.980 .9767	.0002	.737 .7967	.0004	.65	.05
Mn_5	.073 .0457	.0003	.692 .6938	.0002	.675 .6389	.0004	.93	.06

Table 2.3 cont.

Mn_6***	.855	.405	.600

* Coordinates predicted from crystal chemical evidence following cycle 4.

** $z = 1-z'$ where z' was obtained from the minimum function.

*** False ambiguous peaks in the minimum function.

the computation of the Fourier syntheses $\rho(xy)$ and $\Delta\rho(xy)$. These indicated that the structure was essentially correct; i.e. that the five Mn atoms had been correctly placed with respect to the six observed substructure peaks in the minimum functions.

Two cycles of three-dimensional refinement were therefore carried out. (The IBM 709/7090 program SFLSQ2 (Prewitt, 1962) was used for all structure factor calculations and least-squares refinement in this investigation.) Form factors were used assuming half-ionization of all atoms. Complete disorder of Mn, Ca, Mg and Fe was assumed and the average cation scattering function corrected for the average real component of anomalous dispersion. All reflections having $(F_o-F_c)/F_o > 0.5$ were rejected in the refinement. A weighting scheme recommended by Hughes (1941) was used in a slightly revised version. This weighted reflections in the following way.

$$F_o \leq 4F_{min}, \quad \sigma = 4F_{min}$$

$$F_o > 4F_{min}, \quad \sigma = F_{min}$$

$$F_o = 0 \qquad\qquad \omega = 0$$

where $4F_{min} = 15.0$

$$\omega = (1/\sigma)^{\frac{1}{2}}$$

The scale factor was varied in cycle 1 and the scale factor and all coordinates in cycle 2. Table 3.4 is an outline of the least-squares refinement procedure.

The value of the discrepancy factor, R, was extremely high (76%). It was suspected that this was partially caused by wrongly guessed coordinates for the oxygen atoms O_9, O_{13}, O_{14} and O_{15}. Therefore two cycles (cycles 3 and 4) were executed with these atoms omitted. The value of R decreased to only 69% however. It was then noted that agreement between F_o and F_c was good for hko reflections but bad for all others. Comparison was good between $F_o(hkl)$ and $F_c(\bar{h}k\bar{l})$, however. This indicated that the axes a and b, or c, had somehow become reversed in the calculation of P(xyz). Therefore refinement was continued with all z coordinates replaced by 1-z.

Structure factors were computed for all reflections with $F_o \neq 0$, for which R was only 51%. Approximately 500 reflections having good agreement between F_o and F_c were used to compute the Fourier synthesis $\rho(xyz)$. The atoms O_9, O_{13}, O_{14} and O_{15} were not included in this computation. The electron density function indicated that most atom positions were correct although no peaks corresponding to the atoms O_9, O_{13}, O_{14} and O_{15}, could be identified. Since

Table 2.4

Outline of least-squares refinement

Cycle number	Number of reflections	R	Parameters varied	Weighting scheme	Rejection test	Comments
1	2016	77%	Scale factor, K	Hughes	$\frac{(F_o-F_c)}{F_o} > .5$	Sign of all indices incorrect in cycles 1-4
2	"	76	K, all coord.	"	"	
3	"	73	"	"	"	
4	"	69	"	"	"	
5	"	62	"	"	"	
6	"	49	"	"	"	
7	920	55	Si and Mn coord.	"	"	K constant increased to .67
8	"	59	"	"	"	" Mn_6 replaced Mn_5

Table 2.4 cont.

9	920	54	Si and Mn coord.	Hughes	$\frac{(F_o-F_c)}{F_o} > .5$	Mn_5 replaced Mn_6
10	"	49	K and O coord.	"	"	K decreased to .63
11	"	44	All isotropic	"	"	
12	"	56	K and Si are Mn coord.	"	"	All coord. changed $\pm .02$
13	"	44	"	"	"	Coord. returned to cycle 11 values
14	"	44	"	"	"	
15	1620	47	All coord. and K	"	$\left\|\frac{F_o-F_c}{F_o}\right\| > .6$	Rejection test corrected
16	"	46	"	$\sigma = 1.0$	none rejected	Change reject and weight
17	920	42	Si and Mn coord. and K.	"	"	

Table 2.4 cont.

18	1620	44	K and all coord.	σ=1.0	none rejected	
19	"	42	"	"	"	
20	"	42	"	Hughes	"	O_{11} position corrected
21	"	43	"	"	"	O_{12} position corrected
22	920	41	Si and Mn coord. and K	"	$\left\lvert \frac{F_o - F_c}{F_o} \right\rvert > .6$	$\Delta\rho$ (xyz) indicated change in z of Mn_{4-5}
23	"	35	"	"	"	
24	1620	35	K and all coord.	"	"	
25	920	27.9	K and O coord.	"	"	
26	"	25.2	K, and Si and Mn coord.	"	"	
27	"	23.1	"	"	"	

Table 2.4 cont.

28	920	20.9	K and O coord.	Hughes	$\frac{\lvert F_o - F_c \rvert}{F_o} > .6$	
29	"	18.8	K and Si and Mn coord.	"	"	
30	"	16.4	K, and O coord.	"	"	
31	"	15.2	K, and Si and Mn coord.	"	"	
32	"	14.4	K and O coord.	"	"	
33	"	12.3	5 O and Si coord, and K	"	"	Cations ordered
34	"	12.1	K, and Si and Mn coord.	"	"	
35	"	11.9	K and O coord.	"	"	
36	"	11.7	Isotropic temp. factors.	"	"	
37	"	10.8	"	"	"	

Table 2.4 coord.

38	1620	11.0	All coordinates and K	Hughes	$\frac{\lvert F_o - F_c \rvert}{F_o} > .6$	
39	"	10.5	"	"	"	All coordinate variations $< .0006$
40	920	11.0	Isotropic temp. factors	"	"	

most of the reflections used in the calculation of $\rho(xyz)$ were substructure reflections, and since these oxygen atoms are in the complement structure, this was not unexpected. In addition, peaks of $\rho(xyz)$ indicated that Si was located at the peak labelled Si_1 in Fig. 2.2, not at Si_1^1 as previously concluded.

Cycles 5 and 6 were executed with coordinates derived from the minimum function. Coordinates of Si_1 were substituted for those of Si_1^1 and new coordinates for O_9, O_{13}, O_{14}, and O_{15} (Table 3.1) were obtained from a reinterpretation of the minimum function. The value of R decreased only to 49%. The scale factor, K, attained a value of .5. The value of K should adjust such that $\sum F_o = \sum F_c$. The magnitude of K calculated by equating these terms was 0.67, which is considerably larger than the value obtained from least-squares refinement. The scale factor was therefore set at 0.67 and not varied in cycles 7-9.

The program SFLSQ2 required more than five minutes running time on the IBM 7090 computer at the M.I.T. Computation Center when all reflections were used and all coordinates varied. Such problems are assigned low priority and may require as much as one week for execution. Problems requiring

less than five minutes computation time are quickly expedited however. The number of reflections was therefore reduced to about 920 for some cycles, to reduce computation time to less than five minutes. Cycles in which the limited number of reflections were used are designated with subscript n. For these cycles only Mn and Si coordinates or all oxygen coordinates were varied in order to maintain an acceptable ratio of the number of reflections to the number of variables.

Cycle 7_n was executed varying only Si and Mn coordinates. The value of R increased to 55%, probably because of the increase in K noted above. Since the decrease in R predicted for this cycle was negligible, the Bunn synthesis $\Delta\rho(xyz)$ was computed using all reflections with $F_o = 0$. This function showed considerable variation, but little significance could be attributed to it. A peak at the Mn substructure position labelled Mn_6 in Fig. 2.2 indicated that it may be occupied by Mn. Since peaks in the minimum functions corresponding to Mn_5 were the smallest of the remaining five, it was assumed that this position was vacant. The value of R for cycle 8_n increased to 59%, however, indicating that this Mn distribution was incorrect. Since no other reasonable distribution of Mn atoms could be formulated through interpretation of the Bunn error synthesis or the minimum functions, the original Mn distribution was assumed to be correct.

Only Si and Mn coordinates were varied in cycle 9_n, the scale factor being held constant at 0.67. The values of $\sum' F_o$ and $\sum' F_c$ from this cycle indicated that K should be decreased to 0.63. The least-squares value of K had formerly been thought to be too low. There was then a possibility that refinement had been hindered by using an incorrect value of K, and holding it constant. In cycle 10_n it was allowed to vary, as were all oxygen coordinates. The discrepancy factor, R, decreased to 49%.

Refinement was not progressing satisfactorily. The following tests were therefore made of the validity of the structure. If an atom is in an incorrect position, the value of its temperature factor may refine to an unusually large value. All isotropic temperature factors were therefore varied in cycle 11_n. Although temperature factors varied in an unpredictable way, some attaining negative values, none refined to exceptionally large values. Cycle 12_n was executed with all coordinates altered by $\pm$.02 from their refined values of cycle 10. Only Si and Mn coordinates were varied. If coordinates were refining into substructure positions such shifts might alter this trend. All coordinates shifted toward their original values, however, so the results were inconclusive.

All evidence indicated that the proposed structure was correct. Refinement was therefore continued. Cycles 13_n (R=44%) and 14_n (R=44%) were executed with only the scale factor, K, and Si and Mn coordinates varying. Examination of these results showed that the rejection scheme was not operating correctly. Only those reflections with $(F_o-F_c)/F_o \geq 0.5$ were being rejected while those with $|F_o-F_c|/F_o \geq 0.5$ should be rejected. The rejection test was therefore corrected, and the critical rejection value changed to 0.6 so that more reflections might be included in the refinement. All coordinates were varied in cycle 15. The R-factor increased slightly to 47%. Refinement may not converge properly if inappropriate weighting or rejection schemes are used. Therefore, in subsequent cycles the weighting, and the rejection routine changed so that all reflections were included in the refinement except those with $F_o = 0$. (Only a very few of these reflections were being included as input to each cycle in order to decrease computation time.) Si and Mn coordinates and the scale factor were varied in cycles 16_n and 17_n, in which R decreased to 42%. In two more cycles in which all coordinates were varied R was 44% and 42%. The slight increase in R from cycle 17_n to cycle 18 is caused by the inclusion of about 700 more reflections in cycle 18. These were chiefly

reflections of high $\sin\Theta$, for which discrepancies between F_o and F_c are usually greater than for reflections with low $\sin\Theta$.

Since the refinement still was converging very slowly, an attempt was made to ascertain if there was a basic error in the structure. All evidence indicated that the atoms Mn_{1-4} were correctly located. There was some evidence (see above) that Mn_5 might be in an incorrect position. The relatively heavy Mn atoms control many phases. Structure factors were therefore computed using only Mn_{1-4}. Those structure factors of medium or large magnitude having good agreement between F_o and F_c were used to compute the Fourier synthesis $\rho(xyz)$. This contained the same ambiguities as the minimum function however. This was probably caused by the use only of reflections of at least moderate intensity. These are chiefly substructure intensities and reproduce only the substructure in $\rho(xyz)$. Reflections with small magnitudes very probably have incorrect signs, if R is large as in this case, and should not be used in Fourier calculations. This problem is, of course, inherent in substructure problems.

Examination of the atom coordinates showed that O_{11} was not correctly located. In cycle 20, therefore, it

was shifted to a position consistent with the minimum function. In addition, the use of the Hughes weighting routine was reintroduced. This scheme gives a higher weight to small F's and a lower weight to large F's. This is particularly valuable in a substructure problem since it may prevent refinement into a substructure. Following cycle 20 reexamination of the set of coordinates showed that O_{12} had refined into a position inconsistent with accepted values of interatomic distances and coordination. This was corrected in cycle 21, in which all coordinates and the scale factor were varied.

Structure factors for all F_{hkl} with $F_o = 0$ were calculated using the refined coordinates of cycle 21. These were used to compute the Bunn error synthesis $\Delta\rho(xyz)$. This indicated that the x coordinates of Mn_4 and Mn_5 should be changed by .03 and -.07 respectively. This was confirmed with a difference Fourier synthesis, $\Delta\rho(xyz)$, calculated using all reflections except those with $F_o = 0$.

The discrepancy factor, R, decreased to 35% after cycles 22_n and 23_n, in which only K, and Si and Mn coordinates were varied. After cycle 24, in which all coordinates were varied, R was still 35%. This was expected, however, since the number of reflections was much larger in cycle 24 (see above).

The refinement converged rapidly with further cycling, in which oxygen coordinates, and Si and Mn coordinates were varied in alternating cycles (see table 2.4 for details). Convergence was almost complete after cycle 32, for which R was 14.4%, so an attempt was made to determine the ordering, if any, present among the Ca, Mn, Fe and Mg atoms. Form factors computed assuming complete disorder of these atom had been used throughout the refinement. Structure factors were computed for 1620 reflections for which F_o was non-zero, and these were used in the computation of the difference Fourier synthesis, $\Delta\rho(xyz)$. The only major features in this synthesis were peaks at the positions of Mn_1-Mn_5. The heights of these peaks are listed in table 2.5. The peak heights of Mn_1, Mn_2 and Mn_3 are all positive and approximately equal. Since Mn ions have more electrons than the average atom used in the refinement, this suggests that only Mn, and not Mg, Fe or Ca, occupies these positions. The negative peaks at Mn_4 and Mn_5 suggest that Mg and Ca occupy these positions, since they contain fewer electrons than the average atom. It is also very likely that Fe occupies the same positions as Mg since their ionic radii are very similar, and smaller than either Ca or Mn, and they are known to substitute commonly for each other.

Table 2.5

Peak heights at cation positions of $\Delta\rho(xyz)$ and Mn-O interatomic distances after cycle 32

Cation position	Average cation-oxygen distance	Peak height in $\Delta\rho(xyz)$	Interpretation of ordering
1	2.27 Å	175	Mn
2	2.18	145	Mn
3	2.24	193	Mn
4	2.32	-65	Fe + Mg + Mn
5	2.43	-418	Ca + Mn

Assuming that Mn occupies the positions Mn_1, Mn_2 and Mn_3, all Mg and Fe the position Mn_4, all Ca the position Mn_5, and the remaining Mn the positions Mn_4 and Mn_5, peak heights for $\Delta\rho(xyz)$ of -100 and -400 were predicted for Mn_4 and Mn_5 respectively. This is in good agreement with the peaks actually observed and thus indicates that this ordering scheme is correct.

Interatomic distances were then calculated between Mn_{1-5} and oxygen atoms. The average for each polyhedron is shown in table 2.5. Average distances for Mn_1, Mn_2 and Mn_3 are between 2.18 and 2.27 Å, in good agreement with known Mn-O distances. Average distances for Mn_4 and Mn_5 are greater than those for Mn_{1-3}, that of Mn_5 being the largest (2.43 Å). Since Ca is the largest cation of Ca, Mn, Fe and Mg, this indicates that most, if not all, of the Ca occupies the position Mn_5. The average distance for Mn_4 is large only because one of the six distances for which the average was computed is very large. Two Mn_4-O distances are among the smallest of all Mn-O distances. This indicates that Fe and Mg occupy this position. Thus the interatomic distances verify the conclusions on ordering reached on a basis of the peaks in $\Delta\rho(xyz)$. Mn occupies the positions Mn_1, Mn_2 and Mn_3, Mg and Fe the position Mn_4, Ca the position Mn_5, with the remaining Mn at Mn_4 and Mn_5.

Refinement was continued with form factors computed for Mn_{1-5} assuming the ordering determined above, and taking account of anomalous dispersion of Mn, Fe, and Ca. Oxygen, and Si and Mn coordinates were varied in cycles 33_n - 35_n. Since refinement of coordinates had almost completely converged at this point, isotropic temperature factors were refined in cycles 36_n and 37_n. Refinement was completed with cycles 38 and 39, in which all coordinates and the scale factor were varied, and cycle 40, in which all isotropic temperature factors were varied. The final parameter variations were all less than the standard deviations. Final coordinates and temperature factors, and their standard deviations , are listed in table 2.3 for comparison with values obtained from the minimum function. Final coordinates are also listed in table 2.6 where they are compared with coordinates obtained by Liebau et al (1958). The values obtained by Liebau et al. are reasonably close to the values of this investigation, except in the following instances: Mn_1, $\Delta x = .08$; Mn_3, $\Delta z = .08$; Mn_4, $\Delta z = .10$; O_3, $\Delta z = .26$; O_{14}, $\Delta y = .08$; O_{14}, $\Delta z = .10$; O_{15}, $\Delta z = .09$. The coordinates given by Liebau et al. have been transformed, of course, to a unit cell of the Buerger type. In order to

Table 2.6

Comparison of atom coordinates of Liebau et al. (1959) (below) and this refinement (above). Liebau coordinates transformed to the Buerger cell and values of z replaced by 1-z.

Atom	x	y	z
Mn 1	.8819	.8517	.9697
Kat. 3	.963	.889	.998
Mn 2	.6827	.5548	.8748
Kat. 1	.710	.567	.875
Mn 3	.4916	.2700	.8109
Kat. 2	.505	.309	.734
Mn 4	.3018	.9767	.7967
Kat. 4	.273	.998	.700
Mn 5	.0457	.6938	.6389
Kat. 5	.107	.691	.615
Si 1	.2191	.1246	.4956
Si 3	.145	.105	.533
Si 2	.2687	.4701	.6375
Si 1	.281	.462	.611
Si 3	.4610	.7393	.7092
Si 2	.541	.778	.743
Si 4	.7446	.0891	.7538
Si 4	.728	.059	.794
Si 5	.9263	.3466	.8450
Si 5	.943	.338	.864
O 1	.9544	.6772	.9628
O 15		.643	.971

Table 2.6 cont.

O 2	.6011	.7312	.8855
O 7		.734	.912
O 3	.7485	.3895	.8858
O 3		.398	.626
O 4	.3981	.4375	.8074
O 1		.453	.802
O 5	.5485	.0975	.8053
O 12		.129	.828
O 6	.1970	.1318	.7374
O 8		.141	.766
O 7	.3218	.8149	.7438
O 6		.874	.749
O 8	.9337	.8524	.6591
O 9		.882	.627
O 9	.2560	.9962	.4459
O 11		.998	.451
O 10	.7457	.5871	.5846
O 2		.576	.590
O 11	.8430	.0414	.9433
O 10		.000	.942
O 12	.5819	.7790	.5154
O 5		.739	.530
O 13	.3191	.6142	.6300
O 4		.641	.665
O 14	.0546	.4360	.7006
O 14		.364	.599
O 15	.8607	.2221	.7024
O 3		.209	.790

obtain satisfactory comparison it was necessary to change all z coordinates of Liebau et al. to 1-z.

Liebau has noted that all z coordinates of Mn and Si atoms as published (Liebau et al. 1958) should be changed to 1-z, and z of oxygen atoms to $\frac{1}{2}$-z. This transformation was accordingly applied before transforming coordinates to the Buerger cell. A satisfactory correlation of coordinates of Liebau et al. and this investigation could not be found, however. This indicates that the change recommended by Liebau must also involve a change in the choice of unit cell axes, since a reasonable correlation of coordinates was found, as noted above. Such a change in the unit cell would result in a change in the matrix of the transformation of coordinates.

The satisfactory correlation of coordinates may be obtained if all x coordinates of Liebau et al. are replaced by values of 1-x, retaining the unit cell. The change recommended by Liebau is obviously incorrect, however, although the structure determined by him is basically correct.

Structure factors were calculated following cycle 40, for which the discrepancy factor, R, was 10.5% for all reflections with $F_o \neq 0$, and 15.4% for all reflections. Structure factors are listed in Appendix 4.

Description of the Rhodonite Structure

Peaks of $\rho(xyz)$, computed with structure factors from cycle 37, are shown in Fig. 2.4 projected along c onto (001). Only those peaks from z = 0 - 0.5 are shown. Mn atoms are represented by shaded rather than contoured peaks. Fig. 2.5 is an interpretation of the corresponding projection $\rho(xy)$, and Fig. 2.6 is an interpretation of the projection $\rho(xz)$ (relative to the Hilmer unit cell). The unusual latter projection has been chosen since it is parallel to the chains of silica tetrahedra.

The structure, at least in major features, is similar to the structure proposed by Hilmer et al. (1956) and Liebau et al. (1958), as can be seen from the comparison of coordinates in table 2.6. Planes of approximately close-packed oxygen atoms are arranged parallel to $(1\bar{1}1)$. Planes of Mn, Ca, Mg and Fe ions in octahedral coordination alternate between planes of oxygen atoms with planes of Si ions in tetrahedral coordination. The silica tetrahedra each share two vertices with other tetrahedra to form a chain extending parallel to $[101]$. This chain has a repeat unit of five tetrahedra.

Figure 2.4

Peaks of $\rho(xyz)$, calculated after cycle 38 of refinement, projected onto (001). Only peaks of the asymmetric unit, from Z = 0 to $\frac{1}{2}$, are shown. Peaks are labelled with the level, in 100ths, on which they appear.

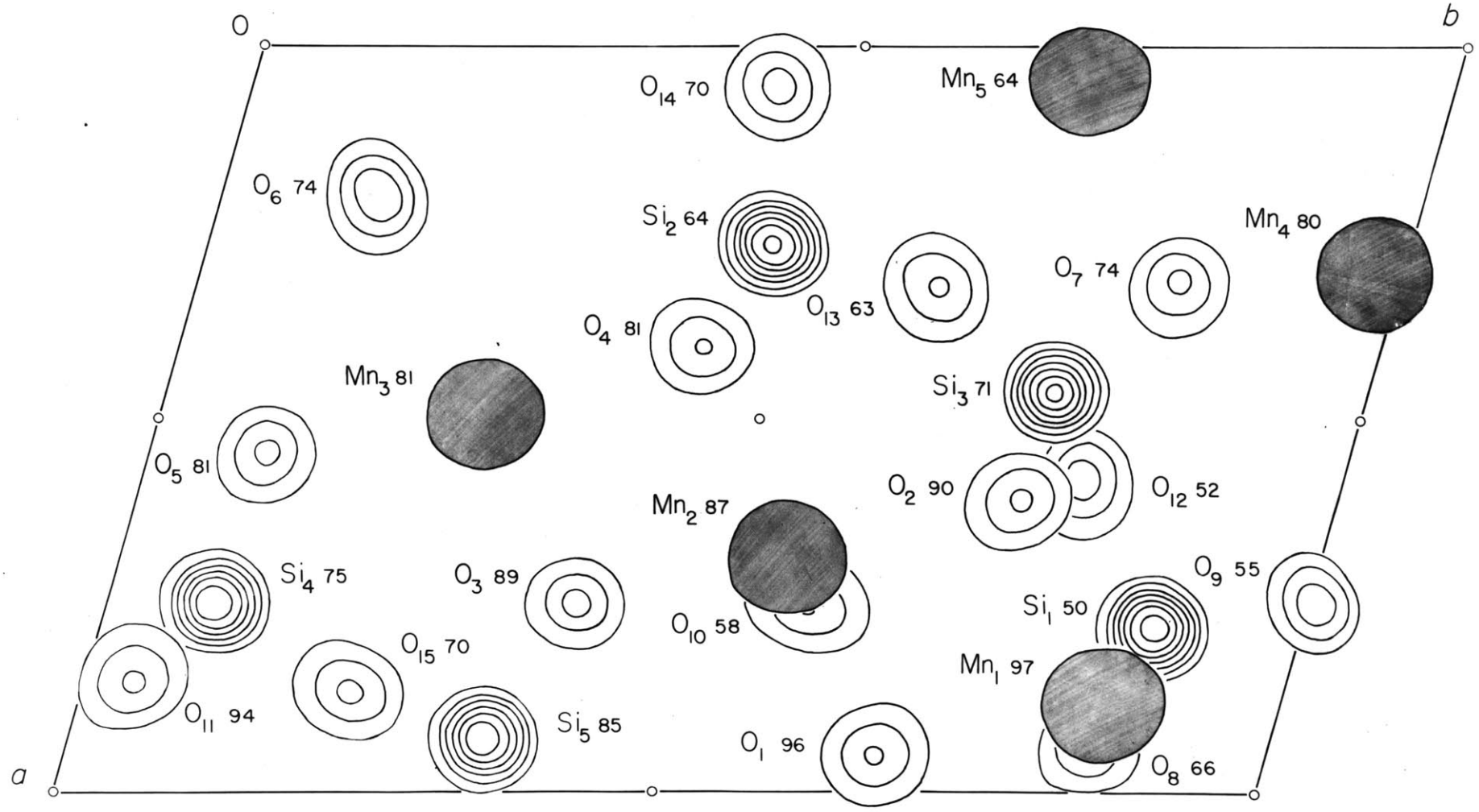

O
b
a
O14 70
Mn5 64
O6 74
Si2 64
Mn4 80
O13 63
O7 74
O4 81
Mn3 81
Si3 71
O5 81
O2 90
O12 52
Mn2 87
Si4 75
O3 89
O9 55
Si1 50
O10 58
O15 70
Mn1 97
O11 94
Si5 85
O1 96
O8 66

Figure 2.5

Projection on (001) of the structure of rhodonite. Mn and Ca atoms, and Si coordination tetrahedra are shown.

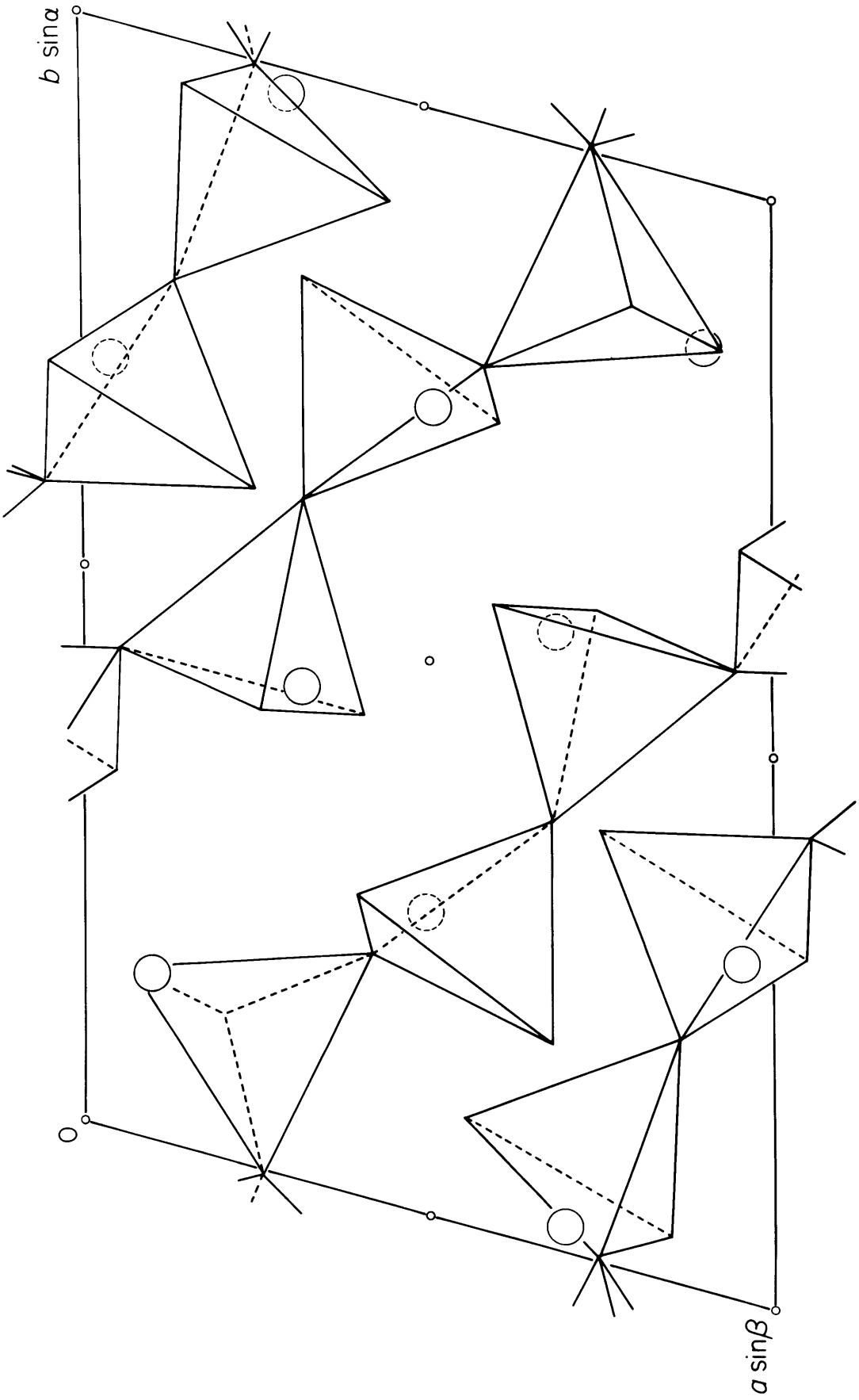
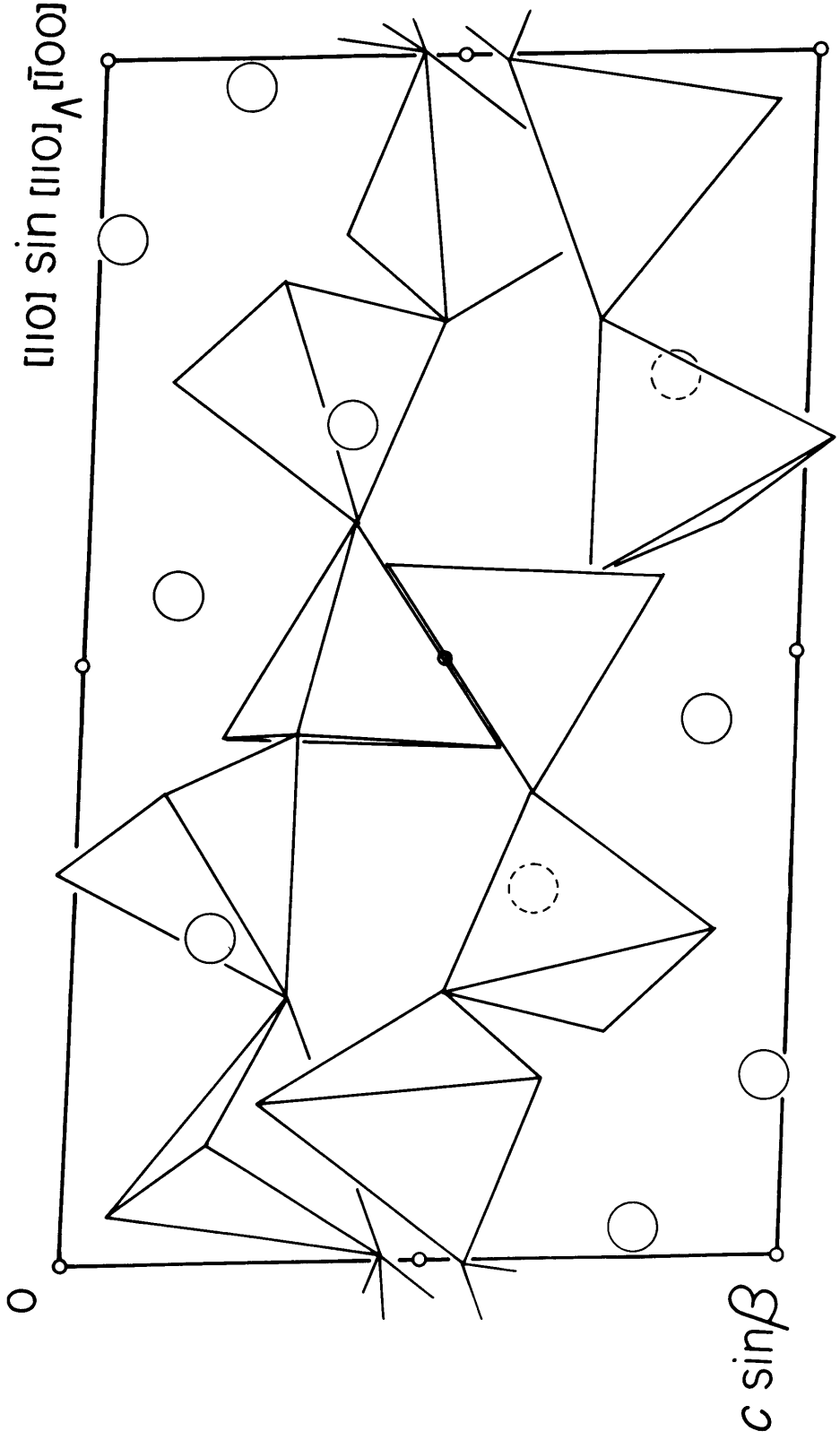

b sinα
a sinβ
O

Figure 2.6

Projection along a of the structure of rhodonite. Mn And Ca atoms, and Si coordination tetrahedra are shown.


[001] V [011] sin [011]
0
c sinβ

Sheet of octahedrally coordinated cations. Fig. 3.3, Chapter 3, is a projection of part of the structure of rhodonite onto the plane parallel to sheets of oxygen atoms described above. One octahedral layer is shown below, with sections of the silica chains in the overlying sheet. The coordination polyhedra of Mn_{1-5} approximate octahedra. These octahedra each share two edges with adjacent tetrahedra to form a chain ten octahedra long. The shared edge at the midpoint of this chain lies on an inversion center so that the two halves of the chain are centrosymmetrically related. These chains are bonded to similar chains through further edge sharing in a staggered manner to form a band of octahedra extending parallel to [101]. One complete band is shown in Fig. 3.3, with the outer edge of a translation related band on the left. Note that these bonds are separated by a rift of unoccupied octahedrally coordinated sites. These relations are treated in more detail in Chapter 3.

Coordination polyhedra and cation ordering. All silica tetrahedra are regular, as can be seen from the Si-O and O-O distances of tables 2.7 and 2.9 respectively. The average of all such O-O distances is 2.65 Å. Individual distances vary from this average by no more than 0.20 Å. All Si-O

Table 2.7

Cation-oxygen interatomic distances

Mn_1-O_1	2.27_6 Å	Mn_2-O_1	2.21_9 Å
O_2	2.24_9	O_2	2.33_5
O_6	2.11_2	O_3	2.14_9
O_8	2.14_8	O_4	2.25_3
O_{11}	2.35_3	O_4	2.26_6
O_{11}	2.17_5	O_{10}	2.06_5
Ave.	2.219	Ave.	2.215

Mn_3-O_2	2.13_9	Mn_4-O_5	2.03_7
O_3	2.10_7	O_6	2.23_1
O_4	2.28_2	O_7	1.97_8
O_5	2.19_6	O_8	2.87_8
O_6	2.41_1	O_9	2.38_6
O_{12}	2.33_3	O_{11}	2.12_0
Ave.	2.228	Ave.	2.272

Table 2.7 cont.

Mn_5-O_1	2.32_9	Ave. excluding O_9,	2.150
O_7	2.26_0		
O_8	2.26_7		
O_{10}	2.30_4	Si_1-O_6	1.64_4
O_{13}	2.52_6	O_8	1.59_9
O_{14}	2.63_5	O_9	1.64_1
O_{15}	2.60_5	O_{12}	1.65_0
Ave.	2.418	Ave.	1.634
Si_2-O_4	1.58_9	Si_3-O_2	1.61_6
O_{10}	1.59_3	O_7	1.59_0
O_{13}	1.64_6	O_{12}	1.66_0
O_{14}	1.67_3	O_{13}	1.62_4
Ave.	1.625	Ave.	1.62_3
Si_4-O_5	1.59_6	Si_5-O_1	1.60_8
O_9	1.64_0	O_3	1.61_6
O_{11}	1.63_3	O_{14}	1.63_8
O_{15}	1.64_9	O_{15}	1.65_6
Ave.	1.630	Ave.	1.628

Table 2.8

Oxygen-cation interatomic distances

O_1-Si_5	1.60_8 Å	O_2-Si_3	1.61_6 Å
Mn_1	2.27_6	Mn_1	2.24_9
Mn_2	2.21_9	Mn_2	2.33_5
Mn_5	2.32_9	Mn_3	2.13_9
O_3-Si_5	1.61_6	O_4-Si_2	1.58_9
Mn_2	2.14_9	Mn_2	2.25_3
Mn_3	2.10_7	Mn_2	2.26_6
		Mn_3	2.28_2
O_5-Si_4	1.59_6	O_6-Si_1	1.64_4
Mn_3	2.19_6	Mn_1	2.11_2
Mn_4	2.03_7	Mn_3	2.41_1
		Mn_4	2.23_1
O_7-Si_3	1.59_0	O_8-Si_1	1.59_9
Mn_4	1.97_8	Mn_1	2.14_8
Mn_5	2.26_0	Mn_4	2.87_8
		Mn_5	2.26_7

Table 2.8 cont.

O_9-Si_1	1.64_1	O_{10}-Si_2	1.59_3
Si_4	1.64_0	Mn_2	2.06_5
Mn_4	2.38_6	Mn_5	2.30_4
O_{11}-Si_4	1.63_3	O_{12}-Si_1	1.65_0
Mn_1	2.35_3	Si_3	1.66_0
Mn_1	2.17_5	Mn_3	2.23_3
Mn_4	2.12_0		
O_{13}-Si_2	1.64_6	O_{14}-Si_2	1.67_3
Si_3	1.62_4	Si_5	1.63_8
Mn_5	2.52_6	Mn_5	2.63_5
O_{15}-Si_4	1.64_9		
Si_5	1.65_6		
Mn_5	2.60_5		

Table 2.9

Oxygen-oxygen interatomic distances of silica tetrahedra (in Angstroms). Distances of shared edges are underlined.

Si_1		O_8	O_9	O_{12}
	O_6	2.81	<u>2.61</u>	<u>2.54</u>
	O_8		2.68	2.70
	O_9			2.61
Si_2		O_{10}	O_{13}	O_{14}
	O_4	2.75	2.64	2.68
	O_{10}		2.63	<u>2.58</u>
	O_{13}			2.59
Si_3		O_7	O_{12}	O_{13}
	O_2	2.75	2.64	2.72
	O_7		2.71	<u>2.45</u>
	O_{12}			2.59

Table 2.9 cont.

Si_4		O_9	O_{11}	O_{15}
	O_5	2.72	2.65	2.61
	O_9		2.65	2.62
	O_{11}			2.71

Si_5		O_3	O_{14}	O_{15}
	O_1	2.75	2.67	2.63
	O_3		2.67	2.65
	O_{14}			2.57

distances are also very close to values found in other silicate structures. The average of all Si-O distances (1.628 Å) is close to the value predicted by Smith and Bailey (in press) for metasilicates (1.623 Å) and to those in bustamite (1.623 Å) and wollastonite (1.626 Å, Prewitt, 1962).

The coordination polyhedra about Mn, Ca, Mg and Fe display some interesting features, however. First, note in table 2.7 that the Mn-O distances of Mn_1, Mn_2 and Mn_3 (Mn occupies these positions) are all close to the average values for these cations, with no large deviations. This is an indication that these polyhedra are reasonably regular octahedra.

Distances for Mn_4 (Mg and Fe occupy this position with Mn) are irregular however. Three of the six distances are short ($\sim$ 2.13 Å), indicating of course that Mg and Fe are distributed there. The Mn_4-O_8 distance (2.88 Å) is exceptionally long though. This indicates that the coordination of this cation actually approaches only five oxygen ions. The average Mn_4-O distances for these five oxygen ions is only 2.150 Å, at least 0.07 Å less than that for any of the Mn ions (Mn_{1-3}).

The coordination polyhedron of Mn_5 (Ca occupies this position with some Mn) lies at the ends of the chain of

ten edge-sharing octahedra. This coordination polyhedron is irregular, and consists of seven oxygen ions. The arrangement is unusual in that O_1, O_7, O_8 and O_{10} (which are each coordinated to one Si ion and one or two other Mn ions) form four vertices approximating one side of an octahedron. However, O_{13}, O_{14} and O_{15} (which are each also coordinated to two Si ions) form the other, irregular, side of the polyhedron. In Fig. 3.3 it can be seen that this polyhedron has vertices in two adjacent close-packed planes, of oxygen atoms, with four vertices in one plane and three in the other.

Interatomic distances. As noted above, the cation-oxygen interatomic distances (table 2.7) of the full refinement substantiate the ordering assumed at an earlier stage. The average cation-oxygen distances of Mn_1, Mn_2 and Mn_3 are very similar, lying between 2.215 and 2.228 Å. Since these distances are almost equal, and since they agree well with other published average Mn-O distances (e.g. 2.203 and 2.245 Å in bustamite) it is very probable that Mn occupies these positions.

Although the average distance (2.27 Å) for Mn_4-O is higher than those of Mn_{1-3}, indicating that Ca (r = 1.06 Å) rather than Mg (r = 0.78 Å) or Fe (r = 0.78 Å) is distributed there, one distance of the six is extremely large. The average

Mn_4-O

distance excluding this is 2.150 Å, in good agreement with the assumption that Mg and Fe occupy this position.

The average distance for Mn_5-O (2.42 Å) is greater than for Mn_{1-4}-O, indicating that Ca is distributed there. Note that the three distances involving O_{13}, O_{14}, O_{15} (each coordinated to two Si ions) are all much larger than distances involving O_1, O_7, O_8 and O_{10} (each coordinated to only one Si ion and one or two other Mn ions). The long Mn_5-O bond lengths and the unusual coordination of this cation clearly shows why Ca occupies this position, and explains why rhodonite may contain up to, but no more than 20 mol. per cent $CaSiO_3$.

The analyses of Pajsberg rhodonite used in this investigation was actually an average of five analyses in which FeO, for instance, varied from 0.36 to 3.31%. There is therefore no guarantee that the specimen used actually contained cations in the ratios of the average analysis. Despite this, the conclusions on cation ordering are still valid and within the accuracy permitted by the data. Although this ordering is certainly not as complete or ideal as assumed from the peaks of the difference synthesis or interatomic distances, it is accurate in principle.

Conformity of rhodonite to Pauling's rules. Several of the Pauling's valency bonds show deviations from ideal values. All oxygen-cation distances are listed in table 2.8. The oxygen ions are of three types: A. Those coordinated by two Si ions and one "Mn" ion. B. Those coordinated by one Si ion and three "Mn" ions. C. Those coordinated by one Si ion and two "Mn" ions. If all Mn ions are considered to be octahedrally coordinated each Mn-O bond has strength $\frac{1}{3}$, while each Si-O bond has strength 1. Thus all type A oxygen atoms have an excess bond strength of $\frac{1}{3}$, those of type B are neutral, and those of type C have a deficiency of $\frac{1}{3}$. This is compensated, in general, by a lengthening of cation-oxygen bonds of type A and a contraction of bonds of type C. For instance, the average Si-O distances for bonds of type A, B and C respectively are 1.648 Å, 1.615 Å and 1.599 Å. A similar situation exists with Mn-O bond lengths, for which the averages are 2.477, 2.280 and 2.137 Å respectively.

A feature of structures of pyroxenes and pyroxenoids is edge sharing between tetrahedra and octahedra. (Chapter 3). In rhodonite there are five such edges shared. In table 2.9 the distances along the tetrahedra edges are underlined. The cation polyhedra and the shared oxygen-oxygen edges are as follows:

Si_1 Mn_4 ; $O_6 - O_9$

Si_1 Mn_3 ; $O_6 - O_{12}$

Si_2 Mn_5 ; $O_{10} - O_{14}$

Si_3 Mn_5 ; $O_7 - O_{13}$

Si_5 Mn_5 ; $O_{14} - O_{15}$

This edge sharing results in a contraction of the length of the edge involved. The average length of all tetrahedra edges is 2.653 Å, while the longest shared edge is only 2.61 Å.

Temperature factors. The temperature factors in general (table 2.3) have values which are consistent with those of other silicate structures refined in the crystallographic laboratory. That is, those of Si are smallest ($\sim$0.2), the average of O are intermediate ($\sim$0.5) and those of the octahedrally coordinated cations largest ($\sim$0.7). Reliance cannot be placed on the absolute values of temperature factors, since they show a wide variation in structures refined in different laboratories with data gathered in different manners, but the relative values of this refinement seem to have some meaning. For instance the temperature factor of Mn_5(Ca) is 0.93. This is the largest of the Mn temperature factors, as expected from the unusual coordination of this cation.

The temperature factors of those four oxygen atoms with a deficiency of bond strength (O_3, O_5, O_7, and O_8; type C above) are the four largest oxygen temperature factors. Those for oxygen atoms with an excess of bond strength (O_9, O_{12}, O_{13}, O_{14} and O_{15}; type A above) are all smaller than the average, and include the smallest oxygen temperature factors. As noted above, bond distances may also be correlated with values of Pauling's valency bonds. Thus there is good correlation between deficiences in bond strength, small bond lengths and large temperature factors on one hand, and an excess of bond strength, large bond lengths and small temperature factors on the other.

Chapter 3

Crystal Chemical Relations Among Some Pyroxenes and Pyroxenoids

Mineralogists have long recognized the close relationship of the minerals of the pyroxene and pyroxenoid groups. Structure determinations have shown that these minerals all contain chains of silica tetrahedra. Liebau has recently systematized these relations (see Chapter 2) and shown that all pyroxenes contain zwierketten, and pyroxenoids drierketten (e.g. wollastonite), funferketten (e.g. rhodonite) or siebenketten (pyroxmangite). Several of these structures have now been refined in detail and it is possible to find further relations among them.

It was noted in Chapter 2 that a unit cell with two axes of related magnitudes, and a third of length proportional to the tetrahedral chain, may be chosen for pyroxenes and pyroxenoids. This is an expression of the structural similarity of these minerals. All are based on an approximately close-packed array of oxygen atoms. Planes of octahedrally coordinated cations alternate with planes of tetrahedrally coordinated Si ions, between sheets of oxygen atoms. The tetrahedra each share two vertices to form a chain.

Figs. 3.1, 3.2, and 3.3 are interpretations of the structures of clinoenstatite (zwierketten) (Morimoto et al., 1960) wollastonite (drierketten) (Buerger and Prewitt, 1961) and rhodonite (funferketten) respectively. Each is a projection onto the planes of oxygen atoms. Oxygen atoms are represented by vertices of polyhedra, all of which occur in only three planes parallel to the plane of the diagram. Tetrahedra are drawn with heavy lines, and two chains in one sheet are shown above the underlying sheet of octahedra. In each chain n + 1 tetrahedra are shown, where n is the number of tetrahedra in the repeat unit. In addition, the chains are not shown in the upper halves of the diagrams, in order to show the nature of the underlying sheet of octahedra more clearly. The magnitudes and directions of the unit translations are shown in the lower left of each figure.

The structures obviously differ in the number of tetrahedra in the repeat unit of the chain. In addition, the arrangement of cations in the octahedral layer is different in each, although there are basic similarities. Each octahedral sheet is defined by two layers of close-packed oxygen atoms. The cation occupancy of the octahedral sites is different in each. In the clinoenstatite structure,

Figure 3.1

Projection along a of the structure of clinoenstatite. Coordination polyhedra are shown for one octahedral layer (below) and for part of the tetrahedral layer (above, heavy lines). Unit translations are shown in the lower left corner of the diagram.

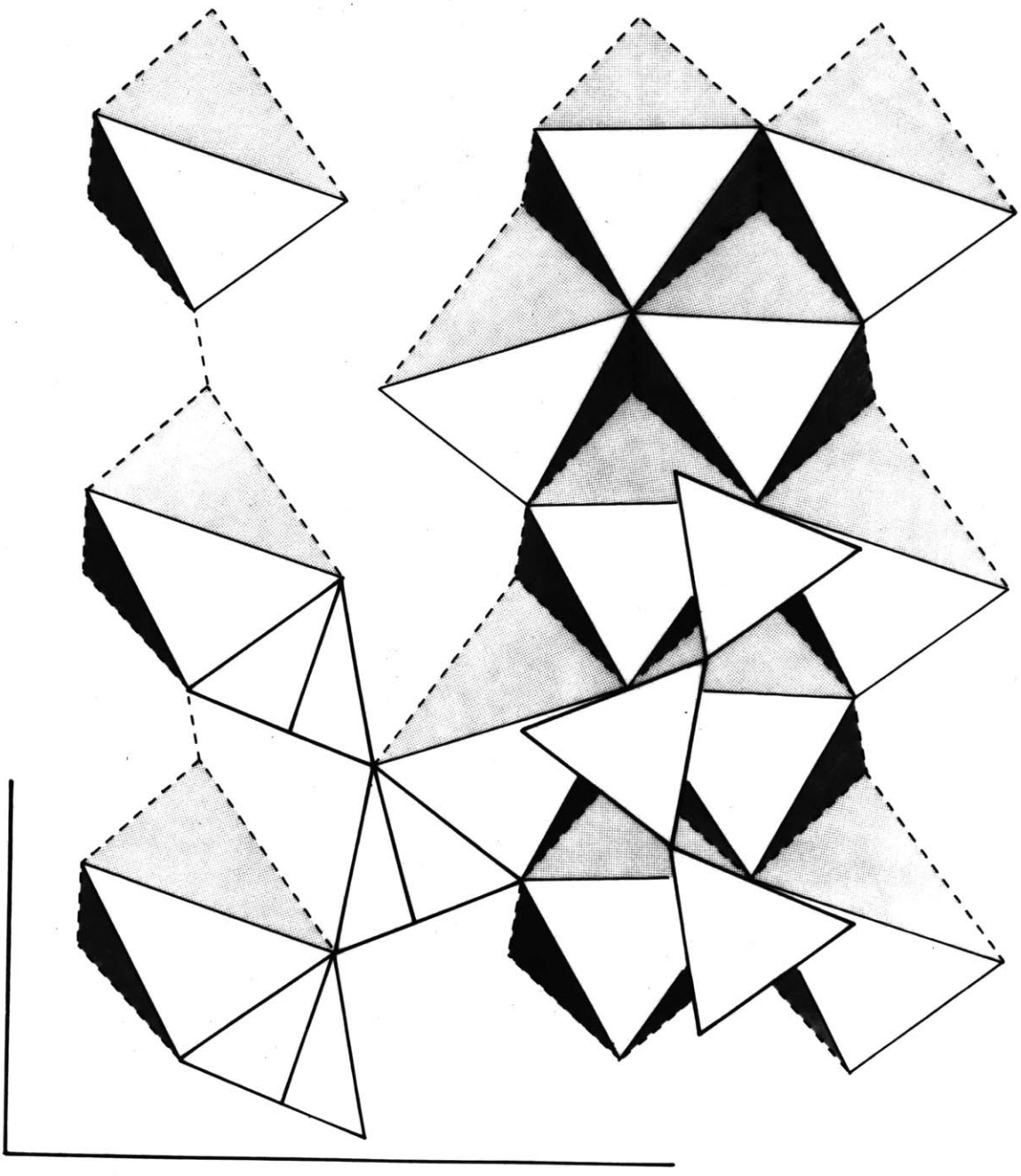


Figure 3.2

Projection along $[\bar{1}0\bar{1}]$ of the structure of wollastonite. Coordination polyhedra are shown for one octahedral layer (below) and for part of the tetrahedral layer (above, heavy lines). Unit translations are shown in the lower left corner of the diagram.

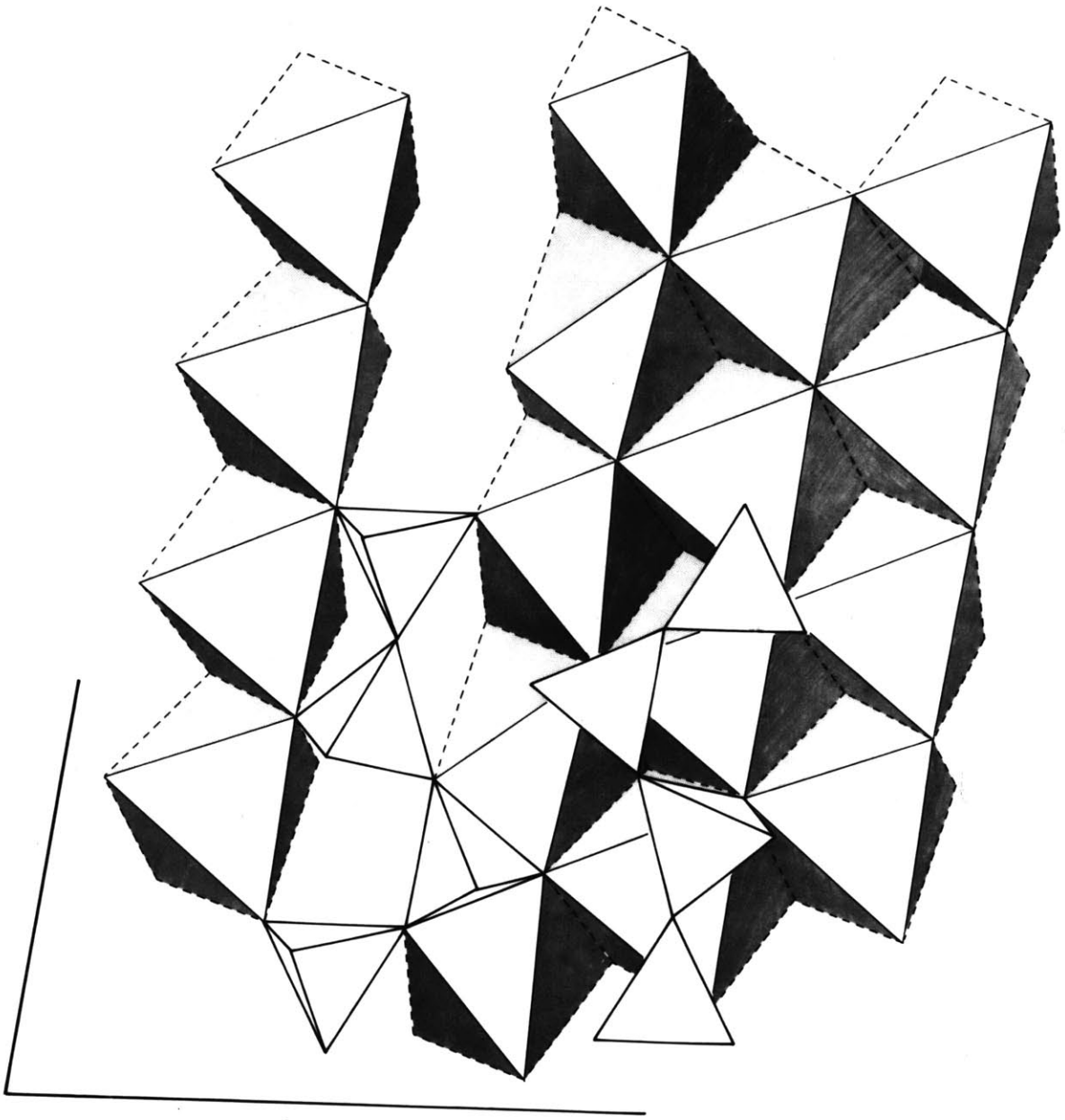
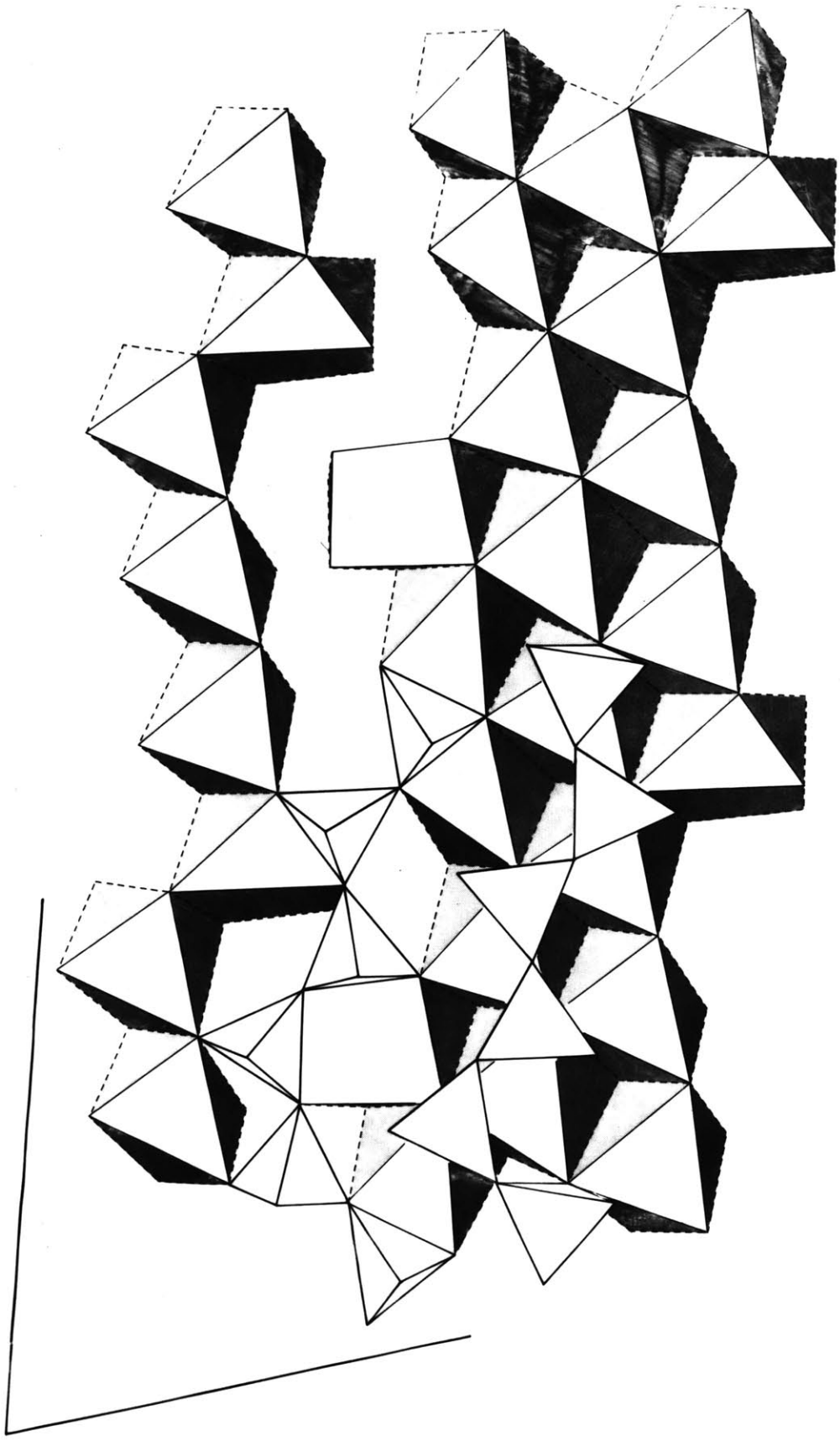


Figure 3.3

Projection along $[10\bar{1}]$ of the structure of rhodonite. Coordination polyhedra are shown for one octahedral layer (below) and for part of the tetrahedral layer (above, heavy lines). Unit translations are shown in the lower left corner of the diagram.



$\frac{1}{3}$ of the octahedrally coordinated sites are occupied, while in wollastonite and rhodonite, the fractions are $\frac{1}{4}$ and $\frac{2}{7}$ respectively. In clinoenstatite octahedra share edges to form a chain four octahedra long. Such chains are bound together through octahedral edge sharing in a staggered manner to form a band whose axis parallels the chain of tetrahedra. Similar bands of octahedra are found in wollastonite and rhodonite. In wollastonite they are formed of three infinitely long chains of edge sharing octahedra which are bound together through further edge sharing. The chains of octahedra in rhodonite are ten octahedra long and they are bound together in a staggered manner to form the band.

All three structures are similar, then, in having a band of edge-sharing octahedra arranged parallel to the chain of tetrahedra, and separated from other bands by a rift of unoccupied octahedrally coordinated sites. In each diagram a single band is shown separated on the left from a portion of another band by the rift. These structures differ, however, in the arrangement of filled and vacant octahedrally coordinated sites.

Two chains are shown in each of Figs. 3.1, 3.2, and 3.3. In each, the chain on the right has vertices pointing

down, bonded to the octahedral sheet. The chain on the left has vertices pointing up, with the triangular bases of the tetrahedra in the upper plane of oxygen atoms coordinating the cations. This chain lies above the rift in the octahedral sheet. There is, in fact, in all three structures, a second chain of tetrahedra arranged along the lower side of the rift. Tetrahedral chains are thus arranged "back-to-back" in each, separated by a column of vacant octahedral sites. The bands of octahedra are knit together by the chains of tetrahedra in this way.

As can be seen in the righthand chain of each figure, each chain fits over the octahedral sheet in a similar manner. That is, lower vertices of paired tetrahedra are bound to the octahedral sheet at either end of an octahedral edge. Thus, in each structure, the vertices of the tetrahedra follow, in zig-zag fasion, a continuous line of octahedral edges. Liebau (1956) proposed that the length of the repeat unit in the tetrahedral chain depends only on the size of the cations in the octahedral sheet. Thus clinoenstatite with a small cation (r_{Mg} = .78 Å) contains zwierketten and wollastonite with a large cation (r_{Ca} = 1.06 Å) contains drierketten. Rhodonite, with an average cation size less than that of wollastonite, contains

funferketten and pyroxmangite with still smaller cations (but still larger than the average of pyroxenes) contains siebenketten. It therefore appears that clinoenstatite and wollastonite represent two extreme cases. If the average cation size is intermediate, the chain tends to have a longer length the smaller the cation. Belov's observations (1960) support this. He noted that in Mg metasilicates paired tetrahedra can "fit over" the smaller octahedron edges. (Fig. 3.1) In wollastonite three tetrahedra (Fig. 3.2) may correspond to a single edge. Rhodonite and pyroxmangite have chains which are combinations of these cases.

The three structures pictured in Figs. 1-3 have other features in common. None have Pauling's valency bonds exactly satisfied. This is caused principally by another unusual feature, the sharing of edges between octahedra and tetrahedra, shown in the lefthand chain of each figure. In clinoenstatite each tetrahedron shares one edge with an octahedron. In wollastonite, the tetrahedron projecting out from the chain shares two edges. Five edges are shared in rhodonite. Note that the top tetrahedron of the chain on the left shares two edges with Mn octahedra. The three tetrahedra immediately be-

low each share one edge with the polyhedron at the end of the chain of octahedra. This coordination polyhedron is unusual, however, in being an irregular polyhedron of seven oxygen atoms.

In each example of edge-sharing above, one of the two oxygen atoms is coordinated to two Si atoms and one other cation. It thus receives bonds of total strength two from the Si atoms, and $\nu\frac{1}{3}$ from the other cation. This results in an excess of $\nu\frac{1}{3}$ in each case. This is usually compensated by Si-O interatomic distances which are larger than average. Each structure also contains other examples of deviations of bond strengths from ideal values. These relations show that Pauling's rules should never be applied too rigidly, for considerable deviation from ideal cases is to be expected.

Other pyroxenes and pyroxenoids. The relations described above are generally applicable to all minerals of these groups. Protoenstatite and enstatite-type structures merely represent different stacking of units approximately similar to that shown in Fig. 3.1 (Morimoto et al., 1960). The diopside structure is merely a distortion of the clinoenstatite structure (Morimoto et al. 1960). The distortion causes coordinating of the cations (Ca) on the edge of the band to change

from 6 to 8. The rift of vacant sites is much less well defined. This structure is unrefined, however, and detailed refinement may alter this interpretation.

Other pyroxenoids with drierketten include bustamite ($CaMnSi_2O_6$) and pectolite ($Ca_2NaHSi_3O_9$), schizolite ($(Ca,Mn)_2NaHSi_3O_9$) and serandite ($(Mn,Ca)_2NaHSi_3O_9$), the latter three forming an isomorphous series. Bustamite is very similar to wollastonite as pictured in Fig. 3.2, except that chains of tetrahedra are displaced in alternating layers. Pectolite, etc., (Buerger and Prewitt, 1961) differ principally in the arrangement of cations in the octahedral layer.

Babingtonite ($Ca_2Fe'''Fe''HSi_5O_{15}$) is probably the only other known pyroxenoid with funferketten. Richmond (1937) found that the unit cell of babingtonite is similar to that of rhodonite. Liebau (1956) proposed that babingtonite contains double-chains of tetrahedra since it contains (OH), as opposed to the single chains in rhodonite. Weissenberg c-axis photographs of each show an identical arrangement of reflections and a similarity in intensities. It is thus highly likely that babingtonite contains funferketten. The presence of hydrogen probably results in a different distribution of cations in the octahedral sheet

as is the case in the wollastonite - pectolite relation.

Classification of pyroxenes and pyroxenoids. It is obvious from the relations discussed above that the classification of these minerals into pyroxene and pyroxenoid groups is an artificial arrangement. Liebau has circumvented this with his classification of structures according to the repeat unit of the tetrahedral chain (zwier-, drier-, funfer-, and siebenketten). Such a classification is perfectly natural, as opposed to the old system which divided the minerals into groups with zwierketten and those with chains with a longer repeat unit. The terms used by Liebau have disadvantages, but are the best proposed until this time, and should be retained.

Phase transformations. Glasser and Glasser (1961) postulated a structural mechanism for the rhodonite-wollastonite transformation. They used crystals of Franklin, N.J. rhodonite, which upon heating transformed to "wollastonite". Using oscillating-crystal and optical goniometer studies of cleavage fragments before and after heating they noted that: 1. The external morphology of the crystals are preserved. 2. The two unit cell axes approximately normal to the silica chains (see Chapter 2) are retained. 3. There is about a 9° difference in the orientation of the axis parallel to the

chains. They concluded that this proves that Si-O bonds are broken and reformed while (Ca,Mn)-O bonds remain intact. They further show that the planes of octahedra in both wollastonite and rhodonite are very similar and that one transforms into the other through simple distortion.

Both structures involved in the transformation have now been well refined and it is possible to review these conclusions in detail. First, it is obvious from the literature on the system $CaSiO_3$ - $MnSiO_3$ of Chapter 1 that rhodonite transforms to bustamite, not wollastonite. Since b-axis photographs of both are very similar, and since the transformed crystals were imperfect, this error is easily explained. Since bustamite and wollastonite are very similar this should not alter their conclusions however. Glasser and Glasser, postulate two possible mechanisms for the transformation: 1. Reorientation of silica chains and reconstruction of the (Mn,Ca) layers. 2. Reconstruction of the chains with simple distortion of the (Mn,Ca) layers. They conclude that the latter mechanism is correct. The silica chains almost certainly undergo reconstruction, based on the evidence presented. However, it was noted above that the arrangement of filled

and vacant octahedrally coordinated sites is entirely different in these structures. A simple distortion is far from sufficient as a transformation mechanism. At least some of the (Mn,Ca)-O bonds must be broken and reformed, with migration of (Mn,Ca) ions. Glasser and Glasser present a detailed mechanism involving migration of only 7 of 15 Si ions and 4 O ions. It can only be concluded that although their conclusion on the reconstruction of the chains is probably correct, that the mechanism for the transformation is extremely complex and cannot be deduced from a simple comparison of the structure involved.

A similar situation exists in the johannsenite-bustamite transformation. Here, too, the axes approximately normal to the chains are probably retained while the chain orientation changes. The arrangement of cations in the octahedral sheet is also different in each, as noted above. This transformation, then, must also involve reconstruction of both the sheets of octahedra and the silica chains.

Appendix I

DCELL: IBM 709/7090 program for the transformation of unit cell parameters and coordinates

When direct and reciprocal cell parameters and atom coordinates are known for one unit cell setting but desired for another, hand calculation or graphical determination may be time consuming under the following conditions: 1. The unit cell is triclinic. 2. Transformations of coordinates are required for many symmetry related atoms. An IBM 709/7090 program has therefore been written in FORTRAN to perform these calculations.

Calculations are performed in the following way. Transformed unit cell vectors a' b' c' are derived where

$$\begin{pmatrix} a' \\ b' \\ c' \end{pmatrix} = (S) \begin{pmatrix} a \\ b \\ c \end{pmatrix}$$

and a, b, c are unit vectors of the original cell and (S) is the transformation matrix. The magnitudes of a',b',c' are computed from relations of the type

$$a' = (a' \cdot a')^{\frac{1}{2}}$$

and interaxial angles from relations of the type

$$\alpha' = \cos^{-1} \frac{b' \cdot c'}{b \times c}$$

Reciprocal transformed cell constants are then computed with relations of the type

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

$$a^{*1} = \frac{1}{a \sin \beta^{*} \sin \gamma}$$

The program then calls the subroutine SYMTRY which calculates the set of coordinates of all atoms in the original cell symmetry related to some atom I whose coordinates are supplied to the program. Transformed coordinates for this set of atoms are obtained with the relation

$$\begin{pmatrix} x' \\ y' \\ z' \end{pmatrix} = \tilde{S}^{-1} \begin{pmatrix} x \\ y \\ z \end{pmatrix}$$

where $\tilde{S}^{-1}$ is the reciprocal of the transform of the matrix (S). This calculation is repeated for each atom, I, supplied as input data.

Directions for operation of DCELL

The following data cards must be supplied:

1. Title card. Format (12 A6) Cols. 1-72; Any identification information may be included.

2. Cell card. Format (3(F7.4, 3X), 3(F7.3, 3X))

cols.	parameter
1-7	a Å
11-17	b "
21-27	c "
31-37	α degrees
41-47	β "
51-57	γ "

3. Transformation matrix card. Format (9(F7.4))

(S) is the matrix of the cell transformation

cols.	parameter
1-7	S_{11}
8-14	S_{12}
15-21	S_{13}
22-28	S_{21}
29-35	S_{22}
36-42	S_{23}
43-49	S_{31}
50-56	S_{32}
57-63	S_{33}

4. Coordinate cards. Format (3(F6.4, 4X), I1)

One card per atom

cols.	parameter
1-6	x
11-16	y
21-26	z
31	Blank in all except the final card; integer 1 in the final card

FORTRAN LISTING OF MAIN PROGRAM DCELL

```
      COMMON K
      DIMENSION TITLE(12),DX(3),DY(3),DZ(3),AXNU(3),ZI(3,3),X(200),Y(200
     1),Z(200)
      READ INPUT TAPE 4,9,(TITLE(I),I=1,12)
 9    FORMAT(12A6)
      WRITE OUTPUT TAPE 2,9,(TITLE(I),I=1,12)
      READ INPUT TAPE 4,10,A,B,C,ALPHA,BETA,GAMMA
 10   FORMAT(3(F7.4,3X),3(F7.3,3X))
      WRITE OUTPUT TAPE 2,10,A,B,C,ALPHA,BETA,GAMMA
 11   READ INPUT TAPE 4,  12,DX(1),DY(1),DZ(1),DX(2),DY(2),DZ(2),DX(3),D
     1Y(3),DZ(3)
 12   FORMAT(9(F7.4))
      WRITE OUTPUT TAPE 2,121
 121  FORMAT(24H0COORDINATES OF NEW AXES)
      WRITE OUTPUT TAPE 2,12,DX(1),DY(1),DZ(1),DX(2),DY(2),DZ(2),DX(3),D
     1Y(3),DZ(3)
      WRITE OUTPUT TAPE 2,122
 122  FORMAT(24HONEW CELL A B C AL BE GA)
      ASQ=A**2
      BSQ=B**2
      CSQ=C**2
      PI=.017453
      ALPHA=ALPHA*PI
      BETA=BETA*PI
      GAMMA=GAMMA*PI
      AB=A*B*COSF(GAMMA)
      AC=A*C*COSF(BETA)
      BC=B*C*COSF(ALPHA)
      DO 14 K=1,3
      AXNU(K)=SQRTF(DX(K)**2*ASQ+DY(K)**2*BSQ+DZ(K)**2*CSQ+2.0*DX(K)*DY(
     1K)*AB+2.0*DZ(K)*DX(K)*AC+2.0*DY(K)*DZ(K)*BC)
 14   CONTINUE
      DO 22 K=1,2
      DO 21 J=2,3
      IF(K-J)19,21,19
 19   ZI(K,J)=DX(K)*DX(J)*ASQ+DY(K)*DY(J)*BSQ+DZ(K)*DZ(J)*CSQ+(DX(K)*DY(
     1J)+DY(K)*DX(J))*AB+(DZ(K)*DX(J)+DX(K)*DZ(J))*AC+(DY(K)*DZ(J)+DZ(K)
     2*DY(J))*BC
      ZI(K,J)=ACOSF(ZI(K,J)/(AXNU(K)*AXNU(J)))
      ZI(K,J)=ZI(K,J)/PI
 21   CONTINUE
 22   CONTINUE
      WRITE OUTPUT TAPE 2,23,AXNU(1),AXNU(2),AXNU(3),ZI(2,3),ZI(1,3),ZI(
     11,2)
 23   FORMAT(4X,6(F7.3,2X))
C     ROUTINE TO TRANSFORM CELL AXES AND COORDINATES
      WRITE OUTPUT TAPE 2,25
 25   FORMAT(35HONEW RECIPROCAL CELL A B C AL BE GA)
      T23=DX(1)*DY(3)-DX(3)*DY(1)
```

```
      ZI(1,2)=ZI(1,2)*PI
      ZI(1,3)=ZI(1,3)*PI
      ZI(2,3)=ZI(2,3)*PI
      COSA =COSF(ZI(2,3))
      COSB=COSF(ZI(1,3))
      COSC=COSF(ZI(1,2))
      SINA=SINF(ZI(2,3))
      SINB=SINF(ZI(1,3))
      SINC=SINF(ZI(1,2))
      ALS=ACOSF((COSB*COSC-COSA)/SINB*SINC)
      BES=ACOSF((COSA*COSC-COSB)/SINA*SINC)
      GAS=ACOSF((COSA*COSB-COSC)/SINA*SINB)
      AS=1.0/(AXNU(1)*SINF(BES)*SINC)
      BS=1.0/(AXNU(2)*SINF(ALS)*SINC)
      CS=1.0/(AXNU(3)*SINF(ALS)*SINB)
      ALS=ALS/PI
      BES=BES/PI
      GAS=GAS/PI
      WRITE OUTPUT TAPE 2,26,AS,BS,CS,ALS,BES,GAS
26    FORMAT(4X,3(F8.5,2X),3(F7.3,3X))
      T11=DY(2)*DZ(3)-DY(3)*DZ(2)
      T12=DX(2)*DZ(3)-DX(3)*DZ(2)
      T13=DX(2)*DY(3)-DX(3)*DY(2)
      T21=DY(1)*DZ(3)-DY(3)*DZ(1)
      T22=DX(1)*DZ(3)-DX(3)*DZ(1)
      T31=DY(1)*DZ(2)-DY(2)*DZ(1)
      T32=DX(1)*DZ(2)-DX(2)*DZ(1)
      T33=DX(1)*DY(2)-DX(2)*DY(1)
      DELTA=DX(1)*DY(2)*DZ(3)+DY(1)*DZ(2)*DX(3)+DZ(1)*DX(2)*DY(3)-DX(3)*
     1DY(2)*DZ(1)-DY(3)*DZ(2)*DX(1)-DZ(3)*DX(2)*DY(1)
      WRITE OUTPUT TAPE 2,261
261   FORMAT(41HONEW COORDINATES FRACTIONAL AND ANGSTROMS)
27    READ INPUT TAPE 4,28,X(1),Y(1),Z(1),IEND
28    FORMAT(3(F6.4,4X),I1)
      CALL SYMTRY(X,Y,Z)
      WRITE OUTPUT TAPE 2,28,X(1),Y(1),Z(1),IEND
      DO 31 I=1,K
      XX=T11*X(I)-T12*Y(I)+T13*Z(I)
      YY=-T21*X(I)+T22*Y(I)-T23*Z(I)
      ZZ=T31*X(I)-T32*Y(I)+T33*Z(I)
      XX=XX/DELTA
      YY=YY/DELTA
      ZZ=ZZ/DELTA
      XXX=XX*AXNU(1)
      YYY=YY*AXNU(2)
      ZZZ=ZZ*AXNU(3)
      WRITE OUTPUT TAPE 2,30,XX,YY,ZZ,XXX,YYY,ZZZ
30    FORMAT(5X,3(F8.4,2X),10X,3(F8.3,2X))
31    CONTINUE
      IF(IEND)32,27,32
32    CALL EXIT
      END
```

FORTRAN LISTING OF SUBROUTINE SYMTRY
THIS EXAMPLE IS FOR SPACE GROUP P 1BAR

```
SUBROUTINE SYMTRY(X,Y,Z)
COMMON K
DIMENSION X(200),Y(200),Z(200)
K=2
X(2)=1.0-X(1)
Y(2)=1.0-Y(1)
Z(2)=1.0-Z(1)
RETURN
END
```

Appendix II

Comparison of observed and calculated structure factors of bustamite.

H	K	L	FOBS	FCAL	AOBS	BOBS
0	0	4	76.18	77.46	-76.09	-3.76
0	0	6	40.49	37.30	40.24	4.48
0	0	8	122.99	137.03	122.54	10.48
0	0	10	42.47	38.78	42.26	4.24
0	0	12	51.18	50.09	-51.06	-3.43
0	0	14	17.05	14.11	16.48	4.38
0	0	16	38.05	37.12	36.68	10.12
2	0	2	28.56	31.41	26.44	10.81
2	0	-4	97.99	106.45	97.80	6.09
2	0	4	92.35	111.63	92.19	5.44
2	0	-6	115.40	120.83	114.87	11.05
2	0	6	16.09	13.56	-15.58	-4.01
2	0	-8	37.13	35.21	-37.09	1.75
2	0	8	20.09	19.73	20.02	1.73
2	0	-10	14.10	14.47	13.76	-3.06
2	0	10	15.73	17.07	-12.09	10.06
2	0	-12	61.80	63.65	61.53	5.78
2	0	-12	61.80	63.65	61.53	5.78
2	0	12	33.88	32.68	33.33	6.10
2	0	-14	53.89	53.35	52.92	10.17
2	0	14	12.76	12.26	12.41	-2.98
2	0	-16	21.11	20.58	-21.06	1.52
2	0	16	7.58	7.23	-7.42	1.54
4	0	0	36.19	60.16	-36.16	-1.42
4	0	2	30.78	32.17	30.78	-0.45
4	0	-2	33.16	33.24	31.97	8.80
4	0	-4	67.25	68.41	66.44	10.40
4	0	4	56.37	59.10	55.46	10.08
4	0	-6	48.19	46.17	48.19	-0.47
4	0	6	8.03	9.33	-3.23	7.35
4	0	-8	41.81	37.69	-41.74	-2.42
4	0	8	12.00	9.32	-11.65	-2.86
4	0	-10	36.28	33.79	35.21	8.76
4	0	10	26.75	24.80	-26.75	-0.42
4	0	-12	58.71	58.36	57.93	9.55
4	0	12	75.96	74.61	75.35	9.61
4	0	-14	20.66	19.57	20.66	-0.34
4	0	14	12.19	10.57	8.69	8.55

4	0	-16	6.05	7.37	-5.87	-1.46
4	0	16	20.28	18.52	-20.18	-1.97
6	0	0	74.60	78.07	73.93	10.00
6	0	2	38.33	35.42	38.32	-0.68
6	0	-2	16.77	15.73	13.86	9.44
6	0	-4	58.81	56.42	-58.77	-2.27
6	0	4	72.33	76.06	-72.30	-2.07
6	0	-6	6.61	1.96	6.33	-1.90
6	0	6	39.66	36.75	38.56	9.27
6	0	-8	66.29	63.27	65.46	10.43
6	0	8	86.81	85.52	86.23	10.00
6	0	-10	42.49	38.86	41.54	8.93
6	0	10	0.	0.92	0.	-0.
6	0	-12	39.04	39.62	-39.00	-1.86
6	0	12	12.66	11.24	-12.48	-2.13
6	0	-14	3.63	2.74	-3.59	-0.56
6	0	14	16.99	15.26	14.83	8.30
6	0	-16	40.79	39.96	39.87	8.62
8	0	0	49.41	45.10	48.88	7.22
8	0	2	55.84	52.03	54.50	12.17
8	0	-2	17.58	16.52	17.23	-3.50
8	0	-4	22.45	19.64	22.38	1.73
8	0	4	0.	1.94	-0.	0.
8	0	-6	32.10	27.36	29.35	13.01
8	0	6	27.46	26.31	27.26	-3.32
8	0	-8	12.01	12.33	-10.34	6.10
8	0	8	57.78	55.01	57.41	6.54
8	0	-10	25.89	26.42	25.73	-2.91
8	0	10	40.42	38.73	38.95	10.82
8	0	-12	6.93	5.88	6.73	1.67
8	0	12	9.23	7.75	-9.10	1.57
8	0	-14	23.64	20.64	20.87	11.10
8	0	14	14.63	12.93	14.31	-3.06
10	0	0	67.74	67.28	-67.64	-3.66
10	0	2	77.27	79.70	77.17	3.99
10	0	-2	11.84	12.41	11.28	3.60
10	0	-4	97.11	98.43	96.46	11.26
10	0	4	105.44	115.05	104.93	10.39
10	0	-6	76.84	75.24	76.73	4.12
10	0	6	5.43	3.81	1.76	5.14
10	0	-8	52.78	50.64	-52.66	-3.54
10	0	8	45.41	42.45	-45.26	-3.65
10	0	-10	7.04	5.53	5.42	4.50
10	0	10	39.41	37.17	39.21	4.01
10	0	-12	50.46	48.18	49.30	10.75
10	0	12	60.51	59.98	59.65	10.16
10	0	-14	24.26	23.92	23.99	3.64
12	0	0	45.79	44.69	45.39	6.05
12	0	2	13.60	14.44	13.26	-3.04
12	0	-2	82.43	84.63	81.75	10.60
12	0	-4	19.95	20.84	-19.88	1.68
12	0	4	30.23	29.65	-30.18	1.77
12	0	-6	14.46	12.24	-13.99	-3.67
12	0	6	39.51	37.72	37.95	11.00
12	0	-8	64.44	63.68	64.19	5.72

12	0	8	41.30	40.16	40.91	5.68
12	0	-10	58.72	53.98	57.69	10.97
12	0	10	7.75	7.00	7.04	-3.25
12	0	-12	0.	3.24	0.	0.
14	0	0	26.97	24.85	24.88	10.40
14	0	2	22.80	21.05	21.25	8.26
14	0	-2	17.06	18.18	17.06	-0.26
14	0	-4	4.36	5.16	3.97	-1.81
14	0	4	25.06	24.75	-24.96	-2.20
14	0	-6	5.63	7.64	-1.06	5.53
14	0	6	20.97	21.88	20.97	-0.26
14	0	-8	54.34	53.84	53.55	9.23
14	0	8	19.14	17.99	16.58	9.57
14	0	-10	1.28	0.89	1.25	-0.27
14	0	10	20.53	19.22	19.14	7.42
14	0	-12	13.39	15.73	13.30	-1.58
16	0	0	30.14	27.59	-30.07	-1.98
16	0	2	22.79	21.56	21.27	8.17
16	0	-2	23.05	25.44	-23.04	-0.60
16	0	-4	65.94	66.36	65.35	8.78
16	0	4	54.27	53.80	53.55	8.81
16	0	-6	16.13	14.66	13.79	8.36
16	0	6	4.10	1.15	-3.32	-2.40
16	0	-8	13.06	12.73	-12.95	-1.71
18	0	0	34.79	34.33	34.77	1.11
18	0	2	0.	8.69	-0.	-0.
18	0	-2	15.83	13.36	11.15	11.24
18	0	-4	6.63	6.93	3.85	5.40
1	1	-3	28.55	25.70	28.42	-2.70
1	1	3	30.75	32.10	-30.58	-3.24
-1	1	-5	18.07	16.09	-17.99	-1.67
1	1	-5	56.44	55.55	-56.30	-4.01
-1	1	5	43.91	43.09	-43.90	0.83
1	1	5	4.35	3.12	0.13	-4.35
-1	1	-7	12.76	10.00	11.65	-5.21
1	1	-7	14.43	11.60	14.40	-0.91
-1	1	7	25.32	22.91	25.32	-0.05
1	1	7	25.64	24.65	25.64	0.26
-1	1	-9	32.66	30.84	-32.61	-1.77
1	1	-9	6.48	4.68	6.19	1.90
-1	1	9	13.98	14.62	-13.60	-3.23
1	1	9	27.06	24.52	-27.05	0.71
-1	1	-11	20.74	20.36	20.69	1.44
1	1	-11	12.19	11.25	12.05	-1.82
-1	1	11	9.40	8.48	8.78	-3.36
1	1	11	9.75	7.30	9.07	-3.57
-1	1	-13	5.03	3.89	-4.95	-0.88
1	1	-13	27.32	27.08	-26.99	-4.21
-1	1	13	20.22	20.25	-20.21	0.49
1	1	13	15.20	15.97	-14.82	-3.37
-1	1	-15	5.33	4.63	2.64	-4.63
1	1	-15	3.07	2.05	-2.50	-1.78
-1	1	15	9.32	4.95	9.23	1.27
1	1	15	18.06	18.80	18.06	-0.21
3	1	1	21.69	19.88	21.69	0.25

3	1	-1	54.30	53.59	-54.20	-3.24
-3	1	-3	25.59	25.70	-25.52	-1.84
3	1	-3	27.27	21.87	26.93	-4.30
-3	1	3	52.10	48.32	52.09	1.15
3	1	3	5.54	2.53	-5.38	1.34
-3	1	-5	26.51	23.82	26.48	1.25
3	1	-5	8.01	4.27	8.01	0.23
-3	1	5	17.68	15.39	-17.65	-1.05
3	1	5	17.66	15.74	17.41	-2.97
-3	1	-7	11.76	10.40	11.75	-0.59
3	1	-7	0.	1.08	-0.	0.
-3	1	7	15.70	14.29	-15.13	-4.19
3	1	7	29.73	29.79	-29.51	-3.61
-3	1	-9	21.17	19.75	-20.76	-4.13
3	1	-9	20.32	19.87	-20.14	-2.70
-3	1	9	24.41	24.79	-24.31	-2.24
3	1	9	0.	2.02	-0.	-0.
-3	1	-11	2.61	3.00	-1.36	-2.23
3	1	-11	7.51	4.00	1.02	-7.44
-3	1	11	11.57	12.11	11.53	0.94
3	1	11	20.37	20.57	20.34	1.04
-3	1	-13	9.65	8.92	-9.57	1.21
3	1	-13	5.86	1.95	5.80	-0.81
-3	1	13	2.54	1.40	2.54	-0.10
3	1	13	8.00	7.98	-7.80	-1.80
-3	1	-15	20.46	19.88	20.46	0.24
3	1	-15	4.69	4.07	4.36	1.74
-3	1	15	7.99	8.01	-7.20	-3.47
3	1	15	5.25	3.77	-0.87	-5.18
-5	1	1	35.73	33.25	-35.71	1.06
5	1	1	22.61	19.95	22.22	-4.18
-5	1	-1	36.95	36.14	36.95	-0.54
5	1	-1	20.92	19.67	-20.73	-2.85
-5	1	-3	4.73	4.09	-2.05	-4.26
5	1	-3	11.91	10.23	-11.88	0.88
-5	1	3	9.24	7.49	8.95	-2.28
5	1	3	15.16	13.17	-15.15	-0.67
-5	1	-5	3.95	2.80	-1.00	-3.82
5	1	-5	5.34	0.67	-4.79	2.36
-5	1	5	6.71	4.80	-3.94	-5.43
5	1	5	10.72	9.00	10.66	1.17
-5	1	-7	29.61	26.43	-29.60	0.85
5	1	-7	6.85	7.42	6.09	-3.14
-5	1	7	1.12	1.89	-0.76	-0.82
5	1	7	21.45	19.81	-21.37	-1.89
-5	1	-9	18.97	18.54	18.97	0.34
5	1	-9	8.06	9.29	-7.50	-2.95
-5	1	9	2.83	3.92	-2.70	0.86
5	1	9	14.30	13.83	13.76	-3.90
-5	1	-11	0.	5.86	0.	-0.
5	1	-11	8.79	5.68	-8.75	0.84
-5	1	11	5.24	3.52	5.05	-1.41
5	1	11	14.20	14.17	-14.14	-1.35
-5	1	-13	13.38	13.02	-12.96	-3.34
5	1	-13	2.22	1.64	1.75	1.37

-5	1	13	6.25	6.94	-5.20	-3.46
5	1	13	2.88	2.50	2.56	1.32
-5	1	-15	4.59	0.55	0.53	4.56
5	1	-15	7.64	3.56	-4.21	-6.38
-5	1	15	9.77	10.44	-9.60	-1.84
5	1	15	3.93	4.84	3.86	-0.72
-7	1	1	0.	2.80	0.	-0.
7	1	1	14.19	12.90	-14.06	-1.93
-7	1	-1	18.87	16.39	18.86	0.67
7	1	-1	7.33	8.01	7.26	0.99
-7	1	-3	23.70	22.22	-23.70	0.30
7	1	-3	21.28	20.63	21.27	-0.60
-7	1	3	5.92	4.03	-2.62	-5.31
7	1	3	24.75	24.25	-24.44	-3.91
-7	1	-5	7.60	6.64	6.72	-3.55
7	1	-5	24.33	22.92	-23.98	-4.10
-7	1	5	14.18	14.26	-14.17	-0.48
7	1	5	7.96	8.54	7.84	-1.36
-7	1	-7	16.81	13.48	-16.28	-4.19
7	1	-7	17.62	17.41	-17.43	-2.61
-7	1	7	14.07	13.08	14.02	1.13
7	1	7	6.62	1.61	-5.11	4.21
-7	1	-9	16.73	15.34	16.73	0.13
7	1	-9	11.82	7.85	11.70	1.68
-7	1	9	15.60	15.63	15.49	-1.88
7	1	9	12.79	12.28	12.76	-0.86
-7	1	-11	15.51	15.53	-15.48	0.95
7	1	-11	7.02	2.28	6.98	0.73
-7	1	11	18.01	16.48	-17.50	-4.25
7	1	11	23.57	22.81	-23.28	-3.69
-7	1	-13	0.	2.49	0.	-0.
7	1	-13	1.58	3.82	0.43	-1.52
-7	1	13	6.74	6.76	-6.65	-1.09
7	1	13	5.48	2.85	3.66	-4.08
-7	1	-15	6.36	4.69	-3.98	-4.96
7	1	-15	16.29	17.55	-16.04	-2.82
-7	1	15	7.36	4.34	6.98	2.34
-9	1	1	14.64	12.07	-14.18	-3.66
9	1	1	6.47	1.75	-5.12	3.96
-9	1	-1	23.34	21.23	-23.05	-3.66
9	1	-1	11.52	11.04	-11.41	-1.57
-9	1	-3	8.72	5.72	-8.72	-0.13
9	1	-3	6.40	4.77	3.55	-5.33
-9	1	3	20.71	18.65	20.71	0.31
9	1	3	3.09	1.72	2.72	-1.47
-9	1	-5	21.05	20.84	21.03	0.85
9	1	-5	7.68	7.94	-7.52	-1.57
-9	1	5	0.	0.60	0.	0.
9	1	5	8.60	10.21	8.05	-3.04
-9	1	-7	26.36	24.36	-26.24	-2.47
9	1	-7	11.81	7.74	-11.62	2.09
-9	1	7	25.11	23.00	-24.93	-2.97
9	1	7	22.07	20.80	-21.94	-2.40
-9	1	-9	0.	4.88	-0.	-0.
9	1	-9	23.94	21.58	23.93	-0.78

-9	1	9	10.81	8.51	9.81	-4.54
9	1	9	7.27	1.73	-6.57	3.12
-9	1	-11	10.94	9.71	-10.91	-0.75
9	1	-11	19.99	21.21	-19.62	-3.83
-9	1	11	1.09	2.11	-1.08	-0.12
9	1	11	3.37	0.76	3.37	-0.06
-9	1	-13	14.92	16.04	14.87	1.18
9	1	-13	2.31	2.20	0.38	-2.28
-9	1	13	17.81	17.04	17.77	1.21
9	1	13	11.65	11.97	11.26	-3.00
9	1	-15	9.14	9.42	-9.02	1.48
-9	1	15	11.49	12.50	-11.33	-1.90
-11	1	1	5.88	4.10	-5.77	1.14
11	1	1	0.	3.39	0.	-0.
-11	1	-1	14.98	13.83	-14.79	-2.39
11	1	-1	7.11	5.23	-5.02	-5.03
-11	1	-3	8.80	5.75	-6.79	-5.59
11	1	-3	18.33	19.03	-18.32	-0.65
-11	1	3	11.05	10.50	-11.05	-0.11
11	1	3	0.	0.73	-0.	0.
-11	1	-5	5.20	2.08	4.70	-2.23
11	1	-5	24.11	22.92	24.07	1.33
-11	1	5	6.49	7.31	5.78	-2.96
11	1	5	0.	0.28	-0.	-0.
-11	1	-7	11.65	11.00	-11.59	1.16
11	1	-7	8.31	8.97	-8.16	-1.56
-11	1	7	19.09	18.29	-18.84	-3.08
11	1	7	14.31	14.66	-13.99	-3.00
-11	1	-9	9.24	8.97	9.13	-1.41
11	1	-9	6.63	6.90	5.34	-3.93
-11	1	9	10.57	9.33	10.56	0.54
11	1	9	9.56	10.66	9.21	-2.58
-11	1	-11	14.20	13.13	-13.62	-4.03
11	1	-11	25.91	26.51	-25.88	-1.17
-11	1	11	18.13	18.64	-18.12	0.62
11	1	11	0.80	2.71	-0.80	0.06
11	1	-13	20.93	21.51	20.87	1.60
-11	1	13	11.07	11.08	10.69	-2.86
-13	1	1	22.01	21.33	21.99	-0.96
13	1	1	23.64	24.43	-23.45	-3.03
-13	1	-1	5.47	4.66	-5.34	1.17
13	1	-1	27.44	29.31	27.44	0.12
-13	1	-3	0.	1.30	0.	-0.
13	1	-3	15.12	14.99	-15.10	0.85
-13	1	3	28.48	28.16	-28.24	-3.67
13	1	3	6.54	6.02	-5.69	-3.23
-13	1	-5	13.67	11.74	-13.00	-4.24
13	1	-5	4.98	3.85	3.75	-3.28
-13	1	5	5.11	6.42	-4.82	-1.70
13	1	5	0.	2.86	0.	0.
-13	1	-7	0.	3.49	-0.	-0.
13	1	-7	17.78	19.01	-17.43	-3.50
-13	1	7	0.	8.33	-0.	0.
13	1	7	5.80	3.91	5.74	0.85
-13	1	-9	9.63	8.38	9.56	1.18

13	1	-9	16.10	15.34	16.10	-0.28
-13	1	9	19.33	18.53	19.33	-0.11
13	1	9	0.	3.30	-0.	-0.
-13	1	-11	3.14	3.23	3.10	-0.47
-13	1	11	17.54	18.87	-17.25	-3.18
-13	1	13	7.78	8.28	-7.35	-2.55
-15	1	1	18.34	18.19	17.98	-3.62
15	1	1	22.27	23.75	-22.26	0.65
-15	1	-1	22.86	22.84	-22.79	-1.76
15	1	-1	16.07	16.24	16.07	0.17
-15	1	-3	7.64	7.85	7.59	0.86
15	1	-3	12.29	12.28	-11.88	-3.16
-15	1	3	6.41	7.60	-6.33	-1.04
15	1	3	10.66	11.64	10.44	-2.14
-15	1	-5	1.96	6.03	1.96	-0.14
15	1	-5	0.	3.33	-0.	-0.
-15	1	5	5.82	6.09	5.73	1.03
15	1	5	11.69	10.69	-11.12	-3.61
-15	1	-7	10.33	10.90	9.85	-3.12
15	1	-7	0.	0.50	0.	0.
-15	1	7	0.59	4.51	-0.58	-0.13
15	1	7	7.58	7.73	7.56	-0.56
-15	1	-9	16.17	16.40	-16.00	-2.37
15	1	-9	3.78	4.62	-3.71	0.72
-15	1	9	5.88	3.77	-1.27	-5.74
-15	1	11	6.78	7.34	-6.56	-1.73
-17	1	1	4.67	5.91	4.66	-0.31
-17	1	-1	6.93	8.30	-6.39	-2.69
17	1	-1	4.63	3.78	-1.87	-4.24
-17	1	-3	10.47	11.61	10.23	-2.21
17	1	-3	10.12	11.53	-9.92	-1.98
-17	1	3	6.42	4.66	-6.30	1.25
-17	1	-5	11.11	9.76	-11.10	0.56
17	1	-5	6.45	6.22	-6.37	1.02
-17	1	5	6.62	9.17	6.49	-1.30
-17	1	7	3.36	5.96	2.69	-2.02
0	2	-4	46.80	44.03	46.00	8.62
0	2	4	65.49	67.60	65.01	7.92
0	2	-6	4.90	5.45	4.33	-2.29
0	2	6	51.81	51.65	50.68	10.78
0	2	-8	7.13	5.83	7.13	0.21
0	2	8	18.53	19.38	-18.53	0.05
0	2	-10	9.79	10.18	-1.56	9.66
0	2	10	16.92	16.23	-16.72	-2.59
0	2	-12	30.31	27.34	29.23	8.03
0	2	12	66.01	78.46	65.72	6.20
0	2	-14	15.59	15.03	15.44	-2.15
0	2	14	36.51	42.09	35.59	8.15
0	2	-16	5.56	3.31	-5.55	0.36
0	2	16	17.51	24.20	-17.51	0.05
2	2	0	131.24	166.55	130.91	9.37
2	2	-2	30.86	28.18	30.17	6.47
-2	2	-4	72.48	71.79	71.87	9.42
2	2	-4	40.52	36.66	-40.34	-3.86
-2	2	4	49.49	48.35	48.55	9.59

2	2	4	46.77	47.10	-46.64	-3.54
-2	2	-6	46.74	42.81	45.50	10.68
2	2	-6	6.14	3.76	-4.80	3.83
-2	2	6	15.74	13.82	15.61	-2.04
2	2	6	50.35	49.51	50.01	5.88
-2	2	-8	23.65	22.10	-23.63	-1.07
2	2	-8	65.52	66.21	64.58	11.08
-2	2	8	0.	1.16	0.	-0.
2	2	8	103.79	120.74	103.33	9.71
-2	2	-10	11.94	10.20	-11.80	-1.80
2	2	-10	41.57	40.31	41.19	5.62
-2	2	10	3.02	9.50	-0.41	2.99
2	2	10	14.16	13.62	13.98	2.23
2	2	12	20.27	19.74	-20.00	-3.28
-2	2	-12	81.16	83.28	80.76	8.08
2	2	-12	43.38	42.84	-43.27	-3.02
-2	2	12	23.97	26.77	22.75	7.55
-2	2	-14	36.23	33.25	35.04	9.22
2	2	-14	2.14	2.17	0.60	2.05
-2	2	14	14.17	18.53	14.12	-1.18
2	2	14	18.16	17.49	17.38	5.27
-2	2	-16	23.70	23.09	-23.69	-0.73
2	2	-16	26.16	23.45	23.96	10.49
-2	2	16	5.20	6.25	-5.15	-0.73
-4	2	0	124.49	155.57	124.15	9.15
4	2	0	60.87	59.97	60.77	3.51
-4	2	2	45.86	45.30	45.25	7.44
4	2	2	96.46	103.61	95.82	11.09
4	2	-2	31.57	27.02	-31.28	-4.30
-4	2	-4	42.18	40.78	-42.06	-3.14
4	2	-4	60.67	57.48	60.47	4.98
-4	2	4	30.06	28.35	-29.88	-3.30
4	2	4	49.36	50.47	49.15	4.58
-4	2	-6	63.82	60.47	63.38	7.52
4	2	-6	98.47	103.49	97.86	10.97
-4	2	6	17.03	14.70	-17.00	1.07
4	2	6	22.31	21.39	-21.98	-3.80
-4	2	-8	105.85	112.78	105.37	10.05
4	2	-8	26.31	22.56	-26.03	3.85
-4	2	8	54.14	56.62	53.13	10.43
4	2	8	55.01	54.48	54.91	3.32
-4	2	-10	8.58	8.23	8.53	0.94
4	2	-10	14.87	15.56	14.54	-3.11
-4	2	10	47.12	54.28	46.75	5.90
4	2	10	31.86	32.59	29.99	10.74
-4	2	12	30.64	38.13	-30.56	-2.24
4	2	12	17.99	18.27	17.51	4.11
-4	2	-12	18.75	16.15	-18.51	-3.01
4	2	-12	29.59	27.62	29.24	4.55
-4	2	-14	24.09	21.72	23.10	6.82
4	2	-14	42.72	42.29	41.51	10.09
-4	2	14	1.70	5.17	-1.68	0.28
4	2	14	0.	4.05	-0.	-0.
4	2	-16	22.44	21.83	-22.24	2.97
-4	2	16	13.06	19.94	11.55	6.10

-6	2	0	69.77	72.77	69.61	4.74
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6	2	2	32.42	29.94	32.40	1.18
-6	2	-2	89.75	97.74	89.09	10.89
6	2	-2	60.38	59.53	59.96	7.08
-6	2	-4	39.28	38.48	39.14	3.27
6	2	-4	88.90	93.10	88.28	10.51
-6	2	4	39.89	38.17	39.75	3.39
6	2	4	84.05	88.97	83.40	10.43
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6	2	-6	62.00	60.60	61.99	1.12
-6	2	6	87.85	108.65	87.34	9.42
6	2	6	25.82	25.66	24.91	6.81
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6	2	8	24.28	21.18	-24.04	-3.41
-6	2	-10	30.90	28.53	28.60	11.69
6	2	-10	40.90	39.66	40.36	6.63
-6	2	10	10.44	13.46	10.09	-2.67
6	2	10	20.81	20.23	-20.78	1.03
-6	2	12	14.76	16.65	14.53	2.62
6	2	12	57.33	58.42	56.50	9.72
-6	2	-12	9.89	8.88	9.35	3.22
6	2	-12	51.81	53.37	50.92	9.54
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6	2	-14	24.80	25.12	24.78	1.06
-6	2	14	28.22	44.97	27.48	6.42
6	2	14	18.51	18.66	17.56	5.84
-6	2	16	6.55	11.44	-6.13	2.32
-8	2	0	62.21	65.56	-62.12	-3.37
8	2	0	47.71	46.00	46.82	9.16
-8	2	2	49.49	50.94	49.19	5.44
8	2	2	31.78	30.42	31.72	-1.91
-8	2	-2	45.21	46.70	45.15	2.40
8	2	-2	57.35	55.74	56.48	9.97
-8	2	-4	85.44	91.42	84.77	10.66
8	2	-4	51.09	48.19	-51.08	-0.92
-8	2	4	78.93	91.50	78.30	9.95
8	2	4	55.23	54.58	-55.22	-0.93
-8	2	-6	10.37	11.41	9.15	4.89
8	2	-6	5.10	1.68	-0.35	-5.09
-8	2	6	56.40	71.40	56.37	1.90
8	2	6	17.13	15.55	13.61	10.40
-8	2	-8	29.09	23.78	-28.81	-4.00
8	2	-8	65.90	64.91	65.35	8.49
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8	2	8	52.13	48.93	51.37	8.88
-8	2	-10	9.10	9.50	-8.83	2.20
8	2	-10	62.35	59.44	61.65	9.35
-8	2	10	26.18	29.84	25.77	4.59
8	2	10	10.47	8.77	10.27	-2.05
-8	2	12	44.29	58.88	43.59	7.84
8	2	12	18.37	15.86	-18.35	-0.95

-8	2	-12	62.96	62.36	62.13	10.18
8	2	-12	21.19	21.02	-21.18	-0.66
-8	2	-14	10.55	9.24	9.10	5.34
8	2	-14	19.48	18.24	-19.43	-1.45
-8	2	14	19.00	27.34	18.94	1.48
-10	2	0	37.64	36.12	36.78	7.99
10	2	0	7.68	8.59	-3.30	6.94
-10	2	2	59.68	68.52	58.97	9.20
10	2	2	38.99	38.32	37.63	10.21
-10	2	-2	24.99	25.82	24.86	-2.56
10	2	-2	10.63	10.69	10.37	-2.33
-10	2	-4	53.93	53.32	-53.93	0.25
10	2	-4	17.11	14.03	17.11	-0.02
-10	2	4	42.70	41.94	-42.70	0.22
10	2	4	17.32	16.69	-17.32	-0.09
-10	2	-6	30.42	27.62	28.29	11.18
10	2	-6	17.05	15.68	13.34	10.62
-10	2	6	14.82	12.96	-14.52	-2.97
10	2	6	19.89	18.69	19.73	-2.48
-10	2	-8	48.93	42.20	48.22	8.30
10	2	-8	7.04	8.33	3.30	6.22
-10	2	8	54.51	64.27	54.15	6.24
10	2	8	28.30	26.57	27.20	7.82
-10	2	-10	5.30	4.22	4.41	-2.94
10	2	-10	0.	2.98	0.	-0.
-10	2	10	51.80	62.19	51.15	8.18
10	2	10	31.91	31.23	30.49	9.41
-10	2	12	8.83	14.31	-8.83	0.13
10	2	12	18.71	18.15	-18.71	-0.11
-10	2	-12	16.33	12.07	-16.33	0.37
10	2	-12	21.11	20.97	21.11	0.07
-10	2	14	17.17	27.43	-17.11	-1.40
-12	2	0	9.41	10.56	5.09	7.91
12	2	0	35.00	35.27	-34.86	-3.13
-12	2	2	9.96	8.78	9.80	-1.78
12	2	2	50.23	49.13	49.92	5.60
-12	2	-2	36.38	34.73	35.09	9.62
12	2	-2	6.25	5.81	-5.88	2.11
-12	2	-4	22.73	22.85	-22.70	-1.15
12	2	-4	59.37	58.21	58.40	10.68
-12	2	4	16.19	15.76	16.14	-1.21
12	2	4	61.43	62.72	60.57	10.24
-12	2	-6	28.82	27.27	28.78	-1.55
12	2	-6	28.14	25.71	27.52	5.87
-12	2	6	12.28	11.93	7.98	9.34
12	2	6	11.22	9.34	11.00	2.22
-12	2	-8	29.85	24.89	28.15	9.94
12	2	-8	18.36	17.13	-18.10	-3.08
-12	2	8	12.82	15.44	10.70	7.06
12	2	8	36.41	35.40	-36.28	-3.11
-12	2	-10	33.99	31.37	32.77	9.03
12	2	-10	13.90	16.00	-13.80	1.63
-12	2	10	6.73	1.70	-3.49	-5.76
12	2	10	46.33	47.32	46.07	4.92
-12	2	12	10.78	18.44	10.76	-0.60

-12	2	-12	22.97	23.31	-22.95	-0.94
12	2	-12	33.43	34.03	32.14	9.21
-14	2	0	25.09	23.83	-24.92	-2.90
14	2	0	33.68	32.41	33.43	4.13
-14	2	2	16.30	17.46	-16.29	0.63
14	2	2	0.	4.12	-0.	-0.
-14	2	-2	50.76	49.30	50.29	6.92
14	2	-2	49.06	50.11	47.99	10.17
-14	2	-4	60.56	62.32	59.78	9.69
14	2	-4	12.45	10.69	11.88	3.71
-14	2	4	51.40	56.07	50.55	9.29
14	2	4	16.24	16.33	15.94	3.12
-14	2	-6	0.	1.31	0.	0.
14	2	-6	18.35	19.60	-18.12	-2.87
-14	2	6	28.86	32.40	28.25	5.90
14	2	6	40.70	41.73	39.49	9.83
-14	2	-8	35.51	33.28	-35.41	-2.70
14	2	-8	43.56	43.07	43.39	3.86
-14	2	8	9.39	12.57	-9.18	-1.97
-14	2	-10	52.95	53.01	52.60	6.10
14	2	-10	31.51	32.50	30.11	9.28
-14	2	10	12.03	18.19	-12.02	0.44
-14	2	12	18.28	30.06	17.40	5.59
-16	2	0	26.79	26.22	26.65	2.74
16	2	0	49.84	52.72	49.02	9.03
-16	2	2	45.47	49.90	44.47	9.49
16	2	2	6.37	7.57	4.15	4.83
-16	2	-2	7.78	6.88	-6.87	-3.65
16	2	-2	24.29	22.39	24.26	1.21
-16	2	-4	24.63	24.58	24.23	4.40
16	2	-4	4.52	2.76	1.52	-4.26
-16	2	4	14.11	15.16	13.49	4.14
-16	2	-6	35.81	34.56	34.29	10.33
16	2	-6	3.44	5.64	-0.15	3.44
-16	2	6	14.12	17.65	-13.89	-2.55
-16	2	8	25.50	32.20	25.42	2.06
-16	2	10	22.43	33.93	21.49	6.44
-18	2	0	44.99	49.66	44.08	8.99
-18	2	2	27.45	29.25	27.37	2.12
-18	2	4	2.12	3.96	-1.36	-1.63
-18	2	6	1.09	7.54	-0.87	0.65
-1	3	-3	20.72	17.62	-20.40	-3.60
1	3	3	16.63	15.75	16.59	-1.16
-1	3	-5	11.52	9.73	11.48	0.97
1	3	-5	4.45	3.84	-4.44.	-0.26
-1	3	5	13.51	11.79	13.28	-2.46
1	3	5	16.86	15.94	-16.82	1.15
-1	3	-7	16.75	15.52	16.73	0.73
1	3	-7	27.22	25.52	26.87	-4.33
-1	3	7	13.56	13.80	-13.06	-3.66
1	3	7	9.56	9.80	-9.49	-1.19
-1	3	-9	15.38	14.65	-14.95	-3.63
1	3	-9	28.50	29.46	-28.37	-2.77
-1	3	9	19.48	19.21	-19.45	-1.06
1	3	9	0.	5.39	-0.	-0.

-1	3	-11	0.	3.67	0.	-0.
1	3	-11	16.59	15.29	16.52	1.47
-1	3	11	16.81	16.11	16.78	1.07
1	3	11	5.89	3.68	5.07	-3.00
-1	3	-13	8.46	10.38	-8.44	0.57
1	3	-13	12.36	10.65	-12.35	0.56
-1	3	13	4.21	3.41	3.95	-1.47
1	3	13	15.66	13.74	-15.63	1.02
-1	3	-15	24.95	23.38	24.91	1.35
1	3	-15	12.71	12.88	12.13	-3.80
-1	3	15	0.72	3.60	0.13	-0.71
1	3	15	7.85	6.27	-7.84	-0.44
3	3	-1	13.70	10.14	-13.58	1.82
-3	3	-3	11.23	10.81	10.77	-3.18
3	3	-3	45.65	43.43	45.63	-1.29
-3	3	3	11.79	10.59	-11.31	-3.33
3	3	3	32.29	33.86	-32.08	-3.72
-3	3	-5	10.33	8.30	-9.20	-4.69
3	3	-5	54.55	55.31	-54.38	-4.24
-3	3	5	0.	3.43	0.	-0.
3	3	5	10.65	10.54	-10.46	-2.02
-3	3	-7	15.01	14.16	-15.01	0.09
3	3	-7	6.75	7.34	-6.52	-1.73
-3	3	7	29.41	27.74	29.41	-0.22
3	3	7	17.60	17.30	17.58	0.92
-3	3	-9	2.05	1.49	0.92	1.83
3	3	-9	5.74	1.70	-0.68	5.70
-3	3	9	11.67	10.19	-11.63	0.95
3	3	9	10.23	8.77	-10.22	-0.40
-3	3	-11	8.09	5.08	6.97	-4.10
3	3	-11	29.93	29.78	29.93	-0.51
-3	3	11	8.42	8.74	8.18	-2.00
3	3	11	8.94	11.12	-8.54	-2.65
-3	3	-13	12.61	11.75	-11.80	-4.45
3	3	-13	10.97	11.39	-10.14	-4.19
-3	3	13	22.61	23.33	-22.35	-3.45
3	3	13	10.74	12.08	-10.50	-2.28
-3	3	-15	4.90	1.46	-4.87	-0.56
3	3	-15	29.02	29.92	-28.94	-2.19
-3	3	15	20.64	20.56	20.62	-0.87
3	3	15	9.02	10.17	9.01	0.44
-5	3	1	24.08	21.37	-23.73	-4.08
5	3	1	31.26	29.60	31.24	1.14
5	3	-1	49.24	49.06	-49.19	-2.20
-5	3	-3	0.	1.83	-0.	0.
5	3	-3	1.64	4.49	0.63	-1.51
-5	3	3	18.62	16.21	18.34	-3.23
5	3	3	29.85	20.18	-29.85	-0.38
-5	3	-5	33.09	30.70	-33.01	-2.35
5	3	-5	0.	3.85	-0.	-0.
-5	3	5	36.37	33.98	-36.37	0.53
5	3	5	20.09	18.87	19.75	-3.69
-5	3	-7	12.98	11.27	-12.07	-4.78
5	3	-7	15.20	12.40	15.06	2.04
-5	3	7	18.01	16.75	18.01	0.36

5	3	7	20.95	19.91	-20.75	-2.88
-5	3	-9	7.97	7.39	7.92	-0.88
5	3	-9	0.	3.92	-0.	-0.
-5	3	9	6.99	8.50	-6.58	-2.36
5	3	9	5.03	5.38	-5.01	0.40
-5	3	-11	4.91	4.68	4.59	1.74
5	3	-11	34.38	35.80	-34.11	-4.30
-5	3	11	21.07	19.59	20.78	-3.50
5	3	11	4.07	4.43	4.06	0.32
-5	3	-13	16.81	15.88	-16.73	-1.64
5	3	-13	15.82	14.85	15.76	-1.32
-5	3	13	13.66	13.75	-13.66	-0.10
5	3	13	7.13	6.05	6.41	-3.13
-5	3	-15	9.98	10.95	-9.19	-3.89
5	3	-15	6.20	5.49	5.77	2.26
-5	3	15	6.83	5.17	-6.74	1.13
-7	3	1	51.78	51.03	-51.74	-2.00
7	3	1	15.48	14.38	15.14	-3.21
-7	3	-1	11.30	11.07	-10.56	-4.02
7	3	-1	9.33	8.65	-8.47	-3.91
-7	3	-3	24.52	24.54	-24.49	-1.18
7	3	-3	11.02	11.05	-11.02	0.07
-7	3	3	42.03	39.70	42.02	1.01
7	3	3	16.17	12.28	-16.16	0.67
-7	3	-5	30.27	28.40	30.23	1.46
7	3	-5	11.47	10.45	11.39	1.39
-7	3	5	15.90	15.54	-15.89	-0.41
7	3	5	17.48	18.07	17.47	0.43
-7	3	-7	3.90	2.67	-3.49	-1.73
7	3	-7	19.09	18.60	-18.91	-2.65
-7	3	7	17.45	17.65	-17.11	-3.41
7	3	7	32.62	33.18	-32.51	-2.72
-7	3	-9	25.86	23.80	-25.46	-4.53
7	3	-9	17.88	15.11	17.17	-4.98
-7	3	9	17.96	15.39	-17.69	-3.10
7	3	9	25.55	24.38	25.33	-3.38
-7	3	-11	13.21	13.29	-13.09	-1.75
7	3	-11	19.26	19.00	-19.26	-0.23
-7	3	11	0.	1.44	-0.	0.
7	3	11	6.08	1.15	-5.95	-1.27
-7	3	-13	14.19	13.33	14.08	1.73
7	3	-13	7.45	8.23	7.27	1.63
-7	3	13	21.52	19.99	21.52	0.36
-7	3	15	18.46	19.47	-18.26	-2.68
-9	3	1	15.15	14.94	-15.11	1.11
9	3	1	22.67	22.34	-22.49	-2.89
-9	3	-1	28.63	25.79	28.61	-1.14
9	3	-1	23.88	24.00	23.87	0.76
-9	3	-3	25.20	22.70	-24.83	-4.33
9	3	-3	0.	3.69	-0.	0.
-9	3	3	13.33	11.06	-13.24	-1.53
9	3	3	8.71	7.00	-7.56	-4.33
-9	3	-5	11.78	9.95	11.52	-2.48
9	3	-5	7.51	5.87	6.16	-4.30
-9	3	5	7.31	6.08	-5.77	-4.48

9	3	5	8.42	9.09	8.42	-0.23
-9	3	-7	31.32	23.83	-31.28	1.62
9	3	-7	25.46	25.40	-25.21	-3.59
-9	3	7	14.23	14.27	-14.11	-1.85
9	3	7	6.36	1.93	-5.70	2.83
-9	3	-9	28.48	27.80	28.48	-0.22
9	3	-9	16.53	14.02	16.51	0.76
-9	3	9	18.61	15.62	18.58	1.10
9	3	9	14.77	16.14	14.67	-1.75
-9	3	-11	0.	3.87	-0.	-0.
9	3	-11	8.15	5.47	7.93	1.87
-9	3	11	33.18	32.88	-33.18	-0.40
9	3	11	27.60	28.18	-27.40	-3.32
-9	3	-13	7.89	7.41	-7.39	-2.77
-9	3	13	8.54	6.40	7.27	-4.48
-11	3	1	19.97	18.72	19.84	-2.28
11	3	1	23.34	20.55	-23.30	1.28
-11	3	-1	0.	2.92	-0.	0.
11	3	-1	13.20	13.05	13.20	-0.30
-11	3	-3	5.82	4.00	5.82	-0.20
11	3	-3	6.96	7.03	-5.84	-3.79
-11	3	3	15.52	15.38	-15.07	-3.69
11	3	3	8.42	9.69	8.25	-1.66
-11	3	-5	12.67	12.49	12.16	-3.56
11	3	-5	0.	2.70	0.	-0.
-11	3	5	5.99	4.28	5.83	-1.37
11	3	5	8.94	5.96	-7.10	-5.43
-11	3	-7	24.96	23.14	-24.77	-3.10
11	3	-7	7.83	3.77	-7.39	2.60
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11	3	7	0.	2.03	0.	-0.
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11	3	-9	3.58	3.86	3.56	0.40
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11	3	9	11.57	9.93	-11.52	1.11
-11	3	-11	7.52	6.11	-7.48	0.73
11	3	-11	6.44	8.04	-5.69	-3.02
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13	3	1	3.24	4.72	3.13	-0.83
-13	3	-1	31.54	30.25	-31.40	-2.99
13	3	-1	3.90	4.33	-1.68	-3.52
-13	3	-3	4.26	7.65	4.25	0.24
13	3	-3	25.08	23.98	-25.02	-1.78
-13	3	3	0.	3.07	0.	-0.
13	3	3	10.52	10.44	10.46	1.16
-13	3	-5	7.12	5.96	7.09	0.70
13	3	-5	0.	4.78	0.	0.
-13	3	5	15.60	14.10	15.58	0.86
13	3	5	18.07	16.62	-18.04	-1.07
-13	3	-7	3.25	4.96	2.67	-1.86
13	3	-7	16.53	14.90	16.52	-0.59
-13	3	7	13.18	11.80	-12.97	-2.32
13	3	7	4.79	3.83	-2.12	-4.29

-13	3	-9	8.83	6.69	-7.59	-4.51
13	3	-9	5.58	5.93	4.00	-3.89
-13	3	9	4.19	3.54	-0.62	-4.14
-13	3	11	2.80	2.35	2.62	-1.00
-15	3	1	1.52	2.40	1.49	0.31
15	3	1	14.63	14.85	-14.19	-3.58
-15	3	-1	16.81	14.71	-16.55	-2.96
15	3	-1	13.29	12.62	13.27	-0.77
-15	3	-3	12.12	12.08	11.64	-3.36
15	3	-3	2.02	1.85	1.29	1.55
-15	3	3	14.41	12.26	-14.41	0.33
15	3	3	7.82	7.29	-7.52	-2.16
-15	3	-5	9.29	10.42	-9.29	-0.23
15	3	-5	0.	3.30	0.	-0.
-15	3	5	5.99	5.57	5.20	-2.98
-15	3	-7	1.48	1.46	-1.04	1.05
-15	3	7	8.08	8.84	7.57	-2.83
-15	3	9	4.12	1.48	4.12	-0.20
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-17	3	1	16.72	13.89	16.71	-0.49
-17	3	-1	0.	2.41	-0.	0.
-17	3	-3	10.72	10.82	-10.58	-1.75
-17	3	3	18.33	17.71	-18.02	-3.33
-17	3	-5	21.90	18.74	-21.51	-4.13
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0	4	-4	87.69	88.31	87.37	7.48
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0	4	8	0.	0.38	-0.	0.
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0	4	10	9.69	10.00	-0.58	9.67
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0	4	-14	42.21	40.31	41.18	9.28
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2	4	0	12.93	9.26	-12.82	-1.71
2	4	2	5.96	6.02	-5.78	-1.47
2	4	-2	7.32	15.97	5.92	4.30
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2	4	-4	62.50	60.52	61.80	9.33
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2	4	4	53.47	54.02	52.70	9.04
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2	4	-8	29.67	27.03	-29.65	-1.13
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2	4	8	7.43	5.23	-7.21	-1.79
-2	4	-10	9.27	6.16	8.51	3.67
2	4	-10	40.12	38.38	39.11	8.93

-2	4	10	34.58	32.86	34.17	5.31
2	4	10	18.61	16.84	-18.54	-1.57
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2	4	12	48.19	46.37	47.42	8.59
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2	4	-12	39.19	36.02	38.20	8.74
-2	4	-14	17.39	15.96	16.67	4.96
2	4	-14	21.95	21.05	21.93	-1.00
-2	4	14	3.67	2.24	0.25	3.66
2	4	14	23.76	21.72	22.05	8.84
4	4	0	70.45	69.25	69.62	10.81
4	4	2	19.98	16.87	19.97	0.77
4	4	-2	16.14	14.56	14.05	7.95
-4	4	-4	50.26	49.24	50.02	4.95
4	4	-4	56.51	52.96	-56.44	-2.81
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4	4	4	39.50	36.71	-39.39	-2.98
-4	4	-6	5.99	6.20	-5.06	-3.21
4	4	-6	25.69	23.16	25.68	0.80
-4	4	6	76.05	76.35	75.20	11.32
4	4	6	9.85	9.70	6.79	7.13
-4	4	-8	20.74	19.03	20.49	3.22
4	4	-8	44.01	38.20	42.49	11.46
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4	4	8	76.49	78.74	75.85	9.84
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4	4	10	2.10	2.73	-2.06	0.41
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4	4	12	12.95	9.53	-12.48	-3.45
-4	4	-12	24.38	22.75	23.93	4.67
4	4	-12	35.81	36.22	-35.75	-2.13
-4	4	-14	3.40	2.70	0.34	-3.38
4	4	-14	3.50	2.99	3.40	0.82
-4	4	14	53.78	55.05	52.88	9.80
-6	4	0	31.64	27.83	-31.47	-3.31
6	4	0	14.81	12.23	13.56	5.96
-6	4	2	9.22	10.39	6.70	6.34
6	4	2	55.69	56.50	54.61	10.90
-6	4	-2	19.65	18.60	19.63	0.89
6	4	-2	22.32	21.27	22.05	-3.46
-6	4	-4	61.23	60.70	60.28	10.73
6	4	-4	9.27	7.94	8.68	3.26
-6	4	4	65.00	63.21	64.04	11.12
6	4	4	5.56	4.14	4.17	3.68
-6	4	-6	7.35	7.66	-3.29	6.57
6	4	-6	40.28	36.25	38.50	11.85
-6	4	6	39.86	35.49	39.85	0.86
6	4	6	8.65	6.47	7.41	-4.46
-6	4	-8	17.05	14.80	-16.79	-2.99
6	4	-8	12.88	13.85	-12.12	4.36
-6	4	8	39.63	36.41	-39.51	-3.09
6	4	8	51.07	49.30	50.84	4.84
-6	4	-10	6.43	6.28	-6.37	0.86

6	4	-10	12.49	13.19	12.20	-2.69
-6	4	10	36.02	34.75	35.35	6.93
6	4	10	30.78	29.51	28.86	10.70
-6	4	12	43.37	41.64	42.15	10.22
6	4	12	8.33	8.36	7.97	2.42
-6	4	-12	59.66	57.73	58.87	9.66
6	4	-12	16.34	13.91	16.07	2.98
-6	4	-14	12.00	9.04	9.04	7.89
-6	4	14	22.31	21.22	22.30	0.69
-8	4	0	58.27	55.55	57.51	9.41
8	4	0	56.77	57.47	-56.68	-3.20
-8	4	2	41.90	37.18	40.52	10.67
8	4	2	58.95	59.27	58.89	2.59
-8	4	-2	10.02	7.50	9.80	-2.11
8	4	-2	26.66	25.76	26.17	5.08
-8	4	-4	40.42	37.22	-40.40	-1.13
8	4	-4	79.87	78.68	79.14	10.75
-8	4	4	47.23	43.20	-47.21	-1.25
8	4	4	71.21	75.05	70.49	10.13
-8	4	-6	33.60	29.45	31.97	10.34
8	4	-6	40.49	36.82	40.39	2.85
-8	4	6	8.98	8.34	8.81	-1.73
8	4	6	23.95	23.19	23.44	4.91
-8	4	-8	72.11	67.26	71.55	8.95
8	4	-8	33.74	31.25	-33.60	-3.12
-8	4	8	38.46	33.56	37.16	9.90
8	4	8	38.16	37.46	-38.02	-3.24
-8	4	-10	8.08	7.07	-7.94	-1.50
8	4	-10	13.77	11.18	12.59	5.57
-8	4	10	48.58	45.96	47.67	9.34
8	4	10	23.10	22.06	22.97	2.49
-8	4	12	26.88	28.33	-26.86	-1.01
-8	4	-12	9.14	7.51	-9.09	-1.00
8	4	-12	44.53	43.70	43.49	9.59
-8	4	14	6.84	5.20	-6.58	-1.86
-10	4	0	27.39	24.34	26.05	8.46
10	4	0	46.89	46.30	46.38	6.88
-10	4	2	26.33	25.52	26.20	-2.62
10	4	2	12.49	12.11	12.22	-2.58
-10	4	-2	50.33	46.75	49.13	10.92
10	4	-2	53.49	52.77	52.57	9.89
-10	4	-4	8.36	7.14	-8.36	0.25
10	4	-4	12.66	10.56	-12.64	0.69
-10	4	4	5.42	1.58	-5.39	0.58
10	4	4	27.29	27.17	-27.29	0.49
-10	4	-6	20.57	19.15	20.42	-2.51
10	4	-6	6.85	7.59	-6.53	-2.06
-10	4	6	35.03	30.32	33.05	11.62
10	4	6	36.26	35.70	34.94	9.69
-10	4	-8	51.61	46.18	51.01	7.82
10	4	-8	55.70	55.21	55.32	6.46
-10	4	8	8.17	7.60	2.54	7.76
10	4	8	30.14	29.76	29.43	6.51
-10	4	-10	28.93	26.04	27.08	10.17
10	4	-10	44.02	44.23	43.11	8.89

-10	4	10	14.21	15.15	14.03	-2.26
-10	4	12	9.24	6.16	9.24	0.24
-10	4	-12	4.15	2.63	-4.12	0.47
-12	4	0	49.38	49.25	-49.27	-3.27
12	4	0	23.86	22.24	22.15	8.86
-12	4	2	0.	3.03	0.	0.
12	4	2	19.79	19.08	17.88	8.49
-12	4	-2	70.53	72.52	70.35	5.10
12	4	-2	10.80	9.54	10.73	-1.25
-12	4	-4	68.78	69.65	67.99	10.39
12	4	-4	6.29	2.63	5.70	-2.67
-12	4	4	72.58	71.04	71.75	10.97
12	4	4	8.52	8.33	-8.43	-1.26
-12	4	-6	4.99	3.13	3.58	3.48
12	4	-6	15.54	14.24	12.91	8.65
-12	4	6	57.84	55.17	57.59	5.41
12	4	6	3.32	4.00	3.17	-0.97
-12	4	-8	37.06	32.71	-36.91	-3.32
12	4	-8	37.01	34.41	36.04	8.40
-12	4	8	29.70	26.66	-29.49	-3.55
-12	4	-10	42.22	38.98	41.91	5.14
-12	4	10	5.82	8.49	-5.64	1.44
-12	4	12	44.25	43.96	43.14	9.87
-14	4	0	31.68	29.98	31.35	4.56
14	4	0	31.79	31.31	-31.71	-2.29
-14	4	2	62.04	61.68	61.12	10.67
-14	4	-2	4.11	4.25	2.64	-3.15
14	4	-2	2.30	3.88	-2.28	0.27
-14	4	-4	13.30	13.76	-13.00	2.82
14	4	-4	48.20	47.36	47.34	9.05
-14	4	4	0.	3.26	0.	0.
14	4	4	13.50	46.50	13.25	2.59
-14	4	-6	42.63	40.08	41.26	10.74
-14	4	6	22.82	21.14	-22.54	-3.54
-14	4	-8	21.52	19.13	21.04	4.54
-14	4	8	42.94	42.42	42.73	4.22
-14	4	10	48.54	47.30	47.45	10.23
-16	4	0	32.49	31.86	30.94	9.91
-16	4	2	16.63	13.25	16.60	1.06
-16	4	-2	11.82	10.85	9.75	6.68
-16	4	-4	18.31	16.72	-18.09	-2.83
-16	4	4	0.71	2.72	-0.10	-0.70
-16	4	-6	18.53	18.72	18.51	0.84
-16	4	6	3.05	6.33	0.83	2.93
-16	4	8	46.82	47.10	45.88	9.33
-18	4	0	18.41	15.45	-18.38	-1.05
-18	4	2	21.09	21.78	-21.04	-1.48
1	5	-3	20.91	18.34	20.41	-4.55
-1	5	3	35.65	37.89	-35.47	-3.57
1	5	3	6.32	7.31	6.31	0.35
-1	5	-5	61.06	60.34	-60.89	-4.49
1	5	-5	16.95	14.76	16.95	0.16
-1	5	5	4.48	2.67	-1.35	-4.27
1	5	5	28.87	28.99	28.70	-3.14
-1	5	-7	3.26	3.71	-3.17	-0.75

1	5	-7	5.57	2.02	3.30	4.49
-1	5	7	35.76	37.86	35.75	0.68
1	5	7	17.69	18.69	-17.43	-3.01
-1	5	-9	10.69	9.70	10.46	2.19
1	5	-9	29.76	30.20	-29.65	-2.60
-1	5	9	24.37	22.38	-24.37	0.14
1	5	9	14.65	13.69	-14.65	0.08
-1	5	-11	16.75	15.25	16.66	-1.71
1	5	-11	8.17	8.78	-7.06	-4.12
-1	5	11	3.55	2.93	-0.16	-3.55
1	5	11	20.24	22.56	20.23	0.59
-1	5	-13	28.04	28.25	-27.66	-4.60
1	5	-13	11.64	12.29	11.64	-0.04
-1	5	13	10.54	11.78	-10.22	-2.56
1	5	13	6.23	5.12	5.63	-2.66
3	5	1	43.16	41.14	42.99	-3.80
3	5	-1	14.28	12.64	-13.81	-3.65
3	5	-3	23.68	20.85	-23.66	1.05
3	5	3	0.	0.90	0.	0.
-3	5	-5	20.03	20.48	-20.01	-0.99
3	5	-5	5.63	3.77	5.46	1.39
-3	5	5	44.80	43.73	-44.78	1.16
3	5	5	9.04	8.57	-8.99	0.98
-3	5	-7	18.19	15.39	17.40	-5.30
3	5	-7	28.02	26.50	27.77	-3.75
-3	5	7	10.09	10.22	10.07	-0.63
3	5	7	24.76	23.59	-24.64	-2.43
-3	5	-9	20.05	19.55	-19.95	-1.95
3	5	-9	6.25	5.25	-4.26	-4.58
-3	5	9	7.46	7.99	-6.71	-3.25
3	5	9	28.44	26.56	28.19	-3.73
-3	5	-11	12.79	14.15	12.67	1.78
3	5	-11	12.21	11.97	-12.18	0.91
-3	5	11	13.11	12.63	12.89	-2.38
3	5	11	1.75	3.03	1.70	-0.40
-3	5	-13	10.91	9.84	-10.90	-0.49
-3	5	13	23.64	21.68	-23.63	0.67
5	5	1	20.27	18.96	-20.12	-2.43
5	5	-1	18.93	19.37	18.88	1.36
-5	5	-3	26.56	27.99	-26.47	-2.24
5	5	-3	33.77	32.61	33.77	-0.
-5	5	3	51.88	51.20	51.87	1.24
5	5	3	35.25	35.65	-35.04	-3.86
-5	5	-5	44.66	41.58	44.63	1.58
5	5	-5	27.03	25.41	-26.67	-4.40
-5	5	5	14.11	13.12	-14.01	-1.66
5	5	5	16.61	16.21	16.59	-0.80
-5	5	-7	15.92	15.44	15.92	0.03
5	5	-7	21.15	21.40	-20.95	-2.92
-5	5	7	29.37	31.04	-29.16	-3.53
5	5	7	11.40	11.70	11.35	1.09
-5	5	-9	28.32	25.30	-27.94	-4.63
5	5	-9	15.32	14.08	15.22	1.71
-5	5	9	20.10	20.60	-20.05	-1.48
5	5	9	0.	1.41	0.	-0.

-5	5	-11	6.62	6.40	-5.92	-2.97
5	5	-11	22.51	23.50	22.50	0.60
-5	5	11	14.31	14.17	14.28	0.94
5	5	11	31.50	33.00	-31.33	-3.30
-5	5	-13	5.18	5.52	4.96	1.48
-5	5	13	4.90	6.34	4.87	-0.52
-7	5	1	32.01	29.86	-31.99	1.04
7	5	1	6.43	4.14	-6.00	2.32
-7	5	-1	47.98	47.88	47.98	0.18
7	5	-1	18.80	18.73	-18.77	-1.02
-7	5	-3	12.59	14.22	12.17	-3.23
7	5	-3	6.33	4.42	1.20	-6.22
-7	5	3	18.90	19.07	-18.74	-2.42
7	5	3	4.11	2.53	-3.56	-2.05
-7	5	-5	2.23	4.68	-1.61	-1.54
7	5	-5	2.54	1.94	-0.58	-2.47
-7	5	5	18.81	16.82	18.36	-4.07
7	5	5	9.10	9.60	8.35	-3.62
-7	5	-7	40.47	38.49	-40.46	1.00
7	5	-7	5.84	3.43	-4.86	3.23
-7	5	7	19.43	18.35	19.42	-0.70
7	5	7	20.81	19.54	-20.74	-1.75
-7	5	-9	33.99	33.48	33.98	0.92
7	5	-9	5.95	7.16	5.94	-0.35
-7	5	9	4.52	5.17	-4.44	0.84
7	5	9	10.88	8.70	-10.81	1.23
-7	5	-11	14.30	14.10	13.87	-3.50
7	5	-11	15.59	18.16	-15.10	-3.86
-7	5	11	18.20	19.16	-18.14	-1.43
-7	5	13	1.35	4.58	-0.90	-1.01
-9	5	1	21.46	21.98	21.23	-3.14
9	5	1	15.92	14.16	15.76	-2.22
-9	5	-1	8.54	6.75	8.52	0.52
9	5	-1	16.08	17.71	-15.63	-3.76
-9	5	-3	21.66	18.74	-21.63	1.07
9	5	-3	30.15	29.82	-30.14	-0.83
-9	5	3	4.28	5.17	3.35	-2.66
9	5	3	7.75	7.93	7.66	1.21
-9	5	-5	3.75	3.33	-1.80	-3.29
9	5	-5	22.03	21.07	21.95	1.93
-9	5	5	17.24	16.84	-17.24	0.14
9	5	5	10.37	10.55	-10.36	-0.34
-9	5	-7	7.02	5.73	-5.20	-4.72
9	5	-7	3.28	2.10	2.28	-2.36
-9	5	7	1.34	3.28	1.31	0.27
9	5	7	20.72	22.35	-20.48	-3.15
-9	5	-9	25.07	23.09	25.07	0.20
9	5	-9	3.63	4.63	-0.65	-3.57
-9	5	9	25.78	24.68	25.67	-2.43
-9	5	-11	24.22	23.18	-24.17	1.59
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11	5	1	16.44	18.62	-16.13	-3.17
-11	5	-1	36.37	34.00	-36.15	-3.99
11	5	-1	33.49	34.81	33.49	0.11

-11	5	-3	2.36	1.91	-2.31	-0.46
11	5	-3	2.04	5.15	-1.96	0.57
-11	5	3	28.22	28.45	28.21	0.76
11	5	3	12.59	14.82	-12.37	-2.32
-11	5	-5	24.23	21.44	24.18	1.58
11	5	-5	8.86	8.85	-8.50	-2.50
-11	5	5	2.02	0.69	1.99	0.32
-11	5	-7	15.55	12.61	-15.36	-2.45
-11	5	7	24.13	22.31	-23.91	-3.26
-11	5	-9	25.00	22.39	-24.57	-4.62
-11	5	9	6.81	4.09	4.80	-4.83
-11	5	11	6.99	7.01	6.99	0.11
-13	5	1	15.65	16.51	-15.61	1.07
-13	5	-1	0.	2.44	-0.	-0.
-13	5	-3	6.22	3.97	-0.94	-6.15
-13	5	3	17.02	17.07	-17.01	-0.64
-13	5	-5	6.57	4.44	-6.30	-1.85
-13	5	5	10.52	8.84	9.68	-4.11
-13	5	-7	14.35	15.55	-14.28	1.41
-13	5	7	6.81	7.23	-6.48	-2.11
-13	5	9	3.18	5.56	3.16	0.37
-15	5	1	25.04	24.78	25.00	-1.49
-15	5	-1	9.92	6.86	9.77	1.69
-15	5	-3	4.71	6.82	-4.69	-0.48
-15	5	3	32.78	34.88	-32.61	-3.37
-15	5	-5	17.15	14.45	-16.56	-4.46
-15	5	5	10.44	9.33	-10.32	-1.60
-15	5	7	6.79	8.38	-6.75	0.75
-17	5	1	21.19	23.34	20.96	-3.08
-17	5	3	9.30	8.87	9.28	-0.62
0	6	-4	34.67	31.24	-34.50	-3.43
0	6	4	13.94	14.47	-13.57	-3.19
0	6	-6	24.60	22.62	24.32	3.69
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0	6	8	76.09	83.27	75.49	9.51
0	6	-10	19.18	16.73	18.68	4.33
0	6	10	4.27	3.29	1.06	4.14
2	6	0	9.88	10.07	9.70	1.86
2	6	2	63.08	64.87	62.26	10.16
2	6	-2	7.97	7.09	-7.27	-3.26
-2	6	-4	30.55	27.61	29.80	6.75
2	6	-4	40.35	37.02	39.91	5.97
2	6	4	28.69	27.84	28.12	5.69
-2	6	-6	7.63	3.04	-3.97	-6.51
2	6	-6	55.02	53.85	54.07	10.20
-2	6	6	33.07	31.51	31.26	10.79
2	6	6	13.47	14.36	-13.17	-2.82
-2	6	-8	3.34	1.45	1.14	3.14
2	6	-8	14.02	9.87	-13.76	2.70
-2	6	8	3.91	2.43	3.37	1.99
2	6	8	30.19	27.67	30.13	1.92
-2	6	-10	25.62	22.94	23.41	10.42
2	6	-10	1.96	2.66	0.78	-1.80
-2	6	10	16.40	14.73	-16.10	-3.13

2	6	10	24.30	24.11	22.21	9.86
4	6	0	19.89	18.23	-19.76	-2.23
4	6	2	10.50	9.48	10.50	-0.08
4	6	-2	35.44	33.23	34.56	7.84
-4	6	-4	66.86	62.66	66.14	9.79
4	6	-4	58.39	56.52	57.61	9.50
-4	6	4	39.82	35.73	38.43	10.44
4	6	4	44.07	41.56	42.94	9.90
-4	6	-6	4.52	14.16	3.77	2.49
4	6	-6	20.48	17.84	20.48	0.09
-4	6	6	17.36	16.23	17.35	-0.66
4	6	6	35.65	33.77	34.82	7.64
-4	6	-8	6.80	3.63	-6.18	-2.84
4	6	-8	17.13	17.55	-17.05	-1.70
-4	6	8	14.30	15.26	-14.20	-1.73
4	6	8	12.38	11.42	-12.17	-2.26
-4	6	-10	7.70	6.25	-7.69	-0.43
4	6	-10	34.97	36.09	34.37	6.45
-4	6	10	21.88	22.17	20.54	7.55
6	6	0	40.36	37.72	39.26	9.38
6	6	2	12.65	11.10	12.63	-0.74
6	6	-2	31.27	27.89	30.03	8.72
-6	6	-4	9.39	8.17	-9.12	-2.22
6	6	-4	24.33	24.15	-24.29	-1.45
-6	6	4	26.57	24.62	-26.47	-2.27
6	6	4	23.79	22.01	-23.73	-1.75
-6	6	-6	30.49	26.26	29.25	8.62
6	6	-6	11.02	10.27	11.01	-0.53
-6	6	6	0.	3.88	0.	-0.
6	6	6	11.08	10.62	7.68	7.98
-6	6	-8	73.21	72.70	72.66	8.95
6	6	-8	34.04	30.59	32.81	9.08
-6	6	8	27.54	23.66	25.33	10.80
-6	6	-10	12.91	12.80	-12.91	-0.03
-6	6	10	42.67	41.87	42.02	7.43
-8	6	0	29.42	26.97	28.74	6.27
8	6	0	8.13	8.29	-5.72	5.78
8	6	2	35.84	36.53	34.60	9.35
-8	6	-2	63.62	64.59	62.80	10.18
8	6	-2	9.27	8.67	8.89	-2.63
-8	6	-4	0.	2.06	0.	0.
8	6	-4	2.50	1.36	-1.33	2.12
-8	6	4	9.23	6.66	8.94	2.30
8	6	4	2.59	1.14	-0.96	2.41
-8	6	-6	6.21	4.65	-5.03	-3.64
8	6	-6	31.67	30.29	30.20	9.55
-8	6	6	61.24	60.70	60.35	10.38
-8	6	-8	45.98	42.49	45.62	5.78
-8	6	8	12.97	13.43	11.82	5.34
-8	6	-10	19.87	17.91	16.99	10.30
-8	6	10	6.47	5.13	-5.32	-3.69
-10	6	0	27.70	30.87	-27.55	-2.91
-10	6	2	14.44	15.54	14.01	3.50
-10	6	-2	38.50	36.60	38.32	3.72
-10	6	-4	48.18	43.98	46.84	11.27

-10	6	4	60.76	58.98	59.78	10.87
-10	6	-6	13.15	12.52	12.58	3.83
-10	6	6	37.92	34.51	37.73	3.81
-10	6	-8	25.48	21.54	-25.26	-3.36
-10	6	8	26.67	26.72	-26.47	-3.22
-10	6	10	18.04	17.86	17.68	3.57
-12	6	0	23.74	22.00	22.92	6.20
-12	6	2	48.20	46.56	47.07	10.37
-12	6	-2	6.30	2.88	-1.75	-6.05
-12	6	-4	13.80	12.41	-13.71	1.58
-12	6	4	12.86	11.33	-12.76	1.57
-12	6	-6	34.39	29.39	32.55	11.10
-12	6	6	12.25	9.25	-11.65	-3.79
-12	6	8	25.44	24.61	24.78	5.75
-14	6	0	16.33	14.75	13.11	9.73
-14	6	2	12.43	11.67	12.42	-0.48
-14	6	-2	21.67	27.80	20.90	5.71
-14	6	-4	13.62	13.16	-13.50	-1.78
-14	6	4	2.62	6.02	-2.49	-0.81
-14	6	6	23.97	22.37	22.66	7.83

Appendix III

Comparison of observed and calculated structure factors of rhodonite.

H	K	L	FOBS	FCAL	AOBS	BOBS
0	1	0	6.19	3.45	10.63	1.99
1	0	0	6.14	4.93	-10.34	-2.84
2	0	0	23.43	18.89	-40.91	1.64
3	0	0	17.43	12.79	30.24	3.64
4	0	0	39.79	35.42	69.49	2.22
5	0	0	63.53	57.06	-108.93	-21.36
6	0	0	22.33	13.34	-35.72	15.71
7	0	0	9.10	1.96	-15.61	3.04
8	0	0	10.82	7.06	-18.84	-1.59
9	0	0	10.39	8.57	-18.15	-0.13
1	-1	0	22.35	19.77	38.33	7.46
1	1	0	43.59	2.42	-74.52	-15.74
2	-1	0	22.30	20.87	-38.96	-0.55
2	1	0	28.79	25.77	-50.19	-3.46
3	-1	0	36.25	35.46	-63.33	-1.24
3	1	0	46.85	44.28	-81.68	-5.53
4	-1	0	27.59	24.40	-47.92	-5.23
4	1	0	12.94	12.63	22.60	-0.54
5	-1	0	14.83	11.85	-24.16	-9.38
5	1	0	23.26	19.06	40.55	2.68
6	-1	0	9.98	7.63	4.89	-16.74
6	1	0	5.15	5.40	-7.44	5.06
7	-1	0	10.91	8.93	-18.91	2.44
7	1	0	31.69	26.67	54.57	9.37
8	-1	0	8.08	6.42	13.78	-3.09
8	1	0	18.61	12.99	29.59	13.48
9	-1	0	6.30	4.56	10.63	2.85
0	2	0	8.20	7.02	-14.31	-0.72
1	-2	0	3.52	1.24	-2.45	-5.64
1	2	0	0.	0.87	0.	-0.
2	-2	0	40.83	43.76	-71.23	-4.01
2	2	0	138.28	159.67	-240.61	-22.13
3	-2	0	76.55	83.40	132.35	19.35
3	2	0	22.44	20.57	38.77	5.88
4	-2	0	7.45	5.13	9.85	-8.52
4	2	0	12.08	10.20	20.93	-2.72
5	-2	0	5.06	5.68	-8.76	-1.17
5	2	0	13.42	11.86	-23.25	-3.05

6	-2	0	13.03	11.48	22.71	1.64
6	2	0	25.22	23.05	-44.07	0.26
7	-2	0	19.99	18.11	34.87	1.99
7	2	0	40.23	31.33	67.32	20.24
8	-2	0	27.53	25.19	-46.48	-12.39
8	2	0	12.72	11.93	18.50	-12.32
9	-2	0	7.55	8.15	-7.88	10.58
0	3	0	3.26	1.30	4.68	3.25
1	-3	0	20.31	21.68	35.49	0.47
1	3	0	17.62	19.45	-29.99	-6.95
2	-3	0	47.41	51.31	82.78	3.28
2	3	0	0.	8.19	0.	0.
3	-3	0	27.97	30.14	48.57	5.40
3	3	0	17.99	12.00	31.23	3.57
4	-3	0	42.76	44.99	73.18	15.06
4	3	0	14.82	12.42	25.40	5.06
5	-3	0	8.70	9.28	-15.05	-2.17
5	3	0	6.91	4.74	-10.69	5.62
6	-3	0	9.70	9.99	16.75	2.62
6	3	0	0.	0.92	0.	0.
7	-3	0	4.25	3.84	7.25	-1.60
7	3	0	25.07	19.54	-43.60	-4.24
8	-3	0	23.02	22.46	-39.91	-5.00
8	3	0	9.05	6.30	-13.80	-7.72
9	-3	0	29.42	23.99	-49.24	-14.76
0	4	0	9.74	7.82	15.16	7.73
1	-4	0	100.20	135.88	-174.40	-15.50
1	4	0	6.85	5.11	11.91	1.15
2	-4	0	18.00	18.73	31.41	1.57
2	4	0	28.13	22.85	49.15	0.47
3	-4	0	8.26	8.52	-14.37	1.37
3	4	0	13.32	12.72	22.88	4.26
4	-4	0	17.89	17.70	-31.22	-1.53
4	4	0	54.84	51.28	92.85	23.69
5	-4	0	41.17	43.89	-71.86	-3.32
5	4	0	8.84	7.03	12.15	-9.54
6	-4	0	37.13	38.75	63.79	11.86
6	4	0	18.31	13.82	31.70	4.31
7	-4	0	14.43	15.54	23.74	-8.49
7	4	0	22.44	18.72	39.13	2.50
8	-4	0	9.98	10.41	-16.33	-6.13
8	4	0	9.07	8.47	15.72	-2.04
9	-4	0	17.12	15.84	-29.69	-3.65
0	5	0	14.18	14.04	-24.66	-2.44
1	-5	0	15.10	14.30	-26.19	-3.21
1	5	0	6.78	5.88	-11.85	-0.11
2	-5	0	78.03	96.96	-135.58	-14.42
2	5	0	4.49	4.30	7.67	-1.67
3	-5	0	24.44	26.62	42.66	1.97
3	5	0	24.25	22.38	41.44	8.84
4	-5	0	3.06	1.51	2.09	-4.92
4	5	0	52.95	48.82	-92.41	-4.48
5	-5	0	3.48	2.83	-6.00	0.99
5	5	0	17.09	15.16	-29.64	-3.67
6	-5	0	21.02	23.47	36.57	3.39

6	5	0	5.04	3.86	-6.49	-5.95
7	-5	0	25.49	28.43	42.08	14.59
7	5	0	13.72	13.86	23.82	-2.67
8	-5	0	3.50	3.93	-0.31	-6.11
9	-5	0	3.35	4.04	-5.06	2.94
0	6	0	8.10	6.46	-13.82	3.07
1	-6	0	18.16	15.71	-31.72	-1.02
1	6	0	119.33	130.60	207.78	17.42
2	-6	0	10.26	9.96	-17.87	1.38
2	6	0	9.25	7.31	-13.27	-9.23
3	-6	0	40.51	43.89	70.64	4.52
3	6	0	5.94	1.93	10.31	1.20
4	-6	0	42.75	50.18	-73.98	-10.37
4	6	0	6.28	0.36	2.19	-10.75
5	-6	0	4.44	5.10	5.81	5.14
5	6	0	21.70	17.96	-37.21	-7.30
6	-6	0	9.62	10.62	15.58	6.31
6	6	0	30.61	24.76	-49.00	-21.44
7	6	0	5.66	4.90	-0.62	9.87
7	-6	0	0.	2.11	0.	0.
8	-6	0	0.	7.27	-0.	0.
9	-6	0	12.38	12.24	19.96	8.33
0	7	0	57.39	63.30	98.86	16.81
1	-7	0	3.32	0.84	-0.66	-5.76
1	7	0	9.46	8.59	-16.53	-0.36
2	-7	0	8.10	7.57	-14.02	1.91
2	7	0	18.96	16.21	33.08	1.82
3	-7	0	4.41	6.29	-7.70	-0.29
3	7	0	4.47	1.53	7.81	-0.28
4	-7	0	5.52	7.67	9.56	-1.26
4	7	0	7.14	7.76	12.41	1.29
5	-7	0	11.23	16.50	-14.33	-13.41
5	7	0	20.66	19.22	-35.09	-8.49
6	-7	0	6.70	8.30	-10.81	4.49
6	7	0	32.21	28.72	55.82	7.18
7	-7	0	14.93	17.39	-25.94	-2.73
8	-7	0	0.	2.56	-0.	-0.
9	-7	0	15.97	17.57	27.90	0.24
0	8	0	14.81	12.02	25.84	-1.33
1	-8	0	28.17	24.84	-48.82	-6.29
1	8	0	13.57	14.01	-23.71	-0.12
2	-8	0	30.10	29.73	51.45	10.93
2	8	0	37.58	36.84	-65.42	-5.72
3	-8	0	13.64	14.22	-23.73	-2.25
3	8	0	59.59	57.04	-102.83	-16.37
4	-8	0	6.00	4.27	5.05	-9.19
4	8	0	22.06	19.64	37.64	8.30
5	8	0	3.33	3.31	-5.65	-1.39
5	-8	0	0.	2.16	-0.	-0.
6	8	0	6.81	8.19	-11.86	0.95
6	-8	0	0.	1.89	-0.	-0.
7	-8	0	24.53	29.03	-42.34	-6.64
8	-8	0	0.	1.93	-0.	0.
9	-8	0	17.79	20.67	30.56	5.67
0	9	0	15.75	15.12	27.50	-1.06

1	-9	0	36.10	31.86	63.08	0.49
1	9	0	3.77	3.41	-6.57	0.44
2	-9	0	4.93	4.20	-8.55	-1.03
2	9	0	38.89	38.17	-65.56	-17.88
3	-9	0	29.34	28.28	46.13	22.37
3	9	0	26.57	26.33	46.28	3.65
4	9	0	4.07	0.90	-5.01	-5.05
4	-9	0	0.	3.76	-0.	-0.
5	-9	0	18.93	20.01	32.99	2.39
5	9	0	4.23	0.81	-7.31	1.06
6	-9	0	0.	5.03	-0.	0.
7	-9	0	11.97	13.75	-20.86	1.47
8	-9	0	18.64	21.70	-30.19	-12.23
0	10	0	24.69	23.59	-42.20	-8.98
1	-10	0	6.76	5.51	11.77	-1.04
1	10	0	5.27	7.10	-8.30	3.99
2	-10	0	16.25	13.42	-27.67	6.35
2	10	0	12.95	11.93	-22.61	0.99
3	-10	0	13.18	11.34	22.73	3.71
3	10	0	11.91	10.83	20.76	1.42
4	-10	0	11.08	10.42	19.16	2.77
4	10	0	32.13	29.65	55.57	7.98
5	-10	0	28.98	30.55	50.24	6.35
6	-10	0	6.59	7.91	11.48	-0.92
7	-10	0	3.99	5.14	4.57	-5.27
8	-10	0	9.13	10.22	-15.34	-4.38
0	11	0	15.13	13.21	26.12	4.06
1	-11	0	67.91	57.45	-115.92	-25.36
1	11	0	23.65	21.61	-41.31	-0.93
2	-11	0	7.59	4.26	13.19	1.34
2	11	0	3.95	2.58	-6.87	0.62
3	11	0	13.32	11.43	23.26	0.90
3	-11	0	0.	1.94	-0.	-0.
4	-11	0	6.89	4.52	-11.34	-4.03
4	11	0	36.08	38.16	61.40	14.31
5	-11	0	11.21	9.20	-18.99	-4.81
6	-11	0	19.69	18.50	29.67	17.41
7	-11	0	11.65	14.00	-18.91	-7.54
8	-11	0	7.48	8.06	-12.90	-2.10
0	12	0	6.12	6.01	-10.10	-3.53
1	-12	0	25.05	17.78	-43.66	-3.10
1	12	0	12.88	11.59	22.23	3.51
2	-12	0	10.09	6.65	17.12	-4.22
2	12	0	22.81	21.15	39.32	6.50
3	-12	0	7.96	5.61	-11.95	-7.11
3	12	0	5.13	5.27	-7.81	-4.40
4	-12	0	3.68	0.83	5.46	-3.40
5	-12	0	18.45	16.56	-31.49	6.92
6	-12	0	8.73	9.33	14.58	4.50
7	-12	0	11.67	11.71	18.54	8.48
0	13	0	0.	1.08	0.	0.
1	-13	0	10.06	6.99	-17.49	1.80
1	13	0	46.03	45.90	78.03	19.48
2	-13	0	0.	2.54	-0.	0.
3	-13	0	24.05	19.95	41.39	7.27

4	-13	0	18.01	15.36	-24.41	-19.87
5	-13	0	7.54	6.91	-11.61	6.23
6	-13	0	0.	2.22	-0.	0.
0	14	0	0.	2.30	0.	0.
1	-14	0	4.66	2.76	-6.06	5.44
2	-14	0	11.53	8.86	19.97	2.69
3	-14	0	15.98	14.04	27.31	-5.80
4	-14	0	14.95	12.59	-25.70	-4.68
5	-14	0	19.58	17.49	-32.41	-10.96
1	0	1	0.	1.76	-0.	-0.
-1	0	1	0.	2.87	-0.	-0.
2	0	1	12.06	10.97	-20.77	-3.54
-2	0	1	44.19	42.63	77.15	-3.14
3	0	1	8.34	6.56	-14.45	-1.85
-3	0	1	9.70	8.83	-16.74	-2.64
4	0	1	35.14	31.18	-61.32	-3.11
-4	0	1	42.02	40.30	-73.15	-6.27
5	0	1	22.02	21.79	-38.08	-5.53
-5	0	1	46.76	42.69	-79.38	-19.37
6	0	1	15.28	13.50	26.29	4.63
-6	0	1	22.69	22.48	39.36	4.79
7	0	1	34.30	34.10	59.54	6.83
-7	0	1	24.25	22.34	-42.36	-1.01
8	0	1	9.81	6.85	14.96	8.37
-8	0	1	3.86	0.71	-6.72	0.58
9	0	1	0.	4.72	0.	0.
-9	0	1	0.	3.79	0.	0.
0	1	1	3.64	2.85	6.10	1.81
0	-1	1	0.	0.98	-0.	0.
1	-1	1	39.69	44.87	65.73	22.11
-1	-1	1	9.95	9.73	17.39	0.01
1	1	1	0.	8.34	0.	-0.
-1	1	1	0.	3.20	-0.	-0.
2	-1	1	5.01	5.34	-7.40	-4.67
2	1	1	22.29	20.35	-38.60	-5.19
-2	-1	1	14.36	11.87	25.09	-0.33
-2	1	1	33.77	38.58	56.75	16.17
3	-1	1	43.69	39.37	76.17	5.07
3	1	1	96.73	97.18	-167.56	-22.17
-3	-1	1	22.25	19.45	38.56	4.99
-3	1	1	2.95	4.62	-5.05	-1.06
4	-1	1	14.34	12.88	24.77	3.78
4	1	1	6.79	8.67	10.62	5.28
-4	-1	1	59.95	60.81	-103.22	-17.87
-4	1	1	0.	1.00	-0.	-0.
5	-1	1	45.11	38.94	-78.81	-1.49
5	1	1	28.44	25.88	-49.32	-6.12
-5	-1	1	27.98	26.64	48.55	5.74
-5	1	1	0.	4.51	-0.	-0.
6	-1	1	23.14	20.57	-35.58	-19.21
-6	-1	1	21.99	20.78	38.36	2.15
6	1	1	0.	3.09	0.	-0.
-6	1	1	0.	3.53	-0.	0.
7	-1	1	50.69	51.92	87.82	11.50
7	1	1	13.98	15.15	24.27	2.77

-7	1	1	7.31	7.27	-9.09	-8.98
-7	-1	1	0.	0.92	0.	0.
8	-1	1	13.98	13.23	-24.31	-2.40
8	1	1	17.38	17.05	27.45	12.99
-8	-1	1	8.01	7.15	-13.77	-2.50
-8	1	1	41.85	38.31	72.58	8.92
9	-1	1	6.38	5.51	-11.09	-1.16
-9	1	1	15.08	14.42	25.60	6.25
0	-2	1	10.07	2.67	-15.89	7.56
0	2	1	9.13	11.72	15.77	2.41
1	-2	1	7.16	5.97	12.49	0.64
1	2	1	3.21	4.89	5.31	1.81
-1	2	1	23.58	25.98	-41.16	1.80
-1	-2	1	0.	6.86	0.	-0.
2	-2	1	54.13	52.83	94.54	2.95
2	2	1	37.04	39.36	-63.68	-11.57
-2	-2	1	17.01	16.27	-27.91	-10.23
-2	2	1	0.	3.06	0.	0.
3	-2	1	19.06	18.27	32.99	4.58
3	2	1	3.43	4.15	4.54	3.92
-3	-2	1	12.24	11.46	21.06	3.71
-3	2	1	24.00	24.25	36.58	20.50
4	-2	1	13.12	10.12	-22.78	-2.55
4	2	1	12.04	10.72	20.62	4.18
-4	-2	1	38.83	34.86	-67.77	3.22
-4	2	1	16.86	15.71	-29.16	-4.16
5	-2	1	30.97	27.78	-53.56	-7.71
5	2	1	9.89	9.01	17.14	2.19
-5	-2	1	13.40	11.61	23.16	3.43
-5	2	1	24.38	22.41	42.60	0.15
6	-2	1	17.81	14.40	-30.14	-7.76
6	2	1	37.25	37.28	65.03	2.79
-6	-2	1	26.03	22.20	44.55	9.16
-6	2	1	0.	0.74	-0.	0.
7	-2	1	52.21	45.52	-90.62	-10.53
7	2	1	19.08	18.00	32.76	6.20
-7	-2	1	47.01	39.26	80.51	16.31
-7	2	1	9.86	8.54	16.85	-3.58
8	2	1	4.30	3.76	-3.26	-6.77
-8	-2	1	33.86	33.56	-58.97	-4.84
-8	2	1	43.40	39.40	-73.60	-18.28
8	-2	1	0.	1.91	-0.	-0.
9	-2	1	8.53	8.98	-14.83	-1.50
-9	2	1	34.82	35.94	60.28	8.22
0	-3	1	11.21	10.79	-19.42	2.55
0	3	1	22.11	20.95	34.09	-18.17
1	-3	1	26.56	27.34	-46.30	-3.15
1	3	1	26.84	26.39	46.50	6.09
-1	-3	1	15.84	20.81	-19.69	-19.45
-1	3	1	17.72	17.94	-30.89	-2.11
2	-3	1	41.84	35.49	-72.97	-4.58
2	3	1	10.66	10.09	18.45	-2.53
-2	-3	1	16.41	14.82	28.60	2.12
-2	3	1	6.01	5.63	-10.48	0.60
3	-3	1	14.56	13.24	25.41	-1.25

3	3	1	5.17	4.71	-8.92	1.46
-3	-3	1	18.62	15.63	-32.54	-0.10
-3	3	1	0.	2.19	-0.	0.
4	-3	1	48.75	44.15	82.15	22.54
4	3	1	27.48	27.91	47.54	6.73
-4	-3	1	16.23	14.93	-28.35	-0.75
-4	3	1	21.17	18.63	36.76	-4.16
5	-3	1	51.30	46.70	-89.03	-10.45
5	3	1	79.80	55.55	137.02	25.87
-5	-3	1	10.99	12.18	19.05	-2.44
-5	3	1	20.06	21.01	34.04	8.34
6	3	1	37.70	38.79	-65.47	-7.26
-6	-3	1	54.09	47.83	92.72	18.33
-6	3	1	46.02	41.35	-80.15	-6.49
6	-3	1	0.	3.09	0.	0.
7	-3	1	8.05	6.99	13.79	2.76
7	3	1	12.34	10.68	20.43	6.90
-7	-3	1	34.96	29.85	-60.27	-9.98
-7	3	1	23.65	22.00	-40.76	-6.80
8	3	1	3.99	4.68	-6.94	0.65
-8	-3	1	6.58	7.74	-11.40	-1.47
-8	3	1	12.29	11.31	-20.52	-6.34
8	-3	1	0.	4.87	-0.	-0.
9	-3	1	19.13	19.91	-31.72	-10.55
-9	3	1	25.10	24.28	-43.76	-2.98
0	-4	1	14.46	14.65	-25.07	-3.14
0	4	1	0.	1.53	-0.	0.
1	-4	1	14.76	13.49	25.60	-3.13
1	4	1	5.51	4.45	-9.34	-2.32
-1	-4	1	8.52	9.12	-14.87	0.71
-1	4	1	60.79	81.19	-104.93	-16.50
2	-4	1	7.17	4.18	-12.53	-0.06
2	4	1	25.68	25.45	-44.77	-2.95
-2	-4	1	9.38	7.61	16.38	-0.51
-2	4	1	15.37	15.83	-26.77	2.20
3	-4	1	18.99	18.16	32.55	6.47
-3	-4	1	10.98	9.53	18.40	5.42
-3	4	1	5.27	4.68	-9.17	0.84
3	4	1	0.	1.73	-0.	-0.
4	-4	1	24.90	22.11	43.01	6.60
4	4	1	28.47	29.63	48.43	11.36
-4	-4	1	4.67	4.27	0.98	8.10
-4	4	1	0.	1.87	-0.	0.
5	-4	1	102.44	101.25	178.63	11.40
-5	-4	1	34.29	31.84	-59.84	-3.11
-5	4	1	12.80	12.06	-22.34	0.97
5	4	1	0.	4.52	-0.	-0.
6	-4	1	8.33	8.71	14.47	1.53
6	4	1	12.49	13.52	-21.60	-3.15
-6	-4	1	10.41	10.38	17.97	-2.84
-6	4	1	74.97	72.72	129.26	21.29
7	4	1	15.17	14.89	-26.41	-2.29
-7	-4	1	30.04	7.49	-50.66	-13.75
-7	4	1	28.70	29.47	-49.70	-6.72
7	-4	1	0.	2.93	-0.	0.

8	-4	1	8.34	7.92	-14.04	-3.92
-8	-4	1	17.72	14.70	-29.33	-9.91
-8	4	1	11.42	10.35	19.92	1.09
8	4	1	0.	17.69	-0.	-0.
9	-4	1	6.56	7.38	10.82	-3.79
-9	4	1	12.41	11.68	21.58	2.18
0	-5	1	4.73	4.12	-7.18	4.10
0	5	1	0.	3.17	0.	0.
1	-5	1	14.51	14.17	25.06	3.87
1	5	1	27.32	32.92	47.54	4.29
-1	-5	1	10.26	1.26	-7.91	16.09
-1	5	1	12.37	11.56	21.59	-1.05
2	-5	1	83.58	85.43	-144.44	-21.54
2	5	1	7.50	11.31	8.78	9.73
-2	-5	1	19.19	15.73	33.53	0.39
-2	5	1	9.26	10.16	15.86	3.23
3	-5	1	7.84	7.92	12.35	5.92
3	5	1	11.15	12.55	-18.83	-4.99
-3	-5	1	45.38	40.45	74.66	26.71
-3	5	1	17.98	16.97	-30.32	-8.21
4	-5	1	11.39	10.24	19.90	-0.36
4	5	1	22.24	22.42	38.75	2.88
-4	-5	1	9.34	9.00	-15.43	-5.33
-4	5	1	0.	2.43	0.	0.
5	5	1	2.50	6.98	-4.29	-0.82
-5	5	1	24.73	21.57	42.70	6.61
5	-5	1	0.	2.26	0.	-0.
-5	-5	1	0.	0.35	-0.	0.
6	-5	1	8.28	9.26	14.43	-0.99
6	5	1	21.96	21.46	-37.57	-7.79
-6	-5	1	6.23	3.70	-10.69	2.05
-6	5	1	25.11	22.75	43.38	6.56
7	-5	1	13.49	12.87	18.96	14.00
7	5	1	22.99	20.57	-37.41	-14.64
-7	-5	1	9.19	6.76	-16.00	1.32
-7	5	1	6.13	7.79	10.26	3.09
8	-5	1	51.02	45.13	-88.01	-14.18
-8	5	1	8.27	7.59	13.67	4.70
9	-5	1	6.64	6.36	-10.76	-4.33
-9	5	1	13.89	11.64	-24.00	-3.59
0	-6	1	14.09	13.26	24.56	1.65
0	6	1	4.41	3.57	-7.70	-0.28
1	-6	1	2.18	2.84	0.90	-3.70
1	6	1	67.43	85.93	116.63	16.72
-1	-6	1	20.68	20.34	-36.11	1.28
-1	6	1	9.06	7.92	15.75	-1.62
2	-6	1	29.99	27.42	-52.17	-4.89
-2	-6	1	11.38	7.63	19.16	5.30
-2	6	1	32.95	35.35	57.57	-0.79
2	6	1	0.	4.99	0.	-0.
3	-6	1	83.09	80.62	-144.57	-13.37
3	6	1	8.42	9.68	-14.60	1.85
-3	-6	1	52.11	45.95	91.02	-2.61
-3	6	1	0.	3.40	0.	0.
4	-6	1	0.	1.32	0.	-0.

4	6	1	5.08	6.14	-8.65	2.00
-4	6	1	61.11	69.18	-104.80	-20.46
-4	-6	1	0.	3.05	0.	-0.
5	-6	1	14.73	13.29	-25.35	-4.48
5	6	1	6.71	8.60	-11.72	0.14
-5	-6	1	17.12	14.40	-29.05	-7.14
-5	6	1	11.76	13.02	20.20	3.76
6	-6	1	5.94	6.44	9.98	2.86
6	6	1	21.18	21.42	-35.60	-10.12
-6	-6	1	8.90	5.85	-13.61	-7.52
-6	6	1	6.73	6.16	11.76	-0.30
7	-6	1	8.75	5.87	-13.87	6.44
7	6	1	5.14	5.89	2.17	8.72
-7	-6	1	15.45	14.63	26.92	2.04
-7	6	1	0.	2.46	-0.	-0.
8	-6	1	22.68	16.52	36.35	15.78
-8	6	1	31.12	31.48	-54.31	-2.65
9	-6	1	4.61	3.48	5.69	-5.70
-9	6	1	18.82	19.82	30.11	13.21
0	-7	1	41.62	44.62	69.90	20.08
0	7	1	16.89	18.19	-29.39	-2.63
1	7	1	7.66	7.95	-13.38	0.35
-1	-7	1	39.79	37.86	-69.23	-6.38
-1	7	1	16.19	18.15	-27.74	5.56
1	-7	1	0.	1.08	0.	-0.
2	-7	1	10.66	10.44	18.62	-0.29
2	7	1	9.08	11.37	15.74	-1.99
-2	-7	1	22.46	20.28	-39.14	-2.89
-2	7	1	8.84	7.37	15.43	-0.70
3	-7	1	25.59	22.44	44.50	4.32
-3	-7	1	3.09	2.02	-5.16	-1.60
-3	7	1	26.60	28.41	-46.29	-4.16
3	7	1	0.	4.40	-0.	-0.
4	-7	1	12.93	11.27	-22.26	3.88
4	7	1	32.34	33.91	-55.45	-10.89
-4	-7	1	12.04	9.60	-20.75	-3.47
-4	7	1	28.97	30.48	-50.38	-4.95
5	-7	1	9.33	10.55	-9.99	-12.88
5	7	1	10.28	10.15	17.34	4.67
-5	-7	1	54.96	49.55	-93.39	-22.36
-5	7	1	15.49	14.17	-26.49	-5.55
6	-7	1	48.41	44.14	83.91	10.72
6	7	1	10.49	10.48	-18.11	-2.81
-6	-7	1	9.67	9.84	15.25	7.27
-6	7	1	10.65	9.13	18.17	-4.04
7	-7	1	28.17	23.78	48.76	6.73
-7	7	1	10.42	14.58	18.16	1.25
-8	7	1	7.89	6.90	12.37	6.08
8	-7	1	0.	1.14	0.	0.
9	-7	1	14.14	11.79	24.30	4.46
-9	7	1	6.73	6.56	9.89	6.37
0	-8	1	28.80	27.94	50.27	2.34
0	8	1	41.56	46.73	-72.60	1.73
1	-8	1	39.22	40.52	67.19	13.49
-1	-8	1	6.96	4.90	11.26	4.61

-1	8	1	6.43	6.46	-10.29	-4.51
1	8	1	0.	2.06	-0.	0.
2	-8	1	6.91	4.04	-12.07	0.24
2	8	1	13.12	13.84	22.86	-1.69
-2	-8	1	10.70	10.42	18.53	-2.47
-2	8	1	57.85	65.52	98.92	20.82
3	-8	1	21.30	17.81	36.85	5.23
3	8	1	45.07	48.25	-76.78	-17.50
-3	-8	1	9.06	8.10	15.83	0.06
-3	8	1	16.24	15.94	28.37	-0.81
4	-8	1	13.70	13.46	-23.83	-2.25
4	8	1	10.49	12.39	-17.21	6.30
-4	-8	1	5.51	5.08	8.68	-4.17
-4	8	1	4.66	3.33	-8.14	-0.27
5	-8	1	21.84	17.91	-37.92	-4.26
5	8	1	5.09	4.04	-8.27	-3.28
-5	-8	1	16.78	15.69	-29.03	4.10
-5	8	1	22.80	21.76	39.79	1.93
6	-8	1	66.90	60.79	-115.76	-16.24
-6	8	1	29.63	36.30	51.61	4.06
6	8	1	0.	4.91	0.	-0.
-6	-8	1	0.	1.64	0.	0.
7	-8	1	21.29	17.50	36.85	5.08
-7	8	1	41.92	39.89	-71.24	-17.02
8	-8	1	19.30	15.25	-33.07	-6.59
-8	8	1	25.85	25.08	44.10	9.78
9	-8	1	0.	13.02	-0.	0.
-9	8	1	0.	3.43	-0.	0.
0	-9	1	3.53	5.97	-6.16	0.24
0	9	1	0.	13.77	-0.	-0.
1	-9	1	34.98	34.46	-61.01	-3.65
1	9	1	10.65	11.35	18.11	-4.28
-1	-9	1	2.73	1.79	3.65	-3.07
-1	9	1	15.80	17.34	27.50	2.49
2	9	1	14.47	16.87	25.24	1.51
-2	-9	1	16.62	15.54	-20.65	-20.41
2	-9	1	0.	3.45	-0.	-0.
-2	9	1	0.	4.30	0.	0.
3	-9	1	42.91	35.72	72.99	17.16
3	9	1	8.08	8.11	14.11	0.58
-3	-9	1	18.26	17.24	30.90	7.96
-3	9	1	31.69	33.98	55.08	5.71
4	-9	1	25.35	22.31	-43.76	-6.86
-4	-9	1	10.42	8.70	18.14	1.57
-4	9	1	7.55	6.78	-12.91	2.73
4	9	1	0.	3.68	0.	0.
5	-9	1	37.92	33.75	-65.86	-7.26
5	9	1	6.05	6.75	8.20	6.67
-5	9	1	16.75	16.61	-29.26	-0.68
-5	-9	1	0.	1.92	0.	0.
-6	9	1	17.67	20.58	-30.59	-4.22
6	-9	1	0.	4.67	0.	-0.
7	-9	1	14.73	11.98	-25.53	-3.29
-7	9	1	3.55	11.83	-5.94	-1.79
8	-9	1	20.13	16.79	-32.61	-13.18

-8	9	1	39.35	38.87	-67.94	-10.55
0	-10	1	11.94	13.14	-20.86	0.21
0	10	1	46.00	50.85	-77.92	-19.74
1	-10	1	25.44	25.85	-44.27	-3.99
1	10	1	6.19	6.93	9.04	5.94
-1	-10	1	18.47	18.53	-29.15	-13.86
-1	10	1	10.77	11.91	-18.68	-2.28
2	-10	1	6.19	4.08	10.62	2.03
2	10	1	13.66	14.66	23.69	-2.90
-2	-10	1	20.17	19.82	-35.24	0.36
-2	10	1	7.33	6.97	12.81	0.25
3	-10	1	20.74	18.35	36.18	2.08
-3	-10	1	9.10	8.29	-15.77	-2.00
-3	10	1	22.09	23.00	-38.59	-0.88
3	10	1	0.	2.14	0.	-0.
4	-10	1	68.87	84.81	119.53	13.96
-4	10	1	30.27	31.80	-52.47	-6.67
4	10	1	0.	2.84	0.	0.
-4	-10	1	0.	4.15	-0.	0.
5	-10	1	26.97	21.93	-46.94	-4.21
-5	10	1	51.64	50.77	88.56	17.31
6	-10	1	8.13	6.39	12.53	6.70
-6	10	1	10.24	14.89	-17.40	-4.17
7	-10	1	13.58	10.83	23.69	1.27
-7	10	1	14.50	16.77	-25.03	-3.94
8	-10	1	23.37	18.14	40.83	-0.70
-8	10	1	0.	2.36	-0.	-0.
0	-11	1	18.26	17.63	31.19	6.73
0	11	1	0.	4.01	0.	-0.
1	-11	1	31.23	28.36	-52.77	-13.88
1	11	1	5.68	6.94	-9.88	-0.90
-1	-11	1	24.56	22.58	42.79	3.24
-1	11	1	30.09	31.98	-52.18	-6.42
2	-11	1	13.46	13.31	23.43	2.09
2	11	1	0.	4.62	-0.	0.
-2	-11	1	0.	2.46	0.	-0.
-2	11	1	0.	0.92	-0.	-0.
3	-11	1	40.99	38.95	71.32	6.62
3	11	1	6.05	7.55	-10.29	2.43
-3	11	1	9.47	7.97	-16.55	-0.11
-3	-11	1	0.	3.30	0.	0.
-4	-11	1	11.35	10.37	10.66	16.72
-4	11	1	22.34	26.83	38.88	3.48
4	-11	1	0.	3.09	0.	0.
4	11	1	0.	5.62	-0.	-0.
5	-11	1	0.	0.95	0.	0.
-5	11	1	17.36	17.80	29.98	4.61
6	-11	1	8.98	7.86	9.94	12.14
-6	11	1	24.28	27.40	40.88	11.33
7	-11	1	8.80	8.19	-14.85	-3.99
-7	11	1	0.	0.69	0.	0.
8	-11	1	0.	22.58	-0.	-0.
0	-12	1	6.53	5.42	11.38	-0.87
0	12	1	9.77	11.28	17.07	0.16
1	-12	1	15.44	15.31	-26.98	0.36

1	12	1	6.89	8.02	11.21	4.39
-1	-12	1	5.97	5.11	9.69	3.86
-1	12	1	27.87	29.93	48.70	-0.24
2	-12	1	56.33	57.16	-96.77	-17.99
2	12	1	39.50	43.47	66.98	16.66
-2	12	1	16.55	17.46	27.83	7.88
-2	-12	1	0.	0.17	-0.	-0.
3	-12	1	5.10	4.06	8.51	2.66
-3	-12	1	13.17	14.64	19.91	11.54
-3	12	1	37.75	38.29	-64.00	-15.97
3	12	1	0.	8.46	0.	-0.
4	-12	1	20.61	20.61	-35.70	-4.76
-4	12	1	5.79	5.50	9.85	2.30
5	-12	1	13.13	7.37	-22.65	-3.67
-5	12	1	24.48	24.54	42.55	4.34
6	-12	1	6.39	5.70	-11.10	-1.19
-6	12	1	4.27	10.71	-7.44	0.54
7	-12	1	27.87	25.42	46.49	14.50
-7	12	1	39.35	39.99	-68.65	-3.82
0	-13	1	4.75	4.55	-8.18	1.43
0	13	1	8.68	9.17	-15.14	0.86
1	-13	1	15.84	11.97	-26.79	-6.97
1	13	1	7.90	7.96	11.95	6.91
-1	-13	1	16.39	13.85	26.11	11.76
-1	13	1	0.	2.87	0.	0.
2	-13	1	12.15	10.10	21.21	-1.00
-2	13	1	17.86	18.20	-31.03	-3.30
3	-13	1	4.39	4.71	-7.65	-0.60
-3	13	1	5.41	5.86	-9.12	-2.49
4	-13	1	14.42	13.12	-23.09	-10.08
-4	13	1	23.29	23.64	-38.20	-14.04
5	-13	1	16.70	11.03	29.14	1.44
-5	13	1	0.	6.23	0.	-0.
6	-13	1	35.79	36.66	62.12	7.21
-6	13	1	2.45	7.17	-4.21	-0.78
0	-14	1	0.	22.12	0.	0.
0	14	1	0.	10.92	-0.	-0.
1	-14	1	10.35	11.28	18.08	-0.46
-1	14	1	28.20	26.86	47.04	14.69
2	-14	1	12.60	14.33	21.75	3.42
-2	14	1	5.61	6.78	9.74	1.13
3	-14	1	5.12	2.62	7.42	5.00
-3	14	1	12.05	14.87	-20.88	-2.75
4	-14	1	5.30	4.37	-8.52	3.62
-4	14	1	7.91	11.97	13.77	-1.15
5	-14	1	0.	30.96	-0.	-0.
-5	14	1	0.	14.33	0.	0.
-1	0	2	83.57	87.50	145.41	13.36
1	0	2	0.	2.75	-0.	0.
2	0	2	21.74	18.99	-37.87	-2.98
-2	0	2	10.85	10.34	-18.93	0.98
3	0	2	33.96	31.05	-58.93	-6.99
-3	0	2	11.05	9.88	19.30	0.47
4	0	2	68.71	62.59	-118.53	-19.08
-4	0	2	0.	2.12	0.	-0.

5	0	2	12.16	12.24	20.63	5.08
-5	0	2	46.59	40.93	81.38	2.03
6	0	2	13.77	14.16	-22.83	-7.58
-6	0	2	15.46	14.03	-26.51	-5.20
7	0	2	10.86	9.51	-18.98	0.17
-7	0	2	20.60	16.70	35.24	7.32
8	0	2	8.14	10.18	13.87	3.14
-8	0	2	15.51	14.04	26.58	5.31
-9	0	2	17.95	16.33	30.36	7.89
0	-1	2	33.80	36.65	-58.98	-3.07
0	1	2	37.64	42.30	65.72	2.58
1	-1	2	100.40	108.70	174.86	14.18
1	1	2	22.84	23.58	39.52	5.53
-1	-1	2	65.31	68.74	-113.98	-5.59
-1	1	2	10.88	10.46	18.94	-1.61
2	-1	2	27.48	26.71	-47.68	-5.66
2	1	2	33.37	28.89	58.29	1.53
-2	-1	2	8.18	7.10	-14.08	-2.48
-2	1	2	78.15	81.95	134.69	22.50
3	-1	2	14.84	14.24	-25.71	-3.37
3	1	2	91.04	59.74	-157.47	-22.58
-3	-1	2	16.67	14.04	-29.02	-2.56
-3	1	2	4.99	5.17	8.36	-2.49
4	-1	2	7.05	6.43	12.27	1.07
4	1	2	54.96	55.15	95.59	9.17
-4	-1	2	97.70	95.14	-169.26	-22.26
-4	1	2	41.14	37.98	-71.82	-3.11
5	-1	2	47.55	42.13	83.01	-3.48
-5	-1	2	9.73	6.53	-15.43	7.15
-5	1	2	6.24	4.29	-10.87	-0.82
5	1	2	0.	2.69	0.	0.
6	-1	2	23.75	22.80	-40.40	-9.49
-6	-1	2	20.19	17.02	35.21	2.25
-6	1	2	16.51	14.18	-28.85	0.41
6	1	2	0.	1.81	-0.	-0.
7	-1	2	20.40	18.63	34.64	8.40
7	1	2	10.72	10.10	-18.23	4.33
-7	1	2	55.92	49.27	-95.10	-22.42
-7	-1	2	0.	2.44	0.	-0.
8	-1	2	12.67	13.84	21.44	5.51
8	1	2	10.40	12.18	16.79	6.95
-8	-1	2	15.59	14.11	27.17	1.91
-8	1	2	10.89	8.18	-16.36	9.72
-9	1	2	6.67	7.67	11.64	0.68
0	-2	2	24.89	25.04	43.47	1.29
0	2	2	19.24	20.12	-33.45	-3.35
1	-2	2	37.93	34.62	66.10	4.86
1	2	2	58.46	64.91	-101.52	-11.34
-1	-2	2	26.54	25.31	-46.22	-3.81
-1	2	2	14.00	14.05	24.37	-2.17
2	-2	2	28.53	29.94	45.83	19.61
2	2	2	20.33	18.88	35.40	2.95
-2	-2	2	24.04	22.93	41.79	4.27
-2	2	2	10.58	10.01	18.27	2.80
3	-2	2	23.34	23.56	-40.50	-4.78

3	2	2	4.06	4.04	-5.83	-4.04
-3	-2	2	60.18	54.51	-103.94	-15.95
-3	2	2	53.14	51.22	-92.85	-0.83
4	-2	2	14.99	14.07	24.85	8.27
4	2	2	15.51	15.27	26.82	3.88
-4	-2	2	17.47	15.92	30.44	2.32
-4	2	2	7.24	8.12	12.10	3.69
5	-2	2	6.78	4.80	11.63	2.25
5	2	2	12.59	10.71	20.33	8.40
-5	-2	2	27.02	24.75	-47.20	1.10
-5	2	2	18.14	14.42	-31.21	-5.53
6	-2	2	6.78	6.14	11.27	-3.65
6	2	2	49.55	48.15	85.47	13.79
-6	-2	2	7.10	8.20	12.04	3.01
-6	2	2	5.40	4.50	-7.93	-5.11
7	-2	2	40.70	38.02	-69.75	-13.88
7	2	2	8.07	8.49	13.36	-4.50
-7	-2	2	5.92	3.86	-9.74	-3.47
-7	2	2	26.28	22.79	-45.14	-8.45
8	-2	2	9.79	11.06	13.82	10.08
8	2	2	10.91	10.22	17.56	7.43
-8	2	2	11.99	7.04	-18.87	-9.11
-8	-2	2	0.	13.59	0.	0.
-9	2	2	10.68	10.18	18.65	-0.76
0	3	2	35.36	42.35	-58.64	-19.46
0	-3	2	0.	2.75	0.	0.
1	-3	2	18.53	17.11	32.19	3.53
1	3	2	15.57	16.42	26.75	4.98
-1	-3	2	31.62	33.04	-53.52	-13.71
-1	3	2	7.81	7.74	13.65	-0.12
2	-3	2	17.04	15.12	-29.71	-1.98
2	3	2	35.41	40.74	-61.78	-3.37
-2	-3	2	34.70	30.86	60.39	5.41
-2	3	2	10.57	11.90	18.23	2.98
3	-3	2	55.67	51.24	-97.25	2.07
3	3	2	5.60	5.92	-8.67	-4.54
-3	-3	2	80.26	77.30	140.13	5.61
-3	3	2	10.00	9.79	17.36	2.02
4	-3	2	32.40	31.01	55.82	9.44
4	3	2	22.38	20.96	-39.10	0.78
-4	-3	2	18.19	15.42	31.72	2.07
-4	3	2	3.82	2.97	-5.59	-3.65
5	-3	2	16.57	15.22	-28.40	-5.61
5	3	2	22.23	21.65	36.54	13.19
-5	-3	2	7.58	3.01	2.93	12.92
-5	3	2	77.53	71.40	123.22	24.58
6	-3	2	17.08	15.03	-28.66	-8.33
6	3	2	36.50	36.56	-62.69	-11.72
-6	-3	2	56.72	50.07	96.98	20.41
-6	3	2	8.06	7.39	13.23	-4.84
7	-3	2	12.83	21.82	-22.31	-2.16
7	3	2	8.08	7.99	14.06	-1.25
-7	-3	2	14.69	13.76	24.83	-6.52
-7	3	2	0.	3.57	-0.	-0.
8	-3	2	18.09	15.96	-30.30	-9.01

-8	-3	2	0.	1.57	-0.	-0.
-8	3	2	0.	3.20	-0.	0.
9	-3	2	7.98	8.38	-12.74	-5.66
-9	3	2	0.	4.97	-0.	0.
0	-4	2	73.25	81.77	-126.42	-19.99
0	4	2	10.29	10.22	17.94	-1.21
1	-4	2	8.82	10.38	15.07	3.24
1	4	2	21.78	25.04	37.91	3.31
-1	-4	2	28.11	24.17	-49.08	-1.82
-1	4	2	13.53	15.17	23.64	-0.46
2	-4	2	25.43	23.45	-43.81	-7.44
2	4	2	20.47	20.75	35.40	5.12
-2	-4	2	17.87	15.50	-31.22	-0.31
-2	4	2	10.83	11.63	-18.65	-3.20
3	-4	2	8.95	8.79	15.31	-3.17
3	4	2	30.56	29.10	52.23	11.12
-3	-4	2	15.32	14.26	26.62	2.84
-3	4	2	17.49	18.68	30.45	2.63
4	-4	2	10.83	10.96	18.85	1.72
4	4	2	4.16	3.20	-6.99	-1.98
-4	-4	2	34.08	31.02	-59.40	-4.19
-4	4	2	7.24	6.41	12.14	3.57
5	-4	2	73.69	70.66	127.55	17.61
5	4	2	23.91	22.44	-41.64	3.40
-5	-4	2	26.32	23.48	43.31	15.47
-5	4	2	35.90	34.27	62.37	6.66
6	-4	2	23.03	21.96	-38.64	-11.23
6	4	2	19.20	19.74	-33.25	-4.48
-6	-4	2	22.72	21.86	-39.35	-5.23
-6	4	2	15.08	14.03	25.06	8.15
7	-4	2	15.00	11.96	25.59	5.66
7	4	2	7.33	6.95	-10.64	-7.14
-7	-4	2	0.	2.06	0.	-0.
-7	4	2	0.	0.15	0.	0.
8	-4	2	4.71	0.92	6.33	5.26
-8	4	2	6.90	4.69	-11.32	-4.14
-8	-4	2	0.	2.92	0.	-0.
9	-4	2	8.95	10.76	-15.41	-2.66
-9	4	2	12.24	11.30	-21.06	-3.72
0	-5	2	38.22	37.99	66.74	2.41
0	5	2	17.85	20.40	-31.07	-2.74
1	-5	2	9.23	8.68	16.10	-0.93
1	5	2	5.22	4.74	-8.62	2.99
-1	-5	2	12.61	11.62	-21.86	-2.79
-1	5	2	48.31	54.10	-84.35	-3.28
2	-5	2	47.55	42.42	-82.62	-8.83
2	5	2	59.29	64.57	101.81	19.19
-2	-5	2	9.48	9.07	16.37	2.52
-2	5	2	7.24	6.93	11.42	5.45
3	-5	2	21.53	20.17	37.55	2.35
3	5	2	34.39	34.77	-59.54	-8.10
-3	-5	2	37.29	33.65	63.79	13.30
-3	5	2	81.18	95.63	-140.43	-20.00
4	-5	2	23.39	21.25	39.97	8.52
4	5	2	30.85	29.15	53.66	5.10

-4	-5	2	10.86	12.52	18.37	-4.74
-4	5	2	5.83	4.25	10.13	1.10
5	-5	2	13.87	12.13	23.86	4.23
5	5	2	23.39	22.05	40.72	3.47
-5	-5	2	10.72	35.66	-18.68	-1.36
-5	5	2	0.	2.46	0.	0.
6	-5	2	24.58	23.89	-41.98	9.06
6	5	2	9.48	8.25	16.34	-2.72
-6	-5	2	17.91	12.42	-31.20	-2.41
-6	5	2	11.13	11.36	-19.45	-0.29
7	-5	2	15.41	13.52	26.05	6.81
7	5	2	9.36	11.13	-14.07	-8.33
-7	-5	2	34.89	10.26	-56.26	-23.49
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8	-5	2	10.32	8.63	18.00	1.00
-8	5	2	31.68	28.86	53.06	15.79
9	-5	2	8.92	10.75	-15.06	-4.03
-9	5	2	11.38	11.71	-17.76	-8.95
0	-6	2	18.05	18.22	31.09	5.32
0	6	2	37.89	41.12	66.16	2.61
1	-6	2	5.85	5.12	9.13	4.60
-1	-6	2	11.37	9.69	-19.70	-2.61
-1	6	2	8.20	8.35	-14.26	-1.36
1	6	2	0.	1.81	-0.	0.
2	-6	2	9.48	8.52	16.55	0.62
2	6	2	20.60	19.95	-35.99	-0.72
-2	-6	2	96.35	90.41	166.69	23.63
-2	6	2	10.69	11.35	-18.60	-1.75
3	-6	2	61.75	58.80	-105.89	-20.70
3	6	2	23.18	21.75	-40.17	-5.19
-3	-6	2	27.73	25.94	-48.42	-1.75
-3	6	2	0.	2.63	-0.	-0.
4	-6	2	33.02	31.45	56.97	9.11
4	6	2	15.75	13.76	-26.70	-6.69
-4	-6	2	11.05	8.14	19.30	-0.35
-4	6	2	16.27	15.95	26.71	-9.73
5	-6	2	12.96	12.12	-22.31	-3.89
5	6	2	19.31	16.48	-32.28	-9.81
-5	-6	2	11.06	8.15	19.22	-2.06
-5	6	2	12.30	13.22	-21.49	0.13
6	-6	2	10.49	13.27	-18.18	-2.36
-6	-6	2	15.67	12.01	27.10	3.92
-6	6	2	4.66	4.11	-7.57	3.00
6	6	2	0.	11.62	-0.	0.
7	-6	2	9.74	9.49	16.93	1.76
-7	-6	2	25.06	22.93	-41.73	-13.26
-7	6	2	10.32	9.60	17.67	3.59
8	-6	2	32.40	30.18	55.24	12.40
-8	6	2	34.18	32.42	59.38	6.42
9	-6	2	21.67	23.44	-35.54	-13.07
-9	6	2	8.35	7.30	5.37	13.56
0	7	2	24.93	25.53	-43.02	-6.82
0	-7	2	0.	36.76	0.	0.
1	-7	2	9.83	9.51	-17.17	0.61
1	7	2	48.53	54.15	84.67	4.69

-1	-7	2	5.45	0.68	-9.36	1.73
-1	7	2	48.13	53.87	81.70	19.95
2	-7	2	56.89	50.02	-99.07	-8.14
-2	-7	2	47.32	45.75	-82.63	-3.05
2	7	2	0.	1.46	0.	0.
-2	7	2	0.	1.63	0.	0.
3	-7	2	5.98	5.63	-9.86	-3.46
3	7	2	20.27	19.48	-35.08	-4.85
-3	-7	2	5.23	3.13	8.83	2.37
-3	7	2	0.	0.97	0.	-0.
4	-7	2	40.73	38.14	70.46	-10.06
4	7	2	49.53	46.70	-84.66	-17.96
-4	-7	2	12.17	10.68	-20.45	-5.84
-4	7	2	5.66	3.67	-9.79	-1.38
5	-7	2	32.60	30.83	-56.69	-5.57
5	7	2	37.77	39.12	65.31	9.51
-5	-7	2	25.64	22.64	-43.65	-10.08
-5	7	2	0.	5.08	-0.	0.
6	-7	2	12.58	10.47	-21.69	-3.56
6	7	2	17.65	16.81	-30.30	-5.72
-6	-7	2	7.27	6.57	-11.30	5.80
-6	7	2	32.96	29.68	-55.03	-17.00
7	-7	2	14.96	14.53	25.61	5.22
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8	-7	2	26.86	21.24	46.82	3.32
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-9	7	2	2.55	1.86	-2.49	3.69
0	-8	2	12.29	11.78	-21.23	-3.24
0	8	2	18.05	18.42	31.53	0.69
1	-8	2	38.22	37.91	63.40	20.98
1	8	2	12.26	11.19	21.42	0.28
-1	-8	2	9.34	9.25	15.78	-4.15
-1	8	2	3.76	4.09	-6.45	1.26
2	-8	2	11.52	10.42	-19.15	-6.19
2	8	2	16.30	15.44	-28.37	-2.57
-2	-8	2	13.14	12.33	-22.62	-3.93
-2	8	2	24.39	26.64	-41.46	9.85
3	-8	2	12.06	12.83	20.94	2.37
3	8	2	4.17	3.19	6.31	-3.64
-3	-8	2	8.67	8.48	15.14	0.39
-3	8	2	0.	4.92	0.	-0.
4	-8	2	11.40	9.87	19.24	5.14
4	8	2	25.05	23.63	43.68	2.84
-4	-8	2	55.75	52.78	-95.06	-21.29
-4	8	2	0.	2.73	0.	-0.
5	-8	2	8.08	6.65	14.11	0.57
5	8	2	16.57	16.06	28.47	5.28
-5	-8	2	20.91	20.33	36.24	4.63
-5	8	2	13.61	14.25	-23.59	-3.04
6	-8	2	37.79	34.94	-64.29	-15.08
-6	-8	2	12.31	11.69	-21.51	0.26
-6	8	2	26.85	25.12	-46.66	-4.90
7	-8	2	22.53	18.64	36.27	15.30
-7	8	2	26.47	22.73	-42.76	-17.64
8	-8	2	3.75	1.87	4.33	4.91

-8	8	2	10.23	7.73	17.63	2.96
0	-9	2	22.64	19.51	38.99	6.72
0	9	2	14.70	14.52	-25.01	-5.87
1	9	2	28.01	28.78	-45.20	-18.77
1	-9	2	11.37	9.52	-19.68	2.71
-1	-9	2	20.25	18.29	-35.25	-3.02
-1	9	2	14.94	16.28	-26.11	0.04
2	-9	2	9.27	8.16	-11.84	11.05
2	9	2	20.09	19.42	34.16	8.07
-2	-9	2	12.39	11.23	-21.27	-4.02
-2	9	2	27.78	28.95	48.50	2.03
3	-9	2	22.63	19.29	39.26	4.70
3	9	2	32.58	31.42	-56.55	-6.51
-3	9	2	7.77	8.28	-11.14	-7.76
-3	-9	2	0.	0.82	0.	-0.
4	-9	2	12.62	11.38	21.45	5.13
4	9	2	4.33	4.50	-7.52	-0.81
-4	-9	2	35.95	35.42	62.72	3.48
-4	9	2	35.50	36.75	60.35	14.33
5	-9	2	12.33	10.82	-20.89	-5.26
-5	-9	2	11.61	9.68	20.29	-0.19
-5	9	2	0.	2.45	0.	-0.
6	-9	2	14.75	15.02	-25.63	-2.70
-6	9	2	0.	3.05	0.	-0.
7	-9	2	14.80	12.10	-22.45	-12.83
-7	9	2	13.00	11.45	-22.39	-3.81
-8	9	2	18.78	19.82	-32.63	3.45
8	-9	2	0.	2.30	0.	0.
0	-10	2	7.18	5.29	12.22	2.83
0	10	2	13.45	14.06	-21.03	-10.50
1	-10	2	5.03	3.19	8.48	-2.31
1	10	2	5.74	6.55	9.91	1.52
-1	-10	2	48.91	47.24	-82.93	-20.64
-1	10	2	6.52	5.67	-11.39	-0.37
2	-10	2	17.07	15.59	29.29	-5.64
2	10	2	4.66	2.76	8.14	-0.02
-2	-10	2	14.53	14.52	24.82	5.36
-2	10	2	12.04	11.13	20.88	2.53
3	-10	2	11.38	11.44	-19.67	-2.89
3	10	2	6.19	5.43	10.80	0.66
-3	-10	2	3.87	2.91	4.96	4.59
-3	10	2	0.	4.85	0.	0.
4	-10	2	36.97	30.50	61.96	18.27
4	10	2	6.89	6.01	11.76	2.56
-4	-10	2	3.75	4.09	6.24	2.00
-4	10	2	0.	5.60	0.	0.
5	-10	2	21.24	18.46	-35.37	-11.24
-5	10	2	36.20	33.48	60.40	18.78
-6	10	2	7.55	5.55	-13.11	-1.43
6	-10	2	0.	2.64	0.	-0.
7	-10	2	17.91	15.62	-31.29	0.05
-7	10	2	5.92	3.48	-10.34	0.09
8	-10	2	21.86	18.66	-37.84	-5.22
-8	10	2	0.	1.66	0.	0.
0	-11	2	34.51	31.45	-59.37	-10.57

0	11	2	34.36	34.43	-59.96	-3.03
-1	-11	2	9.89	9.23	17.26	-0.88
-1	11	2	27.51	30.35	47.49	7.44
1	-11	2	0.	1.60	-0.	-0.
1	11	2	0.	1.42	-0.	0.
2	-11	2	6.85	5.56	-9.86	-6.78
2	11	2	18.39	17.26	31.12	8.01
-2	-11	2	8.55	7.66	-14.24	-4.52
-2	11	2	26.65	27.90	-44.85	-12.52
3	11	2	28.49	26.50	47.06	16.24
-3	-11	2	12.19	10.83	20.84	4.42
3	-11	2	0.	2.13	0.	0.
-3	11	2	0.	3.20	0.	-0.
4	-11	2	6.74	5.69	-11.47	2.68
-4	11	2	8.77	7.12	-14.70	4.34
5	-11	2	8.97	9.82	10.77	11.39
-5	11	2	19.94	17.49	34.58	4.24
6	-11	2	11.11	10.07	19.39	-1.03
-6	11	2	12.77	13.95	22.00	-3.70
7	-11	2	12.48	10.65	20.55	7.29
-7	11	2	12.36	10.72	19.22	9.85
0	-12	2	9.50	9.52	-15.83	5.01
0	12	2	12.59	12.41	-21.91	-2.00
1	-12	2	29.82	28.02	51.83	5.38
1	12	2	6.90	6.59	12.01	1.01
-1	-12	2	3.96	4.24	-6.89	0.65
-1	12	2	5.98	4.81	-9.64	-4.03
2	-12	2	35.75	31.17	-60.16	-16.82
2	12	2	22.83	21.03	38.35	10.98
-2	-12	2	8.35	8.37	14.54	1.17
-2	12	2	0.	3.80	0.	0.
3	-12	2	8.60	6.88	13.01	7.51
-3	12	2	24.62	25.21	-39.25	-17.60
-4	12	2	7.96	10.33	-13.90	-0.42
4	-12	2	0.	3.85	0.	0.
5	-12	2	6.36	7.79	11.09	-0.64
-5	12	2	0.	1.09	-0.	0.
6	-12	2	7.24	5.91	12.19	3.40
-6	12	2	0.	1.41	-0.	0.
0	-13	2	11.45	11.68	19.25	5.44
0	13	2	19.54	17.93	32.15	11.50
1	-13	2	6.71	5.21	-11.27	-3.23
-1	-13	2	5.05	4.88	-8.74	1.21
-1	13	2	4.55	5.19	7.33	3.07
2	-13	2	10.89	10.59	18.99	-1.18
-2	13	2	3.85	3.29	6.40	-2.06
3	-13	2	6.95	8.35	4.05	-11.45
-3	13	2	21.00	20.50	-36.51	-3.70
-4	13	2	10.61	9.83	18.07	4.15
4	-13	2	0.	1.23	-0.	0.
5	-13	2	8.31	8.47	-12.94	-6.59
-5	13	2	9.97	9.27	-15.61	-7.74
1	-14	2	0.	1.54	-0.	-0.
2	-14	2	12.16	10.39	-20.40	-5.94
3	-14	2	11.92	13.80	-20.80	1.02

4	-14	2	4.54	3.11	7.81	-1.39
1	0	3	18.73	18.37	32.13	6.20
-1	0	3	107.70	115.48	186.95	21.56
2	0	3	29.47	28.55	51.07	6.56
-2	0	3	8.29	7.21	14.48	0.44
3	0	3	13.18	11.74	-22.97	-1.67
-3	0	3	7.69	7.34	12.66	-4.50
4	0	3	27.32	25.47	-45.25	-15.22
-4	0	3	15.66	14.09	-27.08	-3.95
5	0	3	15.20	12.89	22.00	14.87
-5	0	3	0.	3.92	-0.	0.
6	0	3	4.86	6.59	8.47	-0.58
-6	0	3	27.38	24.45	-42.24	-22.47
7	0	3	4.06	1.45	7.05	-0.83
-7	0	3	30.90	27.36	53.77	4.93
8	0	3	12.34	13.70	20.83	5.58
-8	0	3	0.	2.43	-0.	0.
0	-1	3	33.22	34.88	57.27	9.45
0	1	3	43.51	47.80	-75.90	-4.37
1	-1	3	6.08	6.25	10.60	0.67
-1	-1	3	31.40	28.04	54.86	0.93
-1	1	3	5.45	5.34	-9.42	1.37
1	1	3	0.	3.43	-0.	-0.
2	-1	3	38.63	36.32	67.34	4.66
2	1	3	28.59	27.32	-48.98	-9.82
-2	-1	3	8.98	7.43	15.15	4.09
-2	1	3	48.99	49.28	85.51	3.95
3	-1	3	12.56	9.97	-20.91	-6.67
3	1	3	10.97	10.64	-19.04	-2.18
-3	-1	3	19.19	17.89	-33.32	-3.75
-3	1	3	8.47	5.87	-14.75	1.17
4	-1	3	12.74	12.63	-21.60	-5.38
4	1	3	44.85	44.82	-78.32	-2.83
-4	-1	3	53.70	49.83	-93.80	-2.27
-4	1	3	10.50	11.57	-17.68	-4.89
5	1	3	12.96	11.67	21.68	6.53
-5	-1	3	10.27	9.24	-17.93	-0.83
-5	1	3	25.06	21.65	-43.74	-2.12
5	-1	3	0.	8.29	-0.	-0.
6	1	3	19.46	17.70	33.53	5.65
-6	1	3	5.52	4.49	-5.60	-7.86
6	-1	3	0.	5.82	0.	0.
-6	-1	3	0.	3.91	0.	0.
7	-1	3	27.44	27.28	-47.35	-7.54
7	1	3	15.50	12.75	24.03	12.50
-7	-1	3	16.67	12.18	28.93	3.40
-7	1	3	23.79	18.69	-39.75	-12.16
8	-1	3	3.15	6.17	5.32	1.42
-8	-1	3	16.39	14.12	27.27	8.76
-8	1	3	0.	1.77	0.	0.
0	-2	3	24.06	24.26	-41.36	-7.52
0	2	3	18.65	19.41	-32.44	-3.05
1	-2	3	12.34	11.24	-21.54	-1.02
1	2	3	46.17	48.58	-78.11	-20.18
-1	-2	3	4.50	4.29	-6.32	-4.68

-1	2	3	0.	2.28	-0.	0.
2	-2	3	12.11	10.44	-9.64	18.84
2	2	3	23.79	25.34	40.88	7.54
-2	-2	3	23.40	21.62	40.81	2.44
-2	2	3	19.18	19.16	33.03	5.66
3	-2	3	25.23	24.63	-42.90	-10.17
-3	-2	3	85.39	83.49	-147.36	-23.41
-3	2	3	9.36	8.80	15.36	-5.63
3	2	3	0.	7.50	-0.	-0.
4	-2	3	5.14	4.15	8.95	-0.79
4	2	3	22.64	22.65	-39.33	-4.28
-4	-2	3	22.87	21.12	39.87	2.74
-4	2	3	50.40	45.62	84.84	23.63
5	-2	3	5.12	7.19	8.82	1.52
5	2	3	22.79	24.63	39.70	3.10
-5	-2	3	10.40	10.30	17.70	4.12
-5	2	3	27.32	25.12	-47.73	-1.07
6	-2	3	47.36	42.70	-82.55	-5.75
6	2	3	27.85	27.34	47.35	11.24
-6	2	3	7.20	3.68	-11.97	-3.87
-6	-2	3	0.	0.95	0.	0.
7	-2	3	10.20	10.85	-15.13	-9.42
7	2	3	26.32	27.45	-44.07	-13.15
-7	-2	3	0.	9.66	-0.	-0.
-7	2	3	0.	3.54	0.	-0.
8	-2	3	26.32	25.81	44.61	11.19
-8	-2	3	38.80	35.93	65.22	18.53
-8	2	3	15.39	14.13	26.12	6.41
0	3	3	38.29	40.85	-66.71	-5.14
0	-3	3	0.	7.74	-0.	-0.
1	-3	3	10.19	9.13	-17.21	4.56
1	3	3	10.84	11.97	-18.90	1.25
-1	-3	3	19.27	18.24	-33.66	0.87
-1	3	3	9.14	8.88	15.92	-1.30
2	-3	3	7.40	9.16	12.37	3.77
2	3	3	17.45	18.90	30.06	5.11
-2	-3	3	29.55	26.18	-50.36	-11.41
-2	3	3	28.06	27.17	48.79	4.82
3	-3	3	60.09	59.03	103.77	16.02
3	3	3	7.70	7.34	-13.06	3.23
-3	-3	3	25.19	21.76	-44.00	1.15
-3	3	3	11.70	11.15	20.41	1.24
4	-3	3	14.57	12.80	25.37	-2.11
4	3	3	9.38	7.10	11.83	11.35
-4	-3	3	10.08	9.60	17.52	-1.76
-4	3	3	6.98	6.24	-11.35	4.46
5	-3	3	43.54	40.69	75.49	9.48
-5	3	3	82.14	79.32	142.96	12.68
5	3	3	0.	2.87	0.	0.
-5	-3	3	0.	16.06	0.	0.
6	3	3	28.19	29.96	49.25	0.83
-6	3	3	11.56	7.68	-19.92	-3.33
6	-3	3	0.	1.46	-0.	-0.
-6	-3	3	0.	12.37	0.	0.
7	3	3	5.11	4.19	-5.64	-6.92

-7	-3	3	11.70	11.40	-20.42	1.00
-7	3	3	11.67	10.27	-19.68	-5.33
7	-3	3	0.	3.38	0.	-0.
8	-3	3	21.32	19.56	-35.96	-9.72
-8	-3	3	12.66	10.74	-20.89	-7.29
-8	3	3	5.02	6.13	8.63	-1.58
-9	3	3	8.50	10.47	14.24	-4.22
0	-4	3	27.89	27.61	-45.73	-16.85
0	4	3	5.90	6.64	-7.93	-6.59
1	-4	3	17.14	16.34	29.26	6.41
-1	4	3	25.18	27.58	43.61	5.84
1	4	3	0.	3.05	-0.	-0.
-1	-4	3	0.	10.28	0.	0.
2	4	3	32.45	34.48	56.48	4.96
-2	4	3	67.88	81.18	-117.32	-17.45
2	-4	3	0.	3.59	0.	0.
-2	-4	3	0.	4.57	-0.	0.
3	-4	3	11.12	10.29	-19.02	-3.95
3	4	3	14.31	11.04	10.06	22.89
-3	4	3	14.40	14.71	-25.04	-2.47
-3	-4	3	0.	2.00	-0.	0.
4	-4	3	37.34	35.37	65.14	3.63
4	4	3	16.01	12.48	-25.20	-12.14
-4	-4	3	24.27	21.85	42.39	1.08
-4	4	3	7.57	5.00	-13.13	1.60
5	-4	3	15.44	14.06	23.92	12.47
5	4	3	17.40	16.09	29.13	8.71
-5	-4	3	52.40	48.55	88.83	22.21
-5	4	3	10.20	8.34	17.47	3.53
6	-4	3	26.69	23.09	-45.43	-10.53
6	4	3	7.97	7.82	13.81	1.83
-6	4	3	41.28	26.11	-71.29	-10.96
7	-4	3	21.38	18.19	-36.86	-6.09
7	4	3	10.53	12.29	-18.02	-3.70
-7	4	3	23.40	18.91	38.01	15.07
-8	4	3	19.07	18.35	-32.69	-6.45
8	-4	3	0.	1.49	0.	-0.
-9	4	3	6.03	5.34	-9.02	-5.44
0	-5	3	15.36	14.07	-26.63	-3.36
0	5	3	10.02	9.72	-17.09	-3.81
1	-5	3	71.13	71.91	-123.07	-17.36
1	5	3	11.48	12.94	-19.98	1.79
-1	-5	3	16.30	14.40	28.33	-2.91
-1	5	3	17.81	17.57	31.11	-0.80
2	5	3	20.36	20.78	35.04	6.14
-2	-5	3	11.34	10.26	18.96	5.76
-2	5	3	13.38	15.28	-23.37	-0.59
2	-5	3	0.	2.78	0.	0.
3	-5	3	37.28	36.33	-64.45	-9.49
3	5	3	20.15	20.18	34.97	-4.13
-3	-5	3	8.68	9.37	15.05	-1.90
-3	5	3	88.68	109.05	-154.54	-11.37
4	-5	3	20.70	19.30	-36.17	-0.36
4	5	3	15.53	16.64	-26.66	-5.04
-4	-5	3	17.75	17.61	29.39	9.92

-4	5	3	13.03	12.92	22.73	1.34
5	-5	3	12.98	10.52	-22.46	3.17
5	5	3	17.79	17.01	-30.88	-3.59
-5	-5	3	16.42	14.60	28.50	-3.34
-5	5	3	27.24	26.27	47.29	5.40
6	-5	3	35.27	30.50	59.95	14.27
6	5	3	4.37	4.35	-0.06	-7.64
-6	5	3	18.23	17.54	31.75	2.58
-6	-5	3	0.	5.87	-0.	0.
7	-5	3	17.37	17.80	-29.06	-8.75
-7	-5	3	21.79	21.20	-37.73	-5.13
-7	5	3	14.35	14.26	-24.82	3.56
8	-5	3	10.39	10.54	17.02	6.33
-8	5	3	33.35	30.65	55.51	17.72
0	6	3	53.29	61.04	91.68	16.29
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1	-6	3	10.15	8.48	-16.85	5.53
1	6	3	19.76	20.65	-33.93	-6.40
-1	-6	3	6.85	6.45	-11.79	-2.04
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2	-6	3	7.62	8.52	-13.26	-1.24
2	6	3	8.33	7.79	11.43	9.01
-2	-6	3	45.21	40.02	77.05	17.42
-2	6	3	0.	3.45	0.	0.
3	-6	3	17.15	16.50	-27.51	-11.89
3	6	3	15.66	15.63	27.36	0.46
-3	-6	3	15.99	15.82	-27.43	-5.33
-3	6	3	16.61	18.16	-28.80	-3.62
4	6	3	14.21	14.96	-24.10	-5.96
-4	6	3	21.73	21.42	37.26	7.31
4	-6	3	0.	3.67	0.	0.
-4	-6	3	0.	4.12	0.	-0.
5	-6	3	25.09	23.31	43.23	7.29
5	6	3	17.15	16.51	-26.64	-13.73
-5	-6	3	7.88	7.06	-13.64	-1.91
-5	6	3	9.77	8.72	-10.43	-13.51
6	-6	3	15.30	13.50	26.70	1.35
6	6	3	3.61	6.16	2.82	5.64
-6	-6	3	18.79	16.43	-32.58	-4.09
-6	6	3	16.50	16.93	28.64	3.29
7	-6	3	27.82	29.38	47.90	8.30
-7	6	3	6.74	3.91	9.26	7.28
8	-6	3	10.79	10.28	16.46	9.20
-8	6	3	0.	3.32	-0.	0.
0	-7	3	16.81	14.99	-29.28	-2.28
0	7	3	13.99	13.86	24.27	-2.92
1	-7	3	18.36	28.80	31.61	5.48
1	7	3	22.75	22.98	-39.74	0.80
-1	-7	3	57.84	57.44	99.39	18.30
-1	7	3	63.73	76.50	110.72	11.94
2	-7	3	55.01	53.51	96.10	2.04
2	7	3	7.31	8.02	12.57	2.29
-2	-7	3	43.21	40.57	75.50	0.88
-2	7	3	5.52	0.87	-9.64	0.21
3	7	3	8.98	10.00	15.48	-2.57

-3	7	3	15.80	16.09	-27.12	-5.18
3	-7	3	0.	2.83	0.	-0.
-3	-7	3	0.	2.76	-0.	0.
4	-7	3	28.71	29.70	-47.92	-14.86
4	7	3	11.61	11.37	-19.28	-6.31
-4	-7	3	20.76	19.58	-35.96	-4.76
-4	7	3	7.99	9.51	-13.68	-2.77
5	-7	3	12.61	14.68	20.81	7.23
5	7	3	15.28	16.22	-26.02	5.98
-5	7	3	9.28	10.52	16.19	-0.93
-5	-7	3	0.	2.51	-0.	0.
6	-7	3	14.13	16.40	-24.04	-5.61
-6	-7	3	19.05	19.27	-32.06	-8.95
-6	7	3	52.40	53.13	-89.60	-18.83
7	-7	3	6.73	6.37	-11.75	-0.46
-7	7	3	0.	3.55	-0.	0.
8	-7	3	12.92	18.41	-22.47	2.17
-8	7	3	8.13	9.00	-14.08	1.88
0	-8	3	16.12	17.63	-28.16	-0.46
0	8	3	14.16	6.56	-24.30	-4.66
1	-8	3	5.38	5.86	-0.25	9.40
1	8	3	24.21	26.43	-41.78	-6.63
-1	-8	3	19.12	10.82	-32.22	-8.83
-1	8	3	8.66	10.16	-14.64	3.83
2	8	3	27.88	26.55	-45.99	-16.06
-2	-8	3	14.10	13.63	24.51	2.46
-2	8	3	9.09	10.08	-14.71	-5.99
2	-8	3	0.	1.90	0.	-0.
3	-8	3	7.70	8.80	-11.75	-6.55
3	8	3	9.93	9.80	16.18	6.26
-3	8	3	11.29	11.95	16.75	10.42
-3	-8	3	0.	1.12	0.	-0.
4	-8	3	6.87	10.59	-11.99	-0.50
4	8	3	5.72	5.92	-5.78	-8.16
-4	-8	3	36.60	37.12	-62.70	-12.60
-4	8	3	20.16	23.41	-35.22	-0.44
5	-8	3	40.47	46.09	-70.33	-7.34
-5	-8	3	23.99	24.87	41.48	6.05
-5	8	3	16.58	14.66	-28.79	-3.24
5	8	3	0.	2.70	-0.	0.
-6	8	3	5.62	3.12	-1.63	-9.68
6	-8	3	0.	8.24	-0.	-0.
-7	8	3	11.22	12.18	19.48	2.24
7	-8	3	0.	5.11	0.	0.
8	-8	3	6.57	10.84	11.06	3.08
-8	8	3	7.55	7.58	-11.98	-5.52
0	-9	3	35.62	43.01	-62.19	-2.61
0	9	3	0.	2.03	-0.	-0.
1	-9	3	11.43	13.16	19.97	-0.43
1	9	3	22.34	22.74	-36.80	-13.02
-1	-9	3	15.40	15.46	-25.96	-7.09
-1	9	3	13.60	15.11	23.38	4.27
2	-9	3	36.42	43.82	61.98	14.43
2	9	3	0.	4.17	0.	0.
-2	-9	3	0.	3.06	0.	0.

-2	9	3	0.	11.87	0.	0.
3	-9	3	9.12	10.57	-14.78	-5.95
3	9	3	5.77	2.80	-9.78	-2.45
-3	-9	3	28.16	31.45	-46.66	-15.61
-3	9	3	0.	1.13	0.	-0.
4	-9	3	7.80	7.22	12.06	6.35
4	9	3	9.72	11.52	-16.95	-1.01
-4	-9	3	18.88	20.30	-32.95	1.53
-4	9	3	67.76	81.29	117.19	16.85
5	-9	3	10.10	13.50	17.53	2.01
-5	-9	3	0.	1.48	0.	-0.
-5	9	3	0.	3.89	-0.	0.
6	-9	3	0.	9.33	0.	-0.
-6	9	3	0.	1.40	0.	-0.
7	-9	3	9.70	27.07	-16.48	-3.95
-7	9	3	6.36	5.79	11.10	-0.48
-8	9	3	26.53	28.39	46.25	3.10
0	-10	3	0.	5.68	0.	-0.
0	10	3	0.	3.86	-0.	0.
1	-10	3	10.84	18.29	18.45	4.27
1	10	3	14.83	15.02	25.56	-4.28
-1	-10	3	0.	4.61	0.	-0.
-1	10	3	0.	28.01	-0.	-0.
2	10	3	8.44	9.81	14.41	3.15
-2	-10	3	5.87	7.06	10.14	1.52
-2	10	3	7.23	5.25	-12.37	-2.57
2	-10	3	0.	6.11	0.	0.
3	-10	3	15.49	42.74	26.93	2.76
3	10	3	16.97	18.25	28.77	7.20
-3	10	3	14.23	14.81	24.84	1.02
-3	-10	3	0.	6.04	-0.	0.
-4	-10	3	12.64	10.63	-21.98	-2.18
-4	10	3	9.11	9.95	15.28	4.46
4	-10	3	0.	16.59	0.	0.
-5	10	3	10.58	10.57	-18.42	-1.61
5	-10	3	0.	5.53	0.	0.
-6	10	3	6.96	6.92	11.21	4.72
6	-10	3	0.	12.89	-0.	-0.
-7	10	3	6.48	6.51	-10.63	-3.89
0	-11	3	16.60	38.47	-27.97	-7.70
0	11	3	9.21	10.14	-15.36	-4.81
1	11	3	4.75	4.12	-7.17	-4.17
-1	-11	3	8.91	10.89	-15.42	2.11
-1	11	3	7.33	9.42	-12.34	3.44
1	-11	3	0.	2.98	0.	0.
2	-11	3	5.85	16.64	-10.09	-1.66
2	11	3	7.21	7.94	12.33	2.59
-2	-11	3	8.25	15.98	14.30	1.86
-2	11	3	59.29	71.21	-102.33	-16.17
3	-11	3	6.83	38.25	-11.91	-0.79
-3	-11	3	11.75	20.17	20.30	3.04
-3	11	3	0.	1.62	0.	-0.
-4	11	3	7.52	5.77	12.79	3.00
4	-11	3	0.	7.33	-0.	-0.
5	-11	3	8.56	31.04	14.52	3.61

-5	11	3	0.	1.15	-0.	0.
-6	11	3	31.36	31.47	-54.54	-5.29
0	12	3	8.12	7.66	13.72	3.62
0	-12	3	0.	2.65	-0.	0.
1	12	3	13.11	12.08	21.45	8.03
-1	-12	3	6.00	16.80	-10.26	-2.17
1	-12	3	0.	18.62	-0.	-0.
-1	12	3	0.	4.53	-0.	0.
2	-12	3	0.	7.23	-0.	-0.
-2	12	3	0.	4.14	0.	-0.
-3	12	3	7.21	6.78	12.59	0.56
3	-12	3	0.	9.66	-0.	-0.
-4	12	3	4.62	5.65	7.48	-3.04
4	-12	3	0.	17.10	0.	0.
-5	12	3	7.52	10.87	13.03	1.73
-6	12	3	15.56	15.75	26.81	4.53
0	-13	3	0.	14.44	0.	0.
1	-13	3	3.69	43.17	6.43	0.46
-1	13	3	13.37	14.84	22.97	4.25
-2	13	3	0.	3.15	-0.	-0.
-3	13	3	10.46	10.11	-17.92	-3.59
-4	13	3	5.25	6.36	7.22	5.66
1	0	4	15.70	16.33	-26.95	-5.12
-1	0	4	0.	8.04	0.	0.
2	0	4	12.38	11.59	-21.63	0.28
-2	0	4	0.	1.44	-0.	0.
3	0	4	44.27	42.48	-76.82	-9.10
-3	0	4	33.18	35.22	-57.52	-7.24
4	0	4	8.51	7.47	-13.01	-7.20
-4	0	4	0.	3.38	0.	-0.
5	0	4	37.41	38.38	65.36	0.64
-5	0	4	17.85	16.94	-31.04	-3.08
6	0	4	9.28	10.19	15.33	5.29
-6	0	4	20.04	17.31	-21.25	-15.81
7	0	4	7.21	6.56	12.34	2.55
-7	0	4	0.	2.06	0.	0.
-8	0	4	23.89	23.05	41.23	6.52
0	-1	4	91.93	113.70	159.84	15.97
0	1	4	30.02	29.68	52.43	1.52
1	-1	4	25.12	25.99	-43.39	-6.62
1	1	4	17.45	15.69	-30.02	-5.31
-1	1	4	37.58	38.57	65.06	8.88
-1	-1	4	0.	1.69	0.	0.
2	-1	4	16.92	15.14	27.49	10.88
2	1	4	108.50	119.22	-188.95	-15.52
-2	-1	4	20.10	19.04	-34.96	-3.33
-2	1	4	40.63	40.09	-70.82	-4.98
3	-1	4	16.22	14.72	27.93	4.81
3	1	4	11.85	13.64	19.56	6.80
-3	-1	4	14.99	14.29	-25.03	-7.72
-3	1	4	51.63	52.59	88.51	17.48
4	-1	4	7.47	6.65	12.43	-3.98
-4	-1	4	43.71	42.59	76.23	4.75
-4	1	4	36.32	33.72	63.45	1.49
4	1	4	0.	20.66	-0.	-0.

5	-1	4	27.70	27.58	-47.08	-11.22
5	1	4	7.01	5.12	-12.07	-2.09
-5	-1	4	52.78	51.28	-90.43	-18.11
-5	1	4	0.	5.05	0.	-0.
6	-1	4	20.53	23.59	33.95	11.60
6	1	4	14.57	13.55	-25.01	4.78
-6	-1	4	34.21	32.10	-59.76	1.59
-6	1	4	0.	4.06	-0.	-0.
7	-1	4	12.13	14.26	-20.88	-3.64
7	1	4	14.16	13.56	23.38	8.11
-7	1	4	24.15	23.63	41.80	5.82
-7	-1	4	0.	2.33	-0.	0.
-8	-1	4	7.27	6.99	12.24	3.41
-8	1	4	0.	4.94	-0.	-0.
0	-2	4	16.14	16.76	-28.18	-1.21
0	2	4	9.59	8.96	-16.64	-1.98
1	-2	4	27.41	28.02	47.24	7.92
1	2	4	6.11	5.23	1.34	-10.59
-1	-2	4	22.77	21.21	39.41	5.47
-1	2	4	22.99	24.86	39.65	6.44
2	-2	4	22.19	21.60	38.36	5.66
2	2	4	31.55	30.19	54.80	5.98
-2	-2	4	5.59	5.82	-9.74	-0.75
-2	2	4	6.95	6.43	12.04	1.61
3	-2	4	13.96	12.93	-24.32	1.90
3	2	4	13.01	12.56	22.20	4.87
-3	-2	4	9.84	8.59	15.34	-7.76
-3	2	4	0.	1.28	-0.	-0.
4	-2	4	27.77	27.72	-48.09	-6.47
4	2	4	20.02	20.02	34.97	0.71
-4	-2	4	22.86	21.65	39.93	1.23
-4	2	4	13.28	15.33	-18.77	13.64
5	-2	4	8.73	8.54	-15.02	-2.63
5	2	4	32.06	31.81	55.29	9.03
-5	-2	4	23.81	24.12	40.90	7.61
-5	2	4	0.	5.43	-0.	-0.
6	-2	4	21.31	17.82	-34.79	-13.28
6	2	4	9.94	10.36	16.32	5.93
-6	-2	4	10.01	10.12	-17.47	0.84
-6	2	4	17.16	15.39	-28.86	-8.12
7	-2	4	17.32	19.12	-30.18	-2.30
7	2	4	19.04	20.59	-33.17	-2.62
-7	-2	4	15.55	14.42	26.54	5.83
-7	2	4	8.86	8.02	-15.28	-2.49
-8	2	4	17.47	16.97	-30.46	-2.00
0	-3	4	46.28	50.24	-80.51	-7.57
0	3	4	0.	4.44	0.	0.
1	-3	4	20.24	18.96	-34.63	-7.18
1	3	4	29.70	31.72	-51.06	-9.29
-1	-3	4	8.04	7.22	12.90	5.56
-1	3	4	43.95	47.95	-75.25	-15.31
2	-3	4	15.56	13.36	27.11	2.03
2	3	4	6.90	5.55	12.04	0.61
-2	-3	4	56.51	57.41	-96.58	-20.55
-2	3	4	12.36	12.78	-21.27	-3.77

3	-3	4	52.61	53.78	90.89	13.78
3	3	4	10.34	11.71	17.35	5.04
-3	-3	4	12.64	10.84	-22.08	-0.33
-3	3	4	6.68	4.04	-11.41	-2.47
4	-3	4	38.85	37.91	-66.71	-12.55
4	3	4	52.92	53.29	91.51	13.31
-4	3	4	14.09	14.62	24.09	5.09
-4	-3	4	0.	5.40	0.	0.
5	3	4	11.00	12.00	-17.82	-7.20
-5	-3	4	10.08	9.20	16.70	5.59
-5	3	4	32.98	32.74	-57.38	-5.32
5	-3	4	0.	1.83	0.	0.
6	-3	4	7.66	6.63	13.34	1.10
6	3	4	15.88	16.18	26.00	9.68
-6	-3	4	14.41	12.68	-24.82	-4.26
-6	3	4	29.00	25.27	49.72	9.76
7	-3	4	7.89	7.59	11.64	-7.39
-7	-3	4	33.54	34.00	56.43	15.83
-7	3	4	16.01	16.01	27.60	-4.54
-8	3	4	6.74	6.38	-11.37	-3.06
0	4	4	25.71	25.73	-44.86	-2.30
0	-4	4	0.	3.01	0.	-0.
1	-4	4	8.10	6.58	-13.32	-4.78
1	4	4	24.17	25.24	-41.90	-5.27
-1	-4	4	10.88	13.87	-18.14	-5.70
-1	4	4	7.80	7.78	12.99	4.11
2	-4	4	42.60	44.77	74.20	5.95
2	4	4	9.58	8.36	16.23	4.11
-2	-4	4	33.59	32.64	58.65	2.31
-2	4	4	12.67	15.18	-17.46	-13.61
3	-4	4	16.20	13.25	28.14	3.09
3	4	4	15.68	15.17	25.93	8.85
-3	-4	4	6.52	6.54	-10.62	-4.13
-3	4	4	4.90	10.01	8.56	-0.00
4	-4	4	43.90	40.29	75.48	13.66
4	4	4	46.52	49.16	-80.90	-7.86
-4	-4	4	8.06	8.75	-13.73	3.14
-4	4	4	14.73	14.73	24.60	7.57
-5	-4	4	17.45	18.27	-30.18	4.32
-5	4	4	6.70	8.66	-11.31	3.04
5	-4	4	0.	2.32	-0.	0.
5	4	4	0.	6.26	-0.	-0.
6	-4	4	7.57	8.49	11.61	6.33
-6	4	4	18.99	18.81	33.18	-0.40
6	4	4	0.	1.44	0.	-0.
-6	-4	4	0.	3.89	-0.	-0.
-7	-4	4	16.05	19.98	-27.44	-5.79
-7	4	4	46.85	44.74	79.40	19.91
7	-4	4	0.	2.18	0.	-0.
-8	4	4	8.27	7.72	-14.18	-2.79
0	-5	4	16.11	16.65	-28.14	0.62
0	5	4	13.83	15.07	23.62	5.11
1	-5	4	85.38	92.98	-148.47	-14.58
1	5	4	68.01	77.94	118.15	12.73
-1	-5	4	23.24	21.56	39.65	8.76

-1	5	4	9.16	9.96	15.71	3.05
2	-5	4	37.01	36.61	63.91	9.85
-2	-5	4	38.72	36.17	67.34	6.58
2	5	4	0.	8.22	0.	-0.
-2	5	4	0.	3.95	-0.	-0.
3	5	4	20.74	21.32	35.02	9.32
-3	-5	4	11.47	8.52	-19.73	-3.50
-3	5	4	33.60	37.58	58.59	3.74
3	-5	4	0.	1.83	0.	-0.
4	-5	4	10.78	9.28	-18.40	-4.02
4	5	4	14.85	14.99	-25.84	-2.35
-4	-5	4	29.52	26.96	46.63	22.06
-4	5	4	41.63	43.50	-72.31	-7.88
5	5	4	6.84	6.14	-10.20	-6.23
-5	-5	4	15.69	12.47	27.25	-2.97
-5	5	4	25.20	23.70	-43.95	2.77
5	-5	4	0.	4.16	0.	0.
6	-5	4	33.92	33.86	58.29	10.75
-6	-5	4	8.12	6.00	-13.02	-5.64
-6	5	4	0.	3.63	-0.	0.
7	-5	4	12.16	13.10	-18.24	-10.89
-7	5	4	22.30	22.27	38.46	6.25
-8	5	4	10.13	9.04	-17.69	-0.44
0	-6	4	38.70	37.85	-67.41	-5.39
0	6	4	28.45	31.37	47.76	13.79
1	6	4	25.37	25.80	-43.75	-7.15
-1	-6	4	9.46	9.49	15.66	5.29
1	-6	4	0.	2.28	0.	-0.
-1	6	4	0.	3.43	-0.	0.
2	-6	4	53.86	52.57	-93.09	-13.86
2	6	4	23.24	22.62	40.47	3.37
-2	6	4	25.17	30.27	-43.60	-5.75
-2	-6	4	0.	3.28	0.	0.
-3	-6	4	24.81	23.60	42.83	6.72
-3	6	4	8.29	8.63	-13.37	-5.56
3	-6	4	0.	5.78	0.	-0.
3	6	4	0.	2.82	-0.	0.
4	-6	4	9.06	9.83	-13.55	-8.19
4	6	4	22.72	22.76	-39.40	-4.89
-4	-6	4	24.58	21.37	-42.79	-3.67
-4	6	4	0.	4.36	-0.	0.
5	-6	4	10.00	7.08	17.09	3.66
5	6	4	15.47	17.23	-26.27	-6.37
-5	-6	4	9.89	8.85	17.01	3.08
-5	6	4	20.53	20.30	-29.25	-20.77
-6	-6	4	7.24	8.42	11.90	-4.29
6	-6	4	0.	3.68	0.	0.
-6	6	4	0.	3.92	-0.	-0.
7	-6	4	10.92	10.91	-16.89	8.89
-7	6	4	17.54	18.34	30.42	3.74
-8	6	4	7.17	5.59	12.43	1.60
0	-7	4	16.00	16.34	-27.28	-6.13
0	7	4	16.57	17.63	28.64	4.27
1	-7	4	11.16	9.16	19.50	0.32
-1	-7	4	62.88	62.42	108.67	16.21

-1	7	4	24.33	27.35	-42.45	-2.37
1	7	4	0.	4.67	-0.	-0.
2	-7	4	15.65	15.43	26.79	5.50
2	7	4	12.51	12.29	-20.93	-6.32
-2	-7	4	20.10	18.98	-34.97	-3.25
-2	7	4	14.45	17.39	24.44	6.35
3	7	4	52.92	56.57	-91.80	-11.14
-3	-7	4	25.58	23.28	-43.74	-9.18
-3	7	4	10.11	12.98	17.65	-0.62
3	-7	4	0.	3.64	0.	-0.
4	-7	4	31.10	31.27	-52.98	-12.07
4	7	4	4.68	5.48	7.88	2.20
-4	-7	4	4.77	3.48	-6.30	-5.46
-4	7	4	9.62	9.75	16.81	-0.12
5	-7	4	28.84	27.83	49.35	10.18
-5	7	4	11.36	8.47	-18.52	-7.14
-5	-7	4	0.	2.99	-0.	0.
-6	7	4	9.14	10.02	15.94	-0.95
6	-7	4	0.	2.17	0.	0.
7	-7	4	9.40	10.69	-16.42	0.16
-7	7	4	8.34	8.93	-14.44	-1.94
-8	7	4	4.06	5.04	5.42	4.58
0	-8	4	31.44	32.15	53.23	13.58
0	8	4	13.78	15.56	23.61	4.74
1	-8	4	11.26	12.60	19.66	0.69
-1	-8	4	18.97	18.80	-33.13	0.96
-1	8	4	24.62	27.89	42.51	6.60
1	8	4	0.	6.02	-0.	-0.
2	-8	4	15.57	15.17	25.33	9.92
2	8	4	25.94	27.16	-43.67	-12.15
-2	-8	4	13.93	13.71	24.03	3.88
-2	8	4	11.15	10.92	-18.73	-5.36
3	-8	4	43.54	41.14	-76.07	-1.21
3	8	4	27.67	29.04	47.52	8.91
-3	8	4	9.61	11.78	3.45	16.43
-3	-8	4	0.	4.39	-0.	-0.
4	8	4	10.39	9.94	-17.63	-4.33
-4	-8	4	11.35	12.20	19.83	-0.05
-4	8	4	20.79	24.96	36.24	2.46
4	-8	4	0.	2.94	-0.	-0.
5	-8	4	7.52	6.91	-5.02	-12.14
-5	8	4	0.	2.21	0.	-0.
-6	8	4	8.20	10.60	-14.11	-2.49
6	-8	4	0.	3.24	0.	0.
-7	8	4	10.13	9.92	-16.49	6.42
0	9	4	7.70	5.19	-8.78	-10.20
0	-9	4	0.	5.41	0.	-0.
1	-9	4	13.33	13.00	23.26	1.13
-1	-9	4	10.99	12.71	-19.19	0.76
1	9	4	0.	2.06	-0.	0.
-1	9	4	0.	0.65	0.	-0.
2	-9	4	35.18	32.52	60.03	13.25
2	9	4	19.80	21.81	-34.48	-2.83
-2	-9	4	6.77	6.40	-11.53	2.63
-2	9	4	17.96	21.42	-31.36	-1.09

3	-9	4	28.03	26.50	-48.44	-7.24
3	9	4	15.57	18.33	26.79	4.73
-3	-9	4	20.46	19.75	-32.35	-15.22
-3	9	4	0.	2.54	-0.	0.
-4	-9	4	10.07	12.10	17.10	4.15
4	-9	4	0.	4.09	-0.	-0.
-4	9	4	0.	1.50	0.	0.
5	-9	4	12.32	11.02	21.50	1.10
-5	9	4	9.52	9.68	16.53	1.88
6	-9	4	17.92	16.08	-29.57	-10.29
-6	9	4	5.68	8.37	-9.30	-3.46
-7	9	4	0.	2.59	-0.	-0.
0	-10	4	18.69	18.97	-31.34	-9.17
0	10	4	22.56	25.16	38.95	6.09
1	-10	4	30.17	29.49	52.72	-0.41
1	10	4	27.44	29.23	-47.26	-8.08
-1	-10	4	14.48	14.07	-25.30	0.01
-1	10	4	19.09	20.18	-28.71	-16.99
2	-10	4	9.69	9.22	-16.93	0.16
2	10	4	9.50	9.42	-16.29	-3.19
-2	-10	4	26.34	26.09	-43.96	-13.62
-2	10	4	11.30	11.59	-19.05	-5.21
3	-10	4	27.05	25.40	45.19	13.84
-3	-10	4	17.22	20.24	30.09	0.39
-3	10	4	0.	1.42	0.	0.
4	-10	4	16.48	16.29	-28.28	-5.42
-4	10	4	6.87	7.34	10.98	4.85
5	-10	4	23.74	22.38	40.66	8.23
-5	10	4	7.13	4.87	5.93	-10.95
6	-10	4	0.	7.58	-0.	-0.
-6	10	4	25.17	25.84	41.11	15.62
0	-11	4	33.41	33.88	-57.36	-10.88
0	11	4	11.79	13.63	20.51	1.94
1	-11	4	13.80	15.27	23.92	3.06
-1	-11	4	7.48	7.95	-13.02	1.13
-1	11	4	9.58	8.68	-16.69	-1.31
1	11	4	0.	1.90	0.	0.
2	-11	4	13.62	11.71	22.68	7.21
-2	-11	4	7.45	7.73	11.32	6.42
-2	11	4	11.63	10.78	-19.95	-3.88
3	-11	4	8.18	6.35	14.10	-2.34
-3	11	4	0.	9.32	-0.	-0.
4	-11	4	12.72	13.08	20.89	7.60
-4	11	4	0.	3.49	0.	0.
5	-11	4	19.28	19.85	32.02	10.46
-5	11	4	9.61	10.66	-16.54	2.87
0	-12	4	13.56	15.60	23.68	0.89
1	-12	4	33.56	36.35	-57.20	-12.92
-1	12	4	6.75	6.14	-11.77	-0.80
2	-12	4	15.12	16.97	26.11	4.02
-2	12	4	8.10	7.48	-12.14	-7.28
3	-12	4	9.22	9.81	-14.52	-6.98
-3	12	4	17.72	24.07	30.42	5.79
4	-12	4	7.34	6.80	12.69	-1.85
-4	12	4	12.37	11.70	-14.68	-15.87

1	0	5	20.60	19.48	-35.95	-1.81
-1	0	5	16.01	13.37	27.89	-2.16
2	0	5	4.68	6.15	-7.63	-2.94
-2	0	5	28.25	26.03	46.99	15.12
3	0	5	8.36	10.89	10.69	-9.95
-3	0	5	0.	4.22	-0.	0.
4	0	5	10.18	10.04	17.04	5.12
-4	0	5	5.77	4.93	9.57	3.19
-5	0	5	12.66	12.17	-21.30	-5.96
5	0	5	0.	37.15	-0.	-0.
6	0	5	5.97	8.04	10.34	1.40
-6	0	5	0.	1.89	0.	0.
-7	0	5	12.34	14.24	-21.13	-4.28
0	-1	5	20.90	22.75	35.21	9.69
0	1	5	0.	5.84	0.	0.
1	-1	5	26.59	25.87	-45.90	-7.21
1	1	5	8.14	7.09	-13.42	-4.72
-1	-1	5	6.20	6.93	10.71	1.62
-1	1	5	9.70	9.71	16.41	4.25
2	-1	5	0.	4.37	0.	-0.
-2	-1	5	0.	5.69	0.	-0.
-2	1	5	0.	3.01	-0.	-0.
3	-1	5	7.64	8.13	13.23	1.78
3	1	5	18.42	20.41	30.97	8.75
-3	-1	5	5.90	4.99	-9.81	-3.16
-3	1	5	39.11	38.93	66.30	16.58
4	-1	5	24.51	21.32	-41.25	-11.53
4	1	5	9.01	8.88	15.67	1.50
-4	-1	5	0.	2.19	-0.	0.
-4	1	5	0.	4.13	-0.	0.
5	-1	5	26.70	27.94	-46.00	-7.76
-5	-1	5	42.43	38.60	-72.10	-17.29
-5	1	5	17.50	16.98	-29.24	-8.94
5	1	5	0.	2.14	-0.	-0.
6	-1	5	6.37	7.45	-10.42	3.92
6	1	5	31.14	35.43	53.63	9.21
-6	-1	5	16.85	17.13	29.36	2.17
-6	1	5	18.37	16.93	-31.67	-5.22
-7	-1	5	7.64	5.82	7.76	10.86
-7	1	5	3.77	5.07	6.46	1.27
0	-2	5	7.90	7.53	13.40	3.30
0	2	5	10.81	13.45	15.59	-10.66
1	-2	5	30.95	30.16	-51.72	15.79
1	2	5	6.06	7.93	-10.58	0.46
-1	2	5	6.01	6.89	-10.23	-2.37
-1	-2	5	0.	2.01	0.	-0.
2	2	5	25.46	25.46	-43.43	-9.64
-2	-2	5	20.81	21.52	-35.09	-9.52
-2	2	5	12.33	12.67	-21.12	-4.26
2	-2	5	0.	3.64	-0.	-0.
3	-2	5	44.08	45.31	76.18	11.39
-3	-2	5	19.53	18.87	-34.00	2.91
3	2	5	0.	2.06	-0.	0.
-3	2	5	0.	3.30	0.	0.
-4	-2	5	46.99	47.57	-80.95	-13.71

-4	2	5	22.56	22.04	39.40	-1.39
4	-2	5	0.	3.43	0.	0.
4	2	5	0.	2.49	0.	0.
5	-2	5	21.84	22.46	-38.02	-3.33
5	2	5	21.85	19.43	36.42	11.44
-5	-2	5	22.03	24.10	38.49	0.36
-5	2	5	5.64	4.36	6.98	6.95
6	2	5	13.35	14.77	-22.97	-4.04
-6	-2	5	6.62	4.94	11.49	-1.37
-6	2	5	41.72	43.28	-72.74	-4.85
6	-2	5	0.	5.03	0.	-0.
-7	-2	5	10.93	10.52	18.27	5.57
-7	2	5	0.	2.61	0.	-0.
0	-3	5	8.97	11.12	15.31	3.37
0	3	5	30.21	35.55	52.37	6.65
1	3	5	2.81	5.59	-3.97	-2.89
-1	-3	5	25.54	26.21	44.49	3.54
-1	3	5	31.25	34.96	-52.79	-13.95
1	-3	5	0.	2.09	-0.	-0.
2	-3	5	14.76	14.32	24.17	8.99
2	3	5	10.68	11.18	-18.00	-4.92
-2	-3	5	13.97	13.52	-22.11	-10.35
-2	3	5	18.05	19.58	-31.46	-2.25
3	-3	5	17.52	18.68	29.53	8.06
3	3	5	11.74	11.75	19.66	5.87
-3	-3	5	5.69	6.74	9.93	0.41
-3	3	5	12.17	13.05	19.93	7.42
4	3	5	13.57	14.43	22.47	7.58
-4	-3	5	14.45	14.53	23.31	9.71
-4	3	5	22.77	22.38	39.08	7.48
4	-3	5	0.	1.58	-0.	-0.
5	-3	5	7.55	7.49	-12.19	-5.04
5	3	5	7.07	8.57	-8.24	-9.20
-5	3	5	17.12	17.55	-29.69	-3.64
-5	-3	5	0.	4.95	0.	0.
6	-3	5	5.61	2.15	-9.80	-0.18
-6	3	5	48.01	49.90	81.89	18.20
-6	-3	5	0.	0.85	0.	0.
-7	3	5	9.68	10.19	-16.91	-0.13
0	-4	5	5.42	6.89	-8.69	3.78
0	4	5	14.68	17.57	25.23	4.63
1	4	5	14.09	12.96	24.33	3.75
-1	-4	5	9.99	9.96	-4.07	-16.98
1	-4	5	0.	22.82	-0.	-0.
-1	4	5	0.	3.23	-0.	-0.
2	-4	5	18.11	16.25	-31.39	-3.98
2	4	5	19.76	22.53	-32.87	10.57
-2	4	5	23.78	25.42	-41.55	-0.33
-2	-4	5	0.	1.30	0.	-0.
3	-4	5	0.	7.38	0.	0.
3	4	5	0.	2.60	-0.	0.
-3	-4	5	0.	3.88	0.	0.
-3	4	5	0.	3.36	0.	-0.
4	-4	5	17.90	18.11	29.53	10.32
4	4	5	23.40	24.37	40.17	7.61

-4	-4	5	19.68	20.55	33.45	7.96
-4	4	5	30.58	33.38	53.31	3.65
5	-4	5	25.93	23.29	-43.45	-12.84
-5	4	5	10.67	11.28	18.63	-0.67
5	4	5	0.	7.45	-0.	-0.
-5	-4	5	0.	4.16	0.	-0.
6	-4	5	10.93	10.11	17.91	6.64
-6	-4	5	25.12	23.49	41.62	13.94
-6	4	5	7.16	9.12	11.92	3.80
-7	4	5	11.38	11.87	19.60	3.37
0	-5	5	17.36	17.62	-29.56	-6.81
0	5	5	11.41	11.36	19.44	4.41
1	-5	5	14.77	14.80	-24.57	-7.91
1	5	5	29.25	30.94	49.55	12.54
-1	-5	5	21.29	21.23	-36.93	4.49
-1	5	5	4.92	5.09	-6.22	-5.94
2	-5	5	8.22	8.35	-14.36	-0.25
2	5	5	22.53	22.92	-38.20	-9.53
-2	-5	5	22.58	22.36	-39.19	-4.60
-2	5	5	20.53	23.03	-34.84	-8.54
3	5	5	7.00	7.90	10.63	6.05
-3	-5	5	8.85	8.02	15.46	-0.24
-3	5	5	14.34	15.15	24.53	5.12
3	-5	5	0.	3.56	0.	0.
4	-5	5	8.76	6.62	15.30	-0.41
4	5	5	13.58	15.30	23.65	1.90
-4	-5	5	25.37	24.23	43.46	8.74
-4	5	5	54.37	61.67	-93.51	-16.77
5	-5	5	46.95	43.62	81.06	12.62
-5	-5	5	11.41	12.04	-19.82	-2.15
-5	5	5	6.02	6.51	-10.22	-2.48
6	-5	5	9.68	9.38	15.95	5.64
-6	-5	5	10.93	10.76	-16.66	-9.34
-6	5	5	0.	2.38	0.	0.
-7	5	5	0.	3.19	0.	0.
0	-6	5	25.73	24.50	44.53	6.23
0	6	5	10.20	12.89	17.76	1.44
1	-6	5	19.85	18.25	34.66	-1.36
-1	-6	5	11.73	11.67	18.02	9.76
-1	6	5	10.32	7.83	15.99	8.33
1	6	5	0.	3.36	-0.	0.
2	-6	5	6.70	8.41	5.87	-10.13
2	6	5	16.66	18.35	-28.61	-5.40
-2	-6	5	6.51	7.58	-10.89	-3.28
-2	6	5	0.	2.58	0.	-0.
3	-6	5	17.27	17.32	28.26	10.59
3	6	5	4.27	4.48	-6.62	-3.44
-3	-6	5	40.96	37.23	69.03	18.91
-3	6	5	9.03	9.06	-15.71	1.49
4	-6	5	8.20	9.32	-13.52	-4.74
4	6	5	8.35	7.31	-8.33	-11.98
-4	-6	5	4.41	4.00	-7.70	-0.31
-4	6	5	12.79	12.27	-22.18	-2.75
-5	-6	5	9.90	7.32	-16.84	-3.98
-5	6	5	14.81	14.39	-25.31	-5.38

5	-6	5	0.	1.46	0.	-0.
6	-6	5	20.12	18.92	34.37	7.41
-6	6	5	11.09	9.30	19.37	-0.51
-7	6	5	24.58	25.72	42.33	7.29
0	-7	5	11.64	10.72	20.12	2.94
0	7	5	6.28	6.88	4.39	10.06
1	7	5	2.86	2.74	3.34	3.71
-1	-7	5	4.26	4.57	4.60	5.85
-1	7	5	11.22	12.23	-18.70	-5.88
1	-7	5	0.	4.98	-0.	-0.
2	-7	5	17.04	16.59	-29.77	0.64
2	7	5	2.60	4.24	-3.05	-3.37
-2	-7	5	6.75	4.85	9.50	6.99
-2	7	5	43.43	47.76	74.20	15.89
3	-7	5	27.08	23.21	-45.30	-13.66
3	7	5	24.92	24.83	-42.36	-10.08
-3	-7	5	14.78	14.21	25.29	-5.22
-3	7	5	5.63	4.88	7.89	5.88
4	-7	5	20.89	20.44	-36.08	-5.52
-4	-7	5	13.74	13.62	23.63	4.23
-4	7	5	12.80	12.92	-22.25	-2.27
5	-7	5	22.41	22.48	-38.72	-5.86
-5	7	5	9.18	8.23	-14.18	-7.49
-6	7	5	30.58	31.96	52.98	6.95
6	-7	5	0.	5.89	0.	0.
-7	7	5	17.17	19.53	-27.48	-12.03
0	-8	5	7.01	8.26	-3.03	11.87
0	8	5	0.	0.91	0.	0.
1	-8	5	20.77	20.14	-35.20	-8.85
1	8	5	6.43	5.16	7.58	-8.30
-1	-8	5	6.43	5.14	-11.20	-0.89
-1	8	5	10.21	10.70	17.76	-1.72
2	-8	5	8.07	7.06	13.32	4.62
2	8	5	10.72	11.89	18.57	-2.45
-2	-8	5	22.39	21.69	-38.38	-7.59
-2	8	5	0.	2.72	-0.	-0.
3	-8	5	24.91	22.89	43.33	4.14
-3	-8	5	16.43	17.35	-27.83	-7.04
-3	8	5	17.49	19.23	30.01	5.75
4	-8	5	20.47	20.90	-35.35	-5.47
-4	8	5	12.57	13.81	-21.93	1.26
-4	-8	5	0.	10.41	0.	0.
5	-8	5	9.73	9.18	-13.07	-10.87
-5	8	5	24.48	25.18	-42.17	-7.16
6	-8	5	31.96	31.04	54.62	11.63
-6	8	5	11.26	12.01	-19.46	-2.88
0	-9	5	10.97	9.30	19.13	-1.14
0	9	5	32.51	35.67	-55.21	-13.38
1	-9	5	8.93	8.96	10.91	11.16
1	9	5	4.53	4.75	4.83	6.27
-1	-9	5	12.15	11.42	20.32	6.16
-1	9	5	18.09	21.16	-31.10	-5.66
2	-9	5	15.45	14.11	26.52	5.03
-2	-9	5	7.40	7.26	-12.08	-4.61
-2	9	5	0.	2.95	0.	0.

3	-9	5	30.60	30.80	52.89	7.83
-3	-9	5	13.62	13.68	-23.45	-4.03
-3	9	5	14.33	14.15	23.59	8.38
4	-9	5	9.52	7.93	16.15	-4.00
-4	9	5	22.72	26.38	-39.22	-6.16
5	-9	5	8.97	8.17	-15.60	1.52
-5	9	5	36.96	39.51	63.38	12.40
-6	9	5	0.	0.79	0.	0.
0	10	5	12.31	13.81	21.36	2.51
0	-10	5	0.	2.08	0.	-0.
1	-10	5	30.73	29.21	-53.33	-6.28
-1	-10	5	23.89	22.49	41.29	6.14
-1	10	5	14.48	14.54	-24.44	-6.53
2	-10	5	9.47	9.48	16.20	3.38
-2	-10	5	10.68	10.67	-12.44	-13.91
-2	10	5	0.	3.06	0.	-0.
3	-10	5	23.64	21.29	39.30	12.72
-3	10	5	13.50	15.97	22.95	5.44
4	-10	5	19.88	18.87	-33.25	-10.06
-4	10	5	23.37	25.73	40.70	3.38
5	-10	5	28.29	28.86	-49.42	-1.26
-5	10	5	0.	0.52	0.	0.
0	-11	5	5.05	4.65	-8.08	-3.55
1	-11	5	25.28	26.06	-43.31	-8.68
2	-11	5	7.03	6.29	-12.00	2.64
3	-11	5	6.11	7.02	10.61	-1.17
1	0	6	33.61	35.27	58.46	5.59
-1	0	6	19.87	21.17	-34.01	-7.00
-2	0	6	47.40	49.85	81.67	13.75
2	0	6	0.	3.75	-0.	-0.
3	0	6	26.16	26.14	-44.99	-8.07
-3	0	6	14.21	15.36	24.75	1.99
4	0	6	24.82	27.44	42.12	10.32
-4	0	6	28.88	29.69	-49.91	-7.48
-5	0	6	16.73	15.28	-27.70	-9.36
5	0	6	0.	5.06	-0.	-0.
-6	0	6	0.	3.53	-0.	0.
0	1	6	7.06	9.23	-12.34	-0.03
0	-1	6	0.	6.18	-0.	0.
1	-1	6	31.91	33.29	55.15	8.22
1	1	6	59.16	66.46	-102.82	-10.67
-1	1	6	15.58	18.24	-26.80	-4.78
-1	-1	6	0.	47.89	0.	0.
2	-1	6	8.48	9.33	-14.39	-3.54
2	1	6	6.46	8.16	10.96	-2.68
-2	-1	6	0.	0.45	0.	-0.
-2	1	6	0.	4.71	0.	0.
3	-1	6	7.65	6.52	-13.31	-1.26
3	1	6	11.74	12.67	-19.56	-6.19
-3	-1	6	20.53	20.82	35.54	4.87
-3	1	6	18.67	20.33	-32.51	2.72
4	-1	6	30.41	28.97	-51.93	-11.25
4	1	6	11.32	12.43	19.37	3.98
-4	-1	6	7.92	8.74	-13.29	-3.87
-4	1	6	9.02	6.87	14.71	5.65

5	-1	6	6.43	6.45	11.14	1.44
5	1	6	7.18	5.27	12.50	1.05
-5	-1	6	0.	0.79	-0.	-0.
-5	1	6	0.	4.35	0.	-0.
-6	-1	6	6.55	4.34	-10.53	-4.47
-6	1	6	0.	0.77	0.	0.
0	-2	6	6.23	7.35	-10.30	3.51
0	2	6	15.51	21.75	-25.56	-9.00
1	-2	6	30.32	31.80	52.15	9.35
1	2	6	10.26	8.85	14.66	10.32
-1	-2	6	52.11	54.06	-90.67	-8.31
-1	2	6	0.	3.28	0.	-0.
2	-2	6	28.75	27.85	-49.14	-10.42
2	2	6	29.73	32.11	-51.24	-8.56
-2	-2	6	16.06	13.71	-27.11	-7.23
-2	2	6	29.01	31.67	50.41	5.34
3	-2	6	12.01	12.05	-20.97	0.90
-3	-2	6	22.23	21.80	38.48	5.27
-3	2	6	34.99	36.45	60.21	10.62
3	2	6	0.	3.77	-0.	-0.
4	2	6	6.35	6.80	8.99	6.51
-4	-2	6	40.25	41.02	-68.78	-14.70
4	-2	6	0.	4.13	0.	0.
-4	2	6	0.	2.73	-0.	-0.
5	-2	6	9.46	8.97	11.21	-12.14
-5	-2	6	19.99	20.59	-34.93	0.04
-5	2	6	31.45	30.19	52.22	17.10
-6	-2	6	22.92	23.95	39.23	8.06
-6	2	6	18.93	20.96	33.04	1.60
0	3	6	6.36	7.95	-11.11	-0.19
0	-3	6	0.	7.75	0.	0.
1	-3	6	11.77	11.19	20.53	1.16
1	3	6	10.53	11.97	17.76	4.81
-1	-3	6	32.40	33.76	-55.87	-9.17
-1	3	6	12.30	15.57	21.23	-3.36
2	-3	6	44.98	44.21	77.62	12.36
-2	-3	6	10.76	10.12	18.78	-0.99
-2	3	6	10.08	11.67	-16.88	-5.04
2	3	6	0.	0.53	0.	0.
3	3	6	34.12	37.30	58.64	10.76
-3	-3	6	13.44	11.27	-19.51	-13.07
3	-3	6	0.	5.37	-0.	-0.
-3	3	6	0.	5.87	0.	0.
4	-3	6	21.72	23.60	36.62	9.97
4	3	6	5.28	6.30	8.68	3.12
-4	3	6	15.89	17.68	-27.75	-1.02
-4	-3	6	0.	5.39	-0.	0.
5	-3	6	0.	4.54	-0.	-0.
-5	-3	6	0.	23.08	-0.	-0.
-5	3	6	0.	2.85	0.	0.
-6	3	6	15.35	15.48	25.88	7.03
0	-4	6	13.44	12.98	22.12	7.90
0	4	6	13.40	13.94	-23.21	-3.06
-1	-4	6	31.83	29.75	-54.46	-11.28
-1	4	6	34.70	39.37	-59.60	-11.15

1	-4	6	0.	1.10	0.	0.
1	4	6	0.	6.60	0.	0.
2	-4	6	12.28	13.11	-21.16	-3.56
2	4	6	12.01	13.31	18.98	8.95
-2	-4	6	12.68	13.34	-22.10	-1.62
-2	4	6	6.07	5.92	9.22	5.24
3	-4	6	9.88	12.85	15.28	8.03
3	4	6	14.00	16.05	-23.08	-8.10
-3	-4	6	47.90	48.98	83.10	9.98
-3	4	6	41.58	47.48	-71.34	-13.76
4	-4	6	20.23	19.18	34.08	9.38
4	4	6	22.86	24.84	38.98	8.72
-4	-4	6	19.09	18.03	33.08	4.26
-4	4	6	13.16	15.28	-22.76	-3.30
5	-4	6	14.05	13.97	-23.84	-5.87
-5	-4	6	0.	3.33	-0.	-0.
-5	4	6	0.	0.87	-0.	0.
-6	4	6	15.95	15.71	26.77	7.74
0	-5	6	49.71	52.41	-85.96	-12.46
0	5	6	25.87	29.79	44.76	6.29
1	-5	6	17.73	17.05	30.90	2.24
-1	-5	6	6.92	5.98	-12.06	-0.82
-1	5	6	17.59	21.46	-30.49	-3.90
1	5	6	0.	2.76	0.	0.
2	-5	6	23.64	25.64	-39.84	-10.92
-2	5	6	11.83	13.54	20.66	0.60
2	5	6	0.	4.00	-0.	-0.
-2	-5	6	0.	2.65	-0.	-0.
3	-5	6	9.63	8.07	16.83	0.23
3	5	6	10.62	13.00	-18.17	-3.75
-3	-5	6	13.92	14.01	22.45	9.36
-3	5	6	0.	5.21	0.	0.
4	-5	6	7.38	6.78	-12.81	1.52
-4	-5	6	9.19	8.54	-16.05	-0.63
-4	5	6	0.	7.19	-0.	-0.
5	-5	6	22.29	21.39	38.18	7.67
-5	5	6	0.	0.91	-0.	-0.
-6	5	6	12.24	13.15	19.38	9.05
0	-6	6	33.07	35.11	57.53	5.37
0	6	6	8.40	8.33	-13.84	-4.88
1	-6	6	23.61	20.80	-40.14	-9.52
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-1	6	6	27.52	32.39	46.61	11.84
-1	-6	6	0.	2.63	-0.	-0.
2	-6	6	34.33	35.58	-59.28	-9.15
2	6	6	9.43	10.04	16.48	0.28
-2	-6	6	15.38	13.87	-26.41	-4.96
-2	6	6	5.53	9.67	9.20	2.97
3	-6	6	17.37	15.91	30.07	4.12
-3	-6	6	15.39	15.47	24.96	10.01
-3	6	6	7.15	8.45	12.48	0.47
4	-6	6	13.61	13.27	23.52	3.49
-4	-6	6	12.88	14.10	22.50	-0.65
-4	6	6	16.45	18.41	-27.59	-8.06
5	-6	6	9.07	8.86	-15.73	-1.94

-5	6	6	11.41	12.30	-19.25	5.19
-6	6	6	19.48	21.90	-32.69	-9.50
0	-7	6	25.88	25.86	43.71	11.61
0	7	6	0.	2.74	-0.	0.
1	-7	6	0.	1.73	-0.	0.
1	7	6	0.	7.86	0.	0.
-1	-7	6	0.	2.82	-0.	-0.
-1	7	6	0.	6.05	-0.	-0.
-2	-7	6	42.95	46.08	74.00	12.52
-2	7	6	9.38	11.52	-14.99	6.63
2	-7	6	0.	0.71	0.	-0.
3	-7	6	21.73	22.79	-36.95	-8.74
-3	7	6	14.35	17.88	24.97	2.30
-3	-7	6	0.	0.75	-0.	-0.
4	-7	6	21.22	22.56	36.16	8.19
-4	7	6	10.03	9.75	-14.93	-9.18
5	-7	6	16.72	17.06	-28.34	-7.10
-5	7	6	11.47	13.86	-19.64	-3.99
0	-8	6	0.	24.18	0.	0.
0	8	6	0.	7.01	-0.	-0.
1	-8	6	9.76	6.28	-16.95	-1.92
-1	-8	6	9.13	9.23	14.87	5.78
-1	8	6	9.72	12.61	-16.87	-1.97
2	-8	6	14.52	13.91	-24.86	-5.09
-2	-8	6	36.83	40.81	-64.07	-6.07
-2	8	6	22.08	25.99	37.75	7.98
3	-8	6	16.92	17.39	29.43	2.77
-3	8	6	7.48	6.00	11.88	-5.45
4	-8	6	9.36	9.58	11.48	-11.65
-4	8	6	10.16	10.46	14.67	10.00
0	-9	6	0.	2.80	0.	0.
1	-9	6	23.29	23.53	39.33	10.44
-1	-9	6	8.89	7.55	-14.68	-5.09
2	-9	6	11.98	11.44	-19.16	-8.44
3	-9	6	12.34	12.47	20.46	6.80
1	0	7	0.	3.02	0.	0.
-1	0	7	0.	1.25	0.	-0.
2	0	7	18.43	18.05	-29.49	-12.94
-2	0	7	14.25	33.30	24.78	2.43
3	0	7	18.32	21.93	-31.68	-4.63
-3	0	7	11.22	11.83	18.93	5.11
-4	0	7	14.46	15.33	-23.89	-8.22
0	-1	7	13.73	16.98	-23.30	-5.73
0	1	7	9.68	11.80	-16.70	-2.69
1	1	7	17.83	17.36	-29.66	-9.52
-1	-1	7	26.13	26.11	44.29	11.10
-1	1	7	5.73	10.07	-9.93	1.27
1	-1	7	0.	7.69	0.	0.
2	1	7	12.16	12.86	20.12	6.84
-2	1	7	19.56	21.88	32.12	11.69
2	-1	7	0.	6.34	-0.	0.
-2	-1	7	0.	3.79	-0.	0.
3	-1	7	16.31	18.23	-27.98	-5.39
3	1	7	7.67	8.82	-9.51	-9.44
-3	-1	7	0.	6.13	0.	-0.

-3	1	7	0.	1.86	0.	-0.
-4	-1	7	20.05	22.75	-33.53	-10.15
-4	1	7	14.26	16.10	22.02	11.66
0	-2	7	19.40	21.09	32.16	10.73
0	2	7	27.39	33.33	-47.61	-4.83
1	-2	7	17.81	20.25	30.74	4.85
1	2	7	12.41	15.00	21.46	3.13
-1	2	7	19.78	17.38	-33.48	-8.59
-1	-2	7	0.	4.16	0.	-0.
2	-2	7	6.70	8.51	11.08	3.77
2	2	7	11.41	13.35	19.79	2.44
-2	2	7	13.50	16.87	22.86	5.82
-2	-2	7	0.	4.99	0.	0.
3	-2	7	9.58	8.21	16.18	-4.27
-3	2	7	10.45	11.00	18.24	0.86
-3	-2	7	0.	1.27	-0.	-0.
-4	-2	7	13.87	14.51	-23.83	-4.41
-4	2	7	13.03	15.13	-22.61	-2.64
0	-3	7	5.87	8.14	9.44	-4.01
0	3	7	12.70	16.42	-19.66	-10.30
1	-3	7	13.11	14.91	22.45	4.56
-1	-3	7	19.05	18.39	-31.76	-9.96
1	3	7	0.	0.26	0.	0.
-1	3	7	0.	1.66	0.	0.
2	-3	7	10.62	13.28	-17.63	5.81
2	3	7	9.79	13.20	16.93	2.42
-2	3	7	15.21	16.48	-23.91	-11.61
-2	-3	7	0.	4.54	0.	0.
3	-3	7	13.92	14.60	-22.20	-9.94
-3	-3	7	24.56	27.29	-41.49	-10.97
-3	3	7	0.	7.24	0.	-0.
-4	3	7	0.	2.14	-0.	-0.
0	4	7	8.28	7.76	-13.47	-5.28
0	-4	7	0.	4.21	-0.	-0.
1	4	7	5.03	5.50	2.76	8.34
-1	-4	7	17.76	19.14	-30.74	-4.27
1	-4	7	0.	3.19	0.	0.
-1	4	7	0.	2.78	-0.	-0.
2	-4	7	4.87	8.75	-8.44	-1.07
-2	-4	7	18.82	20.37	-31.54	-9.31
-2	4	7	12.26	13.25	20.78	5.20
3	-4	7	23.60	24.01	39.77	10.92
-3	-4	7	5.78	5.22	-9.13	4.32
-3	4	7	35.11	42.35	-60.94	-7.10
-4	4	7	7.19	6.57	-12.12	-3.31
0	-5	7	9.50	8.21	-13.23	-10.03
0	5	7	28.06	32.78	48.05	9.76
1	-5	7	14.49	16.68	23.97	8.14
-1	5	7	15.01	18.83	26.11	2.47
-1	-5	7	0.	2.67	0.	-0.
-2	-5	7	10.79	13.78	-17.72	6.43
2	-5	7	0.	2.78	0.	-0.
-2	5	7	0.	5.95	0.	0.
3	-5	7	6.17	4.96	10.54	-2.25
-3	5	7	15.41	19.52	-26.02	-6.94

0	-6	7	7.28	6.49	-12.53	2.17
1	-6	7	25.68	27.24	-43.62	-10.51
-1	-6	7	0.	4.47	-0.	-0.
2	-6	7	0.	4.28	-0.	-0.

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Miss Deborah Jope typed the final draft of this thesis, and Mrs. Shirley Veale and Miss Gay Lorraine the final drafts of the published papers.

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BIOGRAPHY

The author was born February 15, 1937 at Somerville, Massachusetts to Carroll and Leona Peacor. He has two brothers, C. Norman, and Robert W.

He attended grade school and high school in Stoneham, Massachusetts from 1942 to 1954. Institutions attended include Tufts University (1954-1958), where he received the degree of Bachelor of Science, Magna Cum Laude, and M.I.T. (1958-1962) where he received the degree of Master of Science in 1960. At Tufts University he was a laboratory assistant for three years in the Department of Geology, and both a teaching and research assistant in the Department of Geology & Geophysics at M.I.T.

Professional experience includes the following: Summer of 1955 as a geological field assistant; Summer of 1957 as a field assistant in Greenland involved in permafrost research; Summers of 1959 and 1960 research assistant in crystallography in the Department of Geology of M.I.T.; Summer of 1961, staff member at Lincoln Laboratory.

The author received the Standard Oil of California fellowship at M.I.T., 1961-1962, and is a member of Sigma Xi.

He is a co-author of the following publications.

1. M. J. Buerger, C. W. Burnham and D. R. Peacor (1962) Assessment of the several structures proposed for tourmaline. Acta Cryst., 15, 583-590.

2. D. R. Peacor and M. J. Buerger (1962) The determination and refinement of the structure of narsarsukite, $Na_2Ti^{i}OSi^{i}_4O_{10}$. Am. Mineral.

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He was married to Miss Dorothy Coniaris of Milford, Massachusetts on February 1, 1959. They have a son, Scott David, born February 1, 1962. The author has accepted a position as instructor in the Department of Geology and Mineralogy, University of Michigan, beginning September, 1962.

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