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The crystal structure of hodgkinsonite $Zn_2Mn[(OH)_2|SiO_4]$

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With 8 figures

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Auszug

Hodgkinsonit, $Zn_2Mn[(OH)_2|SiO_4]$, ist ein pneumatolytisches Mineral von Franklin, New Jersey, mit Gitterkonstanten: $a = 8{,}171$, $b = 5{,}316$, $c = 11{,}761$ Å, $\beta = 95°15'$; $Z = 4$, Raumgruppe $P2_1/a$. Die Intensitäten der Reflexe *hkl* wurden mit Hilfe eines Einkristall-Zählrohr-Diffraktometers (equi-inclination) gemessen. Die Struktur wurde aus der dreidimensionalen Patterson-Synthese mit Hilfe der Minimum-Funktion ermittelt. Atom-Koordinaten und isotrope Temperaturfaktoren wurden nach der Methode der kleinsten Quadraten bis zu $R = 0{,}067$ verfeinert. Korrektur für anomale Dispersion in bezug auf die Mn-Atome wurde berücksichtigt.

Das SiO_4-Tetraeder ist fast regelmäßig mit mittlerem Si—O Abstand 1,626 Å und O—O Abstand 2,655 Å. Die zwei Zn-Atome sind von vier O-Atomen in Form eines verzerrten Tetraeders umgeben; mittlere Zn—O-Abstände 1,969 Å und 1,974 Å und O—O-Abstände 3,211 Å und 3,216 Å. Das Mn-Atom ist von fünf OH-Gruppen und einem O-Atom umgeben, welche ein ziemlich stark verzerrtes Oktaeder bilden. Mittlerer Mn—O Abstand 2,222 Å und O—O Abstand 3,133 Å. Die ZnO_4-Tetraeder haben mit den SiO_4-Tetraedern eine gemeinsame Spitze und formen zweidimensionale Zn_2SiO_4-Netze, (*A*), parallel (001). Ähnlicherweise bilden die MnO_6-Oktaeder zweidimensionale Netze, (*B*), parallel (001), welche zwei Zn_2SiO_4-Netze verbinden. Das Bauprinzip ist . . *ABAABA* . . der *c*-Achse entlang. Es besteht keine Isotypie zwischen Hodgkinsonit und Norbergit, $Mg_3[(OH)_2|SiO_4]$; das Mineral gehört der Humit-Gruppe nicht an.

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Abstract

Hodgkinsonite, $Zn_2Mn[(OH)_2|SiO_4]$, is a pneumatolytic mineral of Franklin, New Jersey, with lattice constants: $a = 8.171$, $b = 5.316$, $c = 11.761$ Å, $\beta = 95°15'$; $Z = 4$, space group $P2_1/a$. Intensities *hkl* were collected with a single-crystal equi-inclination diffractometer. The structure was obtained from the three-dimensional Patterson synthesis by applying the minimum function. Atomic parameters and isotropic temperature factors were refined by least squares to $R = 0.067$. Correction for anomalous scattering of the Mn atoms was applied.

The SiO_4 tetrahedron is almost regular with an average Si—O distance of 1.626 Å and average O—O distance of 2.655 Å. The two Zn atoms are surrounded by four O atoms forming a distorted tetrahedron. Average Zn—O distances are 1.969 Å and 1.974 Å and O—O distances 3.211 Å and 3.216 Å respectively. The Mn atom is octahedrally coordinated by five OH groups and one O atom. The average Mn—O distance is 2.222 Å and the corresponding O—O distance is 3.133 Å. The ZnO_4 tetrahedra share a corner with the SiO_4 tetrahedra and form two-dimensional networks Zn_2SiO_4, (*A*), parallel to (001). Similarly the MnO_6 octahedra form two-dimensional networks, (*B*), extending parallel to (001), and link two Zn_2SiO_4 networks together. The structural principle is . . *ABAABA* . . in the direction of the *c* axis. Hodgkinsonite is not isotypic with norbergite, $Mg_3[(OH)_2|SiO_4]$, and does not belong to the humite group.

Introduction

Hodgkinsonite, $Zn_2Mn[(OH)_2|SiO_4]$, is a pink pneumatolytic mineral found at Franklin, New Jersey, U.S.A., in association with other zinc minerals, mostly franklinite and willemite. It was discovered by H. HODGKINSON and first studied morphologically and chemically by PALACHE and SCHALLER (1913), who named the mineral after its discoverer. Detailed optical, morphological and chemical study of the mineral, alone or in connection with other minerals from Franklin, was reported at various times again by PALACHE (1914, 1928, 1935). Recent reexamination of hodgkinsonite crystals by ROBERTS and QUODLING (1962) gave almost identical results. The crystals are monoclinic, usually elongated along the *c* axis, with a perfect (001) cleavage.

X-ray data concerning the unit cell and space group of hodgkinsonite were first given by the author (RENTZEPERIS, 1958). Part of corresponding data recently published by ROBERTS and QUODLING (1962) must, for reasons explained below, be considered as erroneous.

From the similarity of the chemical formula of hodgkinsonite with that of norbergite, $Mg_2Mg[(OH)_2|SiO_4]$ the mineral has been considered isotypic with the latter and grouped with the humite family. However, as hodgkinsonite is monoclinic and norbergite orthorhombic, and as, in many instances, Zn behaves differently from Mg, it was thought very probable that hodgkinsonite might have a different structure from that of norbergite, and this actually proved to be the case. And since the high refractive index (~ 1.74) indicated a very probable oxygen substructure, the mineral was considered as very suitable for testing the resolving power of the three-dimensional minimum function (BUERGER, 1959) in such instances.

Experimental

The desirability of having accurate settings for the single-crystal equi-inclination diffractometer used for collecting intensities led to a careful redetermination of the unit-cell constants with a precession camera and Mo$K\alpha$ radiation ($\lambda = 0.71069$ Å). The new data differ only slightly from those already published by the author (RENTZEPERIS, 1958), the differences being within the experimental errors of the methods used then:

$$\begin{array}{ll} a = 8.170 \pm 0.002 \text{ Å} & \beta = 95°15' \pm 5' \\ b = 5.316 \pm 0.002 \text{ Å} & V = 508.67 \text{ Å}^3 \\ c = 11.761 \pm 0.002 \text{ Å} & a:b:c = 1.5370:1:2.2124 \end{array}$$

The angle β and the axial ratios are in very good agreement with those found by PALACHE (1914): $\beta = 95°25'$, $a:b:c = 1.538:1:1.1075$. As in numerous other cases the c axis of the morphological result proves to be half its true value.

ROBERTS and QUODLING (1962) give the following values for the cell constants: $a = 8.12 \pm 0.05$ Å, $b = 5.30 \pm 0.05$ Å, $c = 11.71 \pm 0.05$ Å, $\beta = 95°15'$. The values for a and c are so close to the value of

$$d_{100} = a \sin\beta = 8.136 \text{ Å} \qquad d_{001} = c \sin\beta = 11.712 \text{ Å},$$

found in this investigation, that it seems almost certain that ROBERTS and QUODLING have actually reported their d_{100} and d_{001} values instead of a and c. Their proposed reorientation of the crystal axes by interchanging a and c in the original setting by PALACHE and SCHALLER (1913) cannot be considered as actually necessary.

For a unit-cell content of four formula units, a density of 4.07 $\text{g} \cdot \text{cm}^{-3}$ is deduced, which compares well with 3.91 $\text{g} \cdot \text{cm}^{-3}$ given by PALACHE and SCHALLER (1913), 3.99 $\text{g} \cdot \text{cm}^{-3}$ by ROBERTS and QUODLING (1962) and 4.01 $\text{g} \cdot \text{cm}^{-3}$ found by us with the help of a Clerici solution.

The observed reflections were: *hkl*, no conditions; 0*kl*, no conditions; *h*0*l*, $h = 2n$; *hk*0, no conditions; 0*k*0, $k = 2n$. The only possible space group is $P2_1/a$.

At first an attempt was made to solve the structure by using two-dimensional data obtained from small, almost cylindrical, crystals by precession and Weissenberg methods. As no satisfactory solution was obtained in this way it was thought best to proceed with three-dimensional data. Small spheres of hodgkinsonite were ground in a device similar to that described by BOND (1951). A sphere of radius $R = 0.185$ mm was selected and mounted optically along the shortest axis, *b*. Intensities were collected with a single-crystal equi-inclination diffractometer (BUERGER, 1960) using Cu$K\alpha$ radiation. The response of the Geiger counter was kept linear during all the measurements by using Al foils of measured absorption coefficient. The counting rate was always below 400 counts/second.

The diffractometer settings Υ and φ were computed on the IBM 7090 computer at M.I.T. using the program written by PREWITT (1960, 1962). Six levels were measured with a total of 946 accessible reflections, none of which was actually zero. Intensities were measured as follows: using the suitable Al foil the background count for 100 sec was first obtained, then the reflection was scanned slowly (2/3 degree/min), and lastly the background on the other side of the reflection was measured again. The reproducibility of the measurements was of the order of 1 to 2%. The integrated intensity was obtained from

$$I = C - \left(\frac{B_1 + B_2}{2}\right) \cdot \frac{T}{100}$$

where C is the total count of the peak, B_1 and B_2 the background counts before and after the measurement of the peak, and T the time required to scan the peak. This data reduction was done on the IBM 7090 computer using the program DTRDA by BURNHAM (1961). The integrated intensities obtained from DTRDA were further corrected for spherical absorption and Lp factor using the program DTRDB by BURNHAM and a special program for spherical absorption by PREWITT (1962). Hodgkinsonite absorbs Cu radiation rather highly, having $\mu = 344.80\ \mathrm{cm}^{-1}$, and for the sphere used, $\mu R = 6.378$. The values of the absorption coefficient A were obtained from the International Tables (1959).

All subsequent computations were carried out on the IBM 7090 computer at the Computation Center of M.I.T.

Determination of the structure

A three-dimensional Patterson synthesis with sections normal to the b axis and at intervals of 1/60 along the three axes was computed using the program ERFR2 written by Sly, Shoemaker and Van den Hende (1962). Figures 1, 2, and 3 show three sections of the Patterson function at heights $y = 0$, 8/60 and 1/2 (Harker section).

The general approach to the solution of the Patterson synthesis was as follows: Since the equipoints of the general position in space group $P2_1/a$ are

$$x, y, z; \qquad \bar{x}, \bar{y}, \bar{z}; \qquad \tfrac{1}{2} - x, \tfrac{1}{2} + y, \bar{z}; \qquad \tfrac{1}{2} + x, \tfrac{1}{2} - y, z;$$

it follows that an atom at a general position xyz, with its symmetry equivalent atoms, gives rise to the following peaks in the Patterson space:

inversion peak at $2x, 2y, 2z$, of weight 1
rotation peak at $\tfrac{1}{2} - 2x, \tfrac{1}{2}, 2z$, of weight 2 (Harker section)
reflection peak at $\tfrac{1}{2}, \tfrac{1}{2} - 2y, 0$, of weight 2 (Harker line).

Owing to the center of symmetry on the Harker section, the peak $\tfrac{1}{2} - 2x\ \tfrac{1}{2}\ 2z$ appears also at $\tfrac{1}{2} + 2x\ \tfrac{1}{2}\ 2z$ and, if the origin of the section is shifted to $\tfrac{1}{2}\ \tfrac{1}{2}\ 0$, then this last peak will have coordinates $2x\ \tfrac{1}{2}\ 2z$. Consequently, a double rotation satellite on the Harker section would fall exactly on the corresponding single inversion peak every time the Harker section, with its origin shifted to $\tfrac{1}{2}\ \tfrac{1}{2}\ 0$, were superposed on a Patterson section at height $2y$ containing the inversion peak $2x\ 2y\ 2z$. The authenticity of the single inversion peak could be further established by referring to the reflection satellite at height $\tfrac{1}{2} - 2y$ on the Harker line $\tfrac{1}{2}\ y\ 0$. In this way one could find image points which would allow the application of the three-dimensional minimum function (Buerger, 1959) and finally lead to the solution of the structure.

Before attempting to solve the Patterson synthesis the expected heights of the single and double peaks due to every kind of atom in the cell, relative to the height of the origin peak, were calculated. This showed that the double peaks due to the heavy atoms Zn and Mn were considerably lower than most of the prominent peaks on the Harker section and consequently the latter were probably multiple. The expected single Zn — Zn and Mn — Mn peaks were also much lower than many on the other sections but they were high enough to promise the possibility of finding image points for the minimum function.

Inspection of the Harker line showed a very intense peak at $y = 22/60$ and a somewhat lower peak at $y = 0$. The second peak, because of its special position, was not considered at first. The height of the first peak suggested an accumulation of reflection satellites accompanying single inversion peaks which, according to the relations

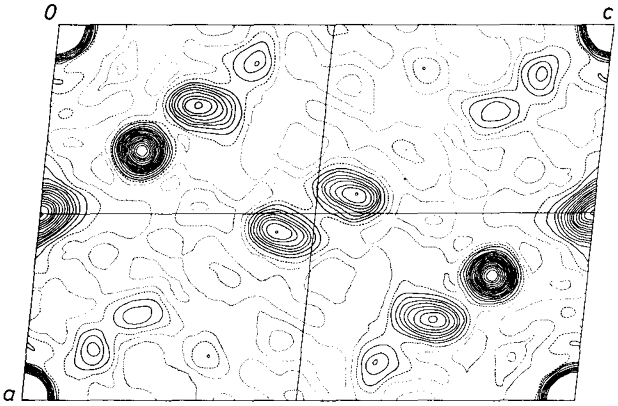

Fig. 1. Three-dimensional Patterson section $P(x0z)$

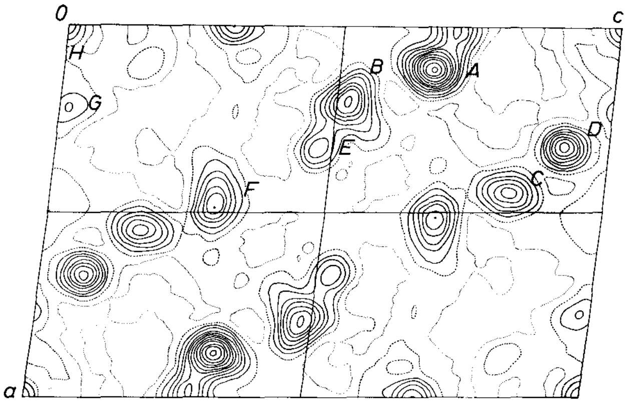

Fig. 2. Three-dimensional Patterson section $P(x\,\frac{8}{60}\,z)$

mentioned above, should lie around $y = \frac{1}{2} - \frac{22}{60} = \frac{8}{60}$. And in fact, superposition of the Harker section on section $y = \frac{8}{60}$, in the way indicated above, brought eight peaks of the asymmetric unit of the former into coincidence with corresponding peaks of the latter (Figs. 2, 3). Peak A on section $y = \frac{8}{60}$, Fig. 2, though certainly a multiple peak, was first considered as a possible Zn — Zn inversion peak and superposed on the origin of section $y = 0$. The minimum function was then drawn in the way described by BUERGER (1959). The first $M_2\,(x\,\frac{4}{60}\,z)$ obtained in this way (Fig. 4) showed six intense and several lower peaks. Of the intense peaks, B and C were attributed to the second Zn and the Mn atom because the corresponding inversion peaks B and C on the Patterson section $y = \frac{8}{60}$ had satisfactory satellites (B and C) on the Harker section and, as mentioned, on the Harker line. Accordingly peaks B and C on section $y = \frac{8}{60}$ were used as image points to form two more minimum functions $M_2\,(x\,\frac{4}{60}\,z)$ in the same way as for peak A. As the atomic numbers of Zn and Mn do not differ very much, and as the peaks on the Patter-

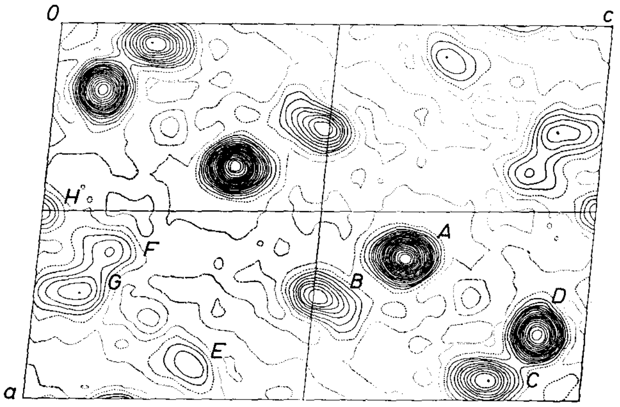

Fig. 3. Harker section $P(x\,\frac{1}{2}\,z)$

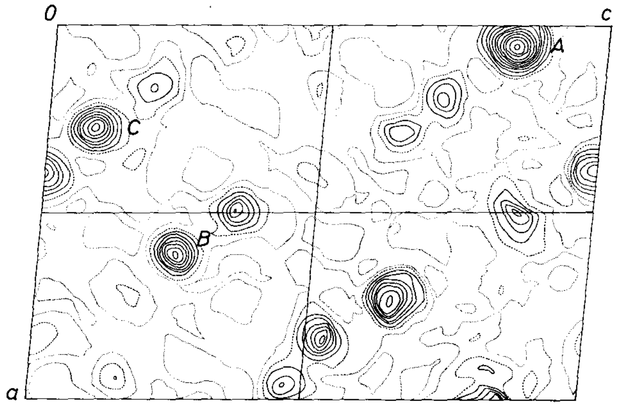

Fig. 4. Minimum function $M_2\,(x\,\frac{4}{60}\,z)$ based on peak A of Fig. 2

son section were certainly multiple, the corresponding M_2's were considered as approximately equivalent, and in this way the three M_2 maps were combined to form a more powerful M_6 $(x\ \frac{4}{60}\ z)$. This showed that very probably almost all the atoms of the asymmetric unit were at, or near, height $y = \frac{4}{60}$. Using the three probable heavy-atom locations as image points the sections of the Patterson synthesis were superposed in pairs differing by $\frac{8}{60}$ (e.g., points A, B, C on section $\frac{10}{60}$ were placed on the origin of section $\frac{2}{60}$, those of section $\frac{12}{60}$ on the origin of section $\frac{4}{60}$, etc.) and the corresponding section of M_6 was formed up to $y = \frac{15}{60}$ (asymmetric unit). Fig. 5 (see p. 133) shows a projection of the maximum heights of M_6 on (010). Most of the peaks lie around $y = \frac{4}{60}$, except for an intense peak at $y = \frac{14}{60}$ and a few weaker peaks at heights $\frac{11}{60}$ and $\frac{14}{60}$. This distribution of the peaks explains very well the appearance of the maxima on the Harker line.

As there were more peaks on the M_6 map than the ten atoms in the asymmetric unit (hydrogen atoms ignored) the assignment of atoms to the peaks on the M_6 was done, at least for some atoms, by taking into account the size of the SiO_4 tetrahedron and interatomic distances Zn — O and Mn — O known from other structures. With the exception of two O atoms, for which there was an alternative position, all other atoms were more or less uniquely allocated, although there was the possibility of an interchange of position among the heavy atoms. The positions originally selected on the M_6 map are marked with letters from A to J in the order $Zn_{(1)}$, $Zn_{(2)}$, Mn, Si, $O_{(1)}$, $O_{(2)}$, $O_{(3)}$, $O_{(4)}$, $OH_{(1)}$, $OH_{(2)}$.

A preliminary scale factor for the F_o values was determined by a structure-factor calculation with the three heavy atoms only. The program SFLSQ3 written by Prewitt (1962) was used for this calculation, as well as for all the subsequent structure-factor calculations and least-squares refinement (full matrix). The discrepancy factor

$$R = \frac{\Sigma \left| \, |F_o| - |F_c| \, \right|}{\Sigma \, |F_o|} \,,$$

obtained from the first calculation, was $R = 0.55$, which dropped to 0.46 in the two subsequent least-squares cycles with all the 10 atoms of the asymmetric unit included. Half-ionized state for all the atoms was assumed and probable isotropic temperature factors, known from other silicates, were assigned to them. Atomic form factors were obtained from the International Tables (1962).

A three-dimensional difference synthesis at this stage indicated an interchange of position between $Zn_{(1)}$ and Mn and between Si and $O_{(3)}$. Further, the weighting scheme by CRUICKSHANK *et al.* (1960) was introduced. With these changes R dropped to 0.35 in the following three least-squares cycles. A three-dimensional Fourier synthesis and the corresponding difference synthesis indicated the right structure immediately: The assumed Si atom ought to be interchanged with the Mn atom, and $O_{(3)}$ and $OH_{(1)}$ should be replaced by peaks K and L on the M_6 map. In the next cycle R dropped to 0.188 and with two further cycles it stopped at 0.137.

Refinement

At this stage examination of F_o and F_c values showed that for all the 90 fifth-level reflections F_c was systematically considerably larger than F_o. The ratio F_o/F_c for the 30 strongest reflections (F_c between 122 and 25) was found to lie close to 0.6, so a systematic error in collecting the intensities of this level was suspected. As the crystal had not been taken off the diffractometer it was found that the Geiger counter had been misset by 1° and consequently counted less than it should. With counter properly set the reflections of the fifth level were measured again. Before and after the measurement, checks were made to see whether reflections from other levels yielded the same number of counts as before. The values agreed to within 1 or 2%.

Before proceeding with further refinement the influence of the weighting scheme on the R value was checked by arranging the F_o values in increasing order, subdividing the set in groups of fifty, finding the R value for 10 reflections around the middle of each group and plotting the R values versus the average F_o value of the ten reflections. It was found that weak reflections were underweighted in comparison with the stronger ones. Constant a in the weighting scheme (CRUICKSHANK *et al.*, 1960) was accordingly increased.

The next cycle brought R down to 0.092 and then to 0.080, at which stage the change in the atomic parameters was so small that refinement of the atomic positions had practically converged. Variation of the isotropic temperature factors of the atoms dropped R to 0.078. Further refinement with anisotropic temperature factors improved R only slightly, 0.075. This, with the practically featureless appearance of the difference map, indicated that the thermal motion was substantially isotropic.

Table 1. *Comparison between observed and calculated structure factors for hodgkinsonite.*

h	k	l	$\lvert F_o \rvert$	$\lvert F_c \rvert$
0	0	1	34.9	33.0
		2	24.9	13.8
		3	97.8	104.2
		4	39.7	39.9
		5	38.4	44.6
		6	168.8	164.1
		7	21.6	21.6
		8	66.0	58.0
		9	25.9	21.3
		10	96.0	96.1
		11	97.5	98.5
		12	57.8	58.5
		13	72.3	75.2
		14	24.0	23.1
2	0	0	14.1	11.2
		1	123.2	126.9
		2	62.3	68.3
		3	107.2	115.5
		4	11.0	13.2
		5	81.7	77.3
		6	34.4	33.1
		7	184.1	191.7
		8	57.0	57.0
		9	49.8	49.6
		10	84.7	83.6
		11	8.1	3.2
		12	30.6	29.2
		13	68.6	71.5
		$\bar{1}$	75.1	76.0
		$\bar{2}$	111.0	106.6
		$\bar{3}$	215.5	243.5
		$\bar{4}$	15.6	11.8
		$\bar{5}$	134.2	135.4
		$\bar{6}$	150.1	164.3
		$\bar{7}$	30.7	31.0
		$\bar{8}$	70.0	75.9
		$\bar{9}$	55.4	60.6
		$\overline{10}$	19.5	17.4
		$\overline{11}$	36.4	39.4
		$\overline{12}$	31.4	32.0
		$\overline{13}$	26.2	28.0
		$\overline{14}$	82.8	89.4
4	0	0	98.9	87.5
		1	93.4	89.3
		2	46.2	41.1
		3	87.7	86.0
		4	230.4	262.7
		5	118.7	119.1
		6	26.8	23.4
		7	7.0	1.2
		8	11.9	10.2
		9	22.8	22.2
		10	94.7	98.7
		11	4.1	11.1
		12	36.5	35.8
		$\bar{1}$	146.4	147.8
		$\bar{2}$	114.0	116.2
		$\bar{3}$	35.6	34.0
		$\bar{4}$	18.4	19.4
		$\bar{5}$	32.4	29.1
		$\bar{6}$	58.5	58.8
		$\bar{7}$	141.3	155.8
		$\bar{8}$	50.1	53.4
		$\bar{9}$	81.5	85.6
		$\overline{10}$	68.2	68.5
4	0	$\overline{11}$	35.2	38.0
		$\overline{12}$	3.0	6.6
		$\overline{13}$	25.1	29.0
6	0	0	103.4	98.2
		1	82.9	74.5
		2	102.7	101.2
		3	43.0	40.4
		4	22.1	20.6
		5	28.6	28.7
		6	68.4	68.4
		7	39.7	38.6
		8	24.8	26.2
		9	17.9	19.1
		10	7.8	7.3
		$\bar{1}$	137.0	139.6
		$\bar{2}$	84.0	80.6
		$\bar{3}$	81.9	74.8
		$\bar{4}$	70.7	74.1
		$\bar{5}$	20.7	21.0
		$\bar{6}$	14.1	10.8
		$\bar{7}$	78.8	84.1
		$\bar{8}$	19.4	20.2
		$\bar{9}$	2.9	3.2
		$\overline{10}$	73.0	79.4
		$\overline{11}$	14.2	17.8
		$\overline{12}$	32.3	33.1
8	0	0	54.4	48.6
		1	9.0	11.5
		2	7.0	10.8
		3	91.3	93.3
		4	35.6	33.7
		5	31.1	35.7
		6	37.9	41.1
		7	56.3	58.0
		$\bar{1}$	51.5	51.4
		$\bar{2}$	17.5	18.2
		$\bar{3}$	111.5	114.5
		$\bar{4}$	36.0	37.1
		$\bar{5}$	18.3	21.0
		$\bar{6}$	83.1	89.7
		$\bar{7}$	30.1	33.8
		$\bar{8}$	26.6	30.7
		$\bar{9}$	13.7	16.1
10	0	0	39.7	41.2
		$\bar{1}$	12.1	15.0
		$\bar{2}$	14.7	15.9
		$\bar{3}$	67.2	70.3
0	1	1	31.0	22.8
		2	91.6	59.9
		3	67.5	60.9
		4	134.9	128.8
		5	10.4	11.5
		6	116.7	110.8
		7	106.1	100.9
		8	7.4	8.0
		9	34.2	31.0
		10	21.1	21.2
		11	17.1	14.1
		12	30.4	28.0
		13	39.0	40.7
		14	24.3	24.6
1	1	0	33.6	32.1
		1	54.9	44.5
		2	19.5	15.4
1	1	3	197.9	198.9
		4	65.9	65.7
		5	29.5	25.8
		6	85.6	77.2
		7	4.0	2.3
		8	35.7	35.1
		9	63.1	63.5
		10	60.1	57.9
		11	28.4	25.3
		12	14.8	12.7
		13	6.5	5.6
		14	4.3	3.9
		$\bar{1}$	37.8	29.8
		$\bar{2}$	100.8	100.3
		$\bar{3}$	109.8	112.7
		$\bar{4}$	2.2	2.1
		$\bar{5}$	7.2	10.1
		$\bar{6}$	102.3	103.5
		$\bar{7}$	40.4	38.1
		$\bar{8}$	151.1	160.3
		$\bar{9}$	96.8	101.1
		$\overline{10}$	5.8	6.0
		$\overline{11}$	34.6	31.7
		$\overline{12}$	22.6	22.3
		$\overline{13}$	33.4	33.7
		$\overline{14}$	28.0	28.0
2	1	0	126.6	121.9
		1	92.1	88.2
		2	95.3	83.8
		3	127.2	128.1
		4	43.7	39.6
		5	10.3	3.4
		6	12.5	8.9
		7	24.3	23.5
		8	11.2	12.9
		9	48.2	46.9
		10	35.6	34.2
		11	59.6	56.7
		12	11.7	11.9
		13	18.8	19.1
		$\bar{1}$	43.1	40.9
		$\bar{2}$	55.6	53.0
		$\bar{3}$	14.8	9.5
		$\bar{4}$	72.9	67.4
		$\bar{5}$	29.5	30.4
		$\bar{6}$	29.6	30.7
		$\bar{7}$	63.3	61.1
		$\bar{8}$	26.4	26.1
		$\bar{9}$	15.1	15.8
		$\overline{10}$	76.4	76.9
		$\overline{11}$	13.0	14.0
		$\overline{12}$	20.6	21.5
		$\overline{13}$	11.1	10.2
		$\overline{14}$	20.6	21.7
3	1	0	24.9	13.3
		1	152.0	158.3
		2	49.6	43.9
		3	21.2	19.1
		4	80.9	74.2
		5	70.3	70.7
		6	23.5	22.4
		7	80.2	82.7
		8	5.0	6.2
		9	7.3	4.7
		10	74.8	69.3
3	1	11	74.8	72.0
		12	43.6	42.6
		13	62.0	62.8
		$\bar{1}$	66.6	66.0
		$\bar{2}$	101.2	99.3
		$\bar{3}$	7.2	2.8
		$\bar{4}$	23.4	21.4
		$\bar{5}$	99.6	104.4
		$\bar{6}$	38.9	41.9
		$\bar{7}$	23.0	22.5
		$\bar{8}$	37.0	41.0
		$\bar{9}$	4.4	4.3
		$\overline{10}$	40.6	42.5
		$\overline{11}$	83.3	90.0
		$\overline{12}$	63.0	64.8
		$\overline{13}$	43.9	48.7
		$\overline{14}$	48.4	53.5
4	1	0	98.2	96.2
		1	11.0	9.3
		2	18.0	14.9
		3	56.2	57.9
		4	24.8	23.9
		5	40.9	38.4
		6	54.2	56.3
		7	47.9	49.1
		8	64.4	61.3
		9	16.0	15.5
		10	55.7	53.9
		11	22.1	21.6
		12	19.9	18.6
		$\bar{1}$	12.8	12.0
		$\bar{3}$	151.7	153.8
		$\bar{4}$	29.3	26.8
		$\bar{5}$	55.7	55.9
		$\bar{6}$	27.2	23.9
		$\bar{7}$	41.3	43.9
		$\bar{8}$	10.1	11.5
		$\bar{9}$	26.9	27.7
		$\overline{10}$	10.1	8.6
		$\overline{11}$	25.6	26.0
		$\overline{12}$	6.0	8.6
		$\overline{13}$	45.7	50.1
5	1	0	9.3	6.5
		1	70.4	69.5
		2	98.9	102.1
		3	3.8	3.3
		4	7.8	7.6
		5	51.8	52.9
		6	39.2	40.3
		7	79.9	77.8
		8	90.3	90.4
		9	32.6	29.4
		10	27.8	27.3
		11	16.1	16.7
		$\bar{1}$	6.5	3.8
		$\bar{2}$	41.0	41.2
		$\bar{3}$	55.8	54.0
		$\bar{4}$	189.4	188.1
		$\bar{5}$	49.9	52.5
		$\bar{6}$	40.9	42.0
		$\bar{7}$	26.2	27.1
		$\bar{8}$	44.4	42.7
		$\bar{9}$	7.8	4.8
		$\overline{10}$	65.3	72.0
		$\overline{11}$	40.1	44.7

Table 1. *(Continued)*

h	k	l	$\vert F_o\vert$	$\vert F_c\vert$
5	1	$\overline{12}$	14.1	16.4
		$\overline{13}$	26.0	29.4
6	1	0	63.5	66.7
		1	16.6	17.5
		2	44.0	46.9
		3	35.3	34.5
		4	63.9	69.3
		5	9.5	10.7
		6	33.1	30.8
		7	50.1	48.3
		8	18.4	17.8
		9	11.0	10.4
		10	19.4	18.5
		$\bar{1}$	30.8	29.8
		$\bar{2}$	2.2	4.2
		$\bar{3}$	24.7	23.2
		$\bar{4}$	10.7	10.0
		$\bar{5}$	16.6	17.8
		$\bar{6}$	60.5	66.6
		$\bar{7}$	24.5	23.9
		$\bar{8}$	22.8	21.9
		$\bar{9}$	31.9	32.4
		$\overline{10}$	27.3	29.4
		$\overline{11}$	35.4	40.3
		$\overline{12}$	4.1	6.7
7	1	0	19.9	21.5
		1	2.1	0.3
		2	69.4	70.8
		3	79.9	80.6
		4	19.4	32.3
		5	71.1	71.4
		6	42.3	41.9
		7	14.8	17.0
		8	27.2	26.4
		9	44.8	47.6
		$\bar{1}$	46.0	46.9
		$\bar{2}$	5.4	4.8
		$\bar{3}$	42.6	41.4
		$\bar{4}$	32.1	32.8
		$\bar{5}$	29.5	29.8
		$\bar{6}$	68.8	70.9
		$\bar{7}$	69.3	74.8
		$\bar{8}$	13.5	12.8
		$\bar{9}$	81.9	93.3
		$\overline{10}$	39.0	45.2
		$\overline{11}$	8.4	8.5
8	1	0	32.1	30.5
		1	70.7	71.1
		2	20.0	19.7
		3	3.9	2.8
		4	20.5	19.1
		5	37.3	38.4
		6	25.0	26.1
		7	35.7	38.8
		$\bar{1}$	27.3	27.1
		$\bar{2}$	31.8	30.4
		$\bar{3}$	46.8	44.7
		$\bar{4}$	43.5	44.3
		$\bar{5}$	6.1	6.7
		$\bar{6}$	17.3	18.6
		$\bar{7}$	3.2	3.2
		$\bar{8}$	8.5	8.3
		$\bar{9}$	21.1	22.2
9	1	0	91.1	97.6
		1	54.7	58.4
		2	4.6	3.4
9	1	3	15.9	18.0
		4	12.5	11.0
		$\bar{1}$	2.7	4.0
		$\bar{2}$	40.4	39.9
		$\bar{3}$	14.1	14.7
		$\bar{4}$	21.1	20.1
		$\bar{5}$	25.2	28.9
		$\bar{6}$	58.5	63.1
		$\bar{7}$	20.8	25.1
0	2	1	143.8	133.8
		2	120.4	111.0
		3	39.2	32.8
		4	12.9	13.4
		5	26.6	23.6
		6	82.2	81.2
		7	71.8	66.8
		8	25.1	22.0
		9	82.1	80.1
		10	16.8	16.0
		11	14.3	13.3
		12	87.8	90.1
		13	13.5	11.6
1	2	0	31.1	29.2
		1	14.0	10.6
		2	81.1	73.2
		3	24.4	23.3
		4	41.6	40.2
		5	86.2	81.8
		6	4.4	3.0
		7	12.2	11.8
		8	67.0	64.0
		9	47.3	45.8
		10	71.3	71.7
		11	67.5	68.4
		12	6.9	5.9
		13	14.8	15.2
		$\bar{1}$	136.6	127.8
		$\bar{2}$	14.2	0.6
		$\bar{3}$	35.0	31.5
		$\bar{4}$	76.7	73.8
		$\bar{5}$	21.1	19.5
		$\bar{6}$	12.0	8.9
		$\bar{7}$	69.8	69.6
		$\bar{8}$	52.1	53.2
		$\bar{9}$	3.8	2.4
		$\overline{10}$	17.2	16.6
		$\overline{11}$	1.8	1.2
		$\overline{12}$	20.8	19.9
		$\overline{13}$	51.9	55.5
2	2	0	62.9	60.4
		1	93.8	91.1
		2	7.5	4.6
		3	11.2	9.0
		4	105.5	102.4
		5	41.5	37.9
		6	105.2	102.3
		7	45.4	38.6
		8	85.5	82.6
		9	76.8	76.5
		10	32.8	31.9
		11	4.0	3.9
		12	19.8	20.1
		13	22.1	22.8
		$\bar{1}$	18.8	15.6
		$\bar{2}$	137.6	129.0
2	2	$\bar{3}$	37.4	31.4
		$\bar{4}$	87.0	78.5
		$\bar{5}$	163.8	171.1
		$\bar{6}$	18.5	12.3
		$\bar{7}$	29.5	26.2
		$\bar{8}$	7.4	5.1
		$\bar{9}$	59.6	60.5
		$\overline{10}$	24.7	25.2
		$\overline{11}$	44.3	44.3
		$\overline{12}$	16.1	17.1
		$\overline{13}$	27.3	28.7
3	2	0	74.4	73.2
		1	6.0	5.6
		2	18.2	19.2
		3	39.7	34.4
		4	17.9	14.9
		5	106.9	106.8
		6	62.8	62.2
		7	10.8	10.1
		8	50.1	49.4
		9	2.0	2.3
		10	30.8	32.3
		11	17.9	18.1
		12	28.9	29.9
		$\bar{1}$	77.1	74.7
		$\bar{2}$	14.7	11.5
		$\bar{3}$	23.0	20.2
		$\bar{4}$	42.7	40.1
		$\bar{5}$	17.1	15.5
		$\bar{6}$	143.6	151.9
		$\bar{7}$	56.6	55.6
		$\bar{8}$	24.0	22.6
		$\bar{9}$	28.6	28.0
		$\overline{10}$	18.0	17.8
		$\overline{11}$	30.7	31.4
		$\overline{12}$	37.9	39.3
		$\overline{13}$	23.5	23.6
4	2	0	30.0	26.8
		1	62.9	58.3
		2	117.6	116.6
		3	39.7	37.2
		4	87.1	84.7
		5	105.1	102.3
		6	12.9	12.6
		7	7.4	4.7
		8	34.2	33.1
		9	20.8	21.0
		10	18.1	16.8
		11	49.2	50.1
		$\bar{1}$	30.3	27.6
		$\bar{2}$	127.8	124.1
		$\bar{3}$	9.7	8.4
		$\bar{4}$	17.8	15.6
		$\bar{5}$	50.9	48.1
		$\bar{6}$	31.7	30.9
		$\bar{7}$	40.8	40.0
		$\bar{8}$	102.8	104.5
		$\bar{9}$	25.5	25.8
		$\overline{10}$	10.8	11.3
		$\overline{11}$	27.5	25.7
		$\overline{12}$	28.5	32.6
		$\overline{13}$	24.7	22.7
5	2	0	71.8	67.5
		1	57.9	55.3
		2	16.2	12.3
		3	71.9	71.3
5	2	4	34.9	31.6
		5	17.5	18.5
		6	49.2	50.0
		7	43.3	42.6
		8	14.2	13.6
		9	36.7	36.9
		10	8.3	9.6
		11	3.1	1.9
		$\bar{1}$	2.0	0.7
		$\bar{2}$	23.8	22.3
		$\bar{3}$	58.1	56.8
		$\bar{4}$	24.3	23.2
		$\bar{5}$	33.4	33.3
		$\bar{6}$	20.9	19.8
		$\bar{7}$	19.0	20.3
		$\bar{8}$	50.0	51.5
		$\bar{9}$	69.7	73.9
		$\overline{10}$	31.5	31.3
		$\overline{11}$	56.6	65.0
		$\overline{12}$	40.2	41.3
6	2	0	20.3	18.2
		1	12.5	10.7
		2	61.7	57.3
		3	35.3	32.0
		4	15.1	13.1
		5	70.3	68.8
		6	9.4	9.8
		7	32.7	33.5
		8	43.2	44.0
		9	28.4	29.0
		$\bar{1}$	135.4	135.3
		$\bar{2}$	35.0	30.0
		$\bar{3}$	22.4	21.4
		$\bar{4}$	26.1	23.0
		$\bar{5}$	76.5	78.2
		$\bar{6}$	29.9	27.8
		$\bar{7}$	33.3	32.9
		$\bar{8}$	16.1	15.0
		$\bar{9}$	19.9	20.9
		$\overline{10}$	25.3	28.5
		$\overline{11}$	46.7	49.2
7	2	0	8.2	3.7
		1	6.6	8.7
		2	3.8	1.0
		3	35.9	32.9
		4	61.0	58.8
		5	12.5	13.1
		6	3.6	4.2
		7	24.3	23.7
		8	34.5	34.8
		$\bar{1}$	48.9	46.4
		$\bar{2}$	108.0	107.7
		$\bar{3}$	7.1	6.2
		$\bar{4}$	29.4	27.9
		$\bar{5}$	16.7	17.5
		$\bar{6}$	25.1	23.3
		$\bar{7}$	7.9	4.9
		$\bar{8}$	53.9	58.1
		$\bar{9}$	24.0	26.5
		$\overline{10}$	11.1	13.7
8	2	0	7.4	6.9
		1	42.0	40.0
		2	63.7	63.7
		3	16.5	15.0
		4	28.5	29.2
		5	29.0	27.9

Table 1. *(Continued)*

h	k	l	$\|F_o\|$	$\|F_c\|$
8	2	6	53.8	53.6
		$\bar{1}$	7.6	6.8
		$\bar{2}$	17.6	17.8
		$\bar{3}$	60.0	57.9
		$\bar{4}$	50.8	50.1
		$\bar{5}$	40.5	42.4
		$\bar{6}$	13.1	12.7
		$\bar{7}$	29.2	30.2
		$\bar{8}$	32.9	34.4
9	2	0	4.8	4.0
		1	24.1	23.2
		2	7.3	6.3
		3	7.0	6.4
		$\bar{1}$	30.7	30.6
		$\bar{2}$	16.8	17.9
		$\bar{3}$	34.3	37.5
		$\bar{4}$	42.5	45.0
		$\bar{5}$	36.4	35.7
0	3	1	113.9	109.6
		2	19.3	18.3
		3	67.9	61.7
		4	48.5	42.7
		5	169.9	166.6
		6	18.8	16.0
		7	66.7	64.4
		8	96.4	91.3
		9	8.1	9.6
		10	40.7	39.8
		11	53.7	52.6
		12	17.5	16.6
1	3	0	5.5	1.9
		1	45.0	40.3
		2	13.7	10.0
		3	67.4	59.1
		4	53.4	48.0
		5	7.9	1.1
		6	31.0	27.2
		7	6.7	6.3
		8	16.7	14.8
		9	8.8	8.3
		10	21.6	20.1
		11	4.2	5.0
		12	8.6	7.6
		$\bar{1}$	7.5	6.2
		$\bar{2}$	19.1	16.5
		$\bar{3}$	40.0	36.2
		$\bar{4}$	26.1	24.2
		$\bar{5}$	5.8	1.1
		$\bar{6}$	45.8	41.4
		$\bar{7}$	25.4	23.1
		$\bar{8}$	35.3	33.4
		$\bar{9}$	43.0	40.4
		$\overline{10}$	2.8	4.2
		$\overline{11}$	5.9	4.9
		$\overline{12}$	12.7	12.8
2	3	0	20.1	19.0
		1	42.0	35.5
		2	260.7	278.2
		3	74.3	67.8
		4	22.4	18.3
		5	41.5	34.8
		6	7.4	6.4
		7	9.5	7.9
		8	97.2	97.2
		9	8.1	9.7
2	3	10	48.5	48.7
		11	17.2	17.7
		12	65.9	72.2
		$\bar{1}$	84.5	76.7
		$\bar{2}$	69.5	63.6
		$\bar{3}$	71.2	69.6
		$\bar{4}$	113.1	112.4
		$\bar{5}$	41.0	37.7
		$\bar{6}$	31.3	28.0
		$\bar{7}$	12.9	12.0
		$\bar{8}$	62.1	60.1
		$\bar{9}$	108.1	111.5
		$\overline{10}$	44.2	44.3
		$\overline{11}$	66.0	67.8
		$\overline{12}$	40.7	42.5
3	3	0	29.5	27.1
		1	61.7	55.7
		2	41.2	36.0
		3	24.4	23.3
		4	7.7	5.7
		5	13.8	13.9
		6	7.6	5.8
		7	26.6	24.8
		8	9.4	10.0
		9	9.6	10.3
		10	27.9	27.4
		11	25.8	25.3
		$\bar{1}$	38.8	36.2
		$\bar{2}$	40.3	35.2
		$\bar{3}$	18.5	13.0
		$\bar{4}$	21.2	19.5
		$\bar{5}$	12.6	10.9
		$\bar{6}$	15.2	14.0
		$\bar{7}$	21.5	20.3
		$\bar{8}$	7.4	8.7
		$\bar{9}$	1.7	1.7
		$\overline{10}$	1.6	1.9
		$\overline{11}$	26.0	24.5
		$\overline{12}$	19.2	19.0
4	3	0	90.0	82.4
		1	42.1	37.8
		2	15.3	14.3
		3	56.3	55.7
		4	66.1	65.3
		5	57.9	54.5
		6	15.4	15.7
		7	40.7	40.2
		8	19.6	16.8
		9	102.5	105.5
		10	45.4	43.8
		$\bar{1}$	118.6	115.2
		$\bar{2}$	65.5	63.2
		$\bar{3}$	111.7	109.2
		$\bar{4}$	96.7	94.1
		$\bar{5}$	54.1	50.3
		$\bar{6}$	59.3	58.3
		$\bar{7}$	27.9	28.9
		$\bar{8}$	21.4	19.6
		$\bar{9}$	40.5	41.2
		$\overline{10}$	23.6	24.1
		$\overline{11}$	5.6	6.7
5	3	0	21.9	21.0
		1	24.7	22.5
		2	20.7	17.3
		3	1.9	0.8
		4	1.9	1.3
5	3	5	26.8	26.3
		6	17.1	16.7
		7	26.8	25.3
		8	32.6	31.7
		9	18.9	18.8
		$\bar{1}$	13.2	11.0
		$\bar{2}$	30.1	27.5
		$\bar{3}$	1.9	1.3
		$\bar{4}$	58.4	55.0
		$\bar{5}$	33.7	32.4
		$\bar{6}$	13.6	11.1
		$\bar{7}$	1.8	1.5
		$\bar{8}$	9.5	11.1
		$\bar{9}$	6.5	7.2
		$\overline{10}$	29.5	32.2
		$\overline{11}$	9.8	9.1
6	3	0	40.5	39.2
		1	101.2	98.6
		2	48.7	44.5
		3	46.6	45.5
		4	29.3	27.1
		5	58.9	57.6
		6	98.9	101.5
		7	72.2	72.5
		8	16.4	12.6
		$\bar{1}$	25.0	23.6
		$\bar{2}$	36.9	34.7
		$\bar{3}$	29.5	27.5
		$\bar{4}$	12.6	10.0
		$\bar{5}$	107.1	111.8
		$\bar{6}$	34.8	35.6
		$\bar{7}$	45.8	45.8
		$\bar{8}$	70.5	75.4
		$\bar{9}$	28.9	31.8
		$\overline{10}$	15.8	15.7
7	3	0	8.7	6.8
		1	7.0	7.1
		2	20.6	19.0
		3	41.3	40.3
		4	5.1	3.1
		5	24.8	24.0
		6	29.1	28.2
		$\bar{1}$	7.6	4.9
		$\bar{2}$	1.7	2.5
		$\bar{3}$	19.9	19.3
		$\bar{4}$	5.8	4.9
		$\bar{5}$	2.8	4.6
		$\bar{6}$	5.9	5.0
		$\bar{7}$	26.4	27.2
		$\bar{8}$	5.4	5.3
8	3	0	18.9	18.9
		1	72.8	70.4
		2	72.2	70.6
		3	5.2	3.6
		4	53.9	53.6
		$\bar{1}$	56.9	53.4
		$\bar{2}$	50.3	49.9
		$\bar{3}$	8.9	9.6
		$\bar{4}$	7.3	8.8
		$\bar{5}$	63.7	64.9
		$\bar{6}$	7.7	7.4
0	4	1	60.0	52.7
		2	34.6	30.3
		3	14.1	11.6
		4	41.0	36.9
0	4	5	13.9	12.0
		6	11.6	10.0
		7	22.8	21.4
		8	24.3	24.7
		9	32.0	32.0
		10	23.5	25.5
		11	23.6	28.3
1	4	0	32.3	28.3
		1	18.9	17.8
		2	22.7	20.4
		3	34.9	33.4
		4	51.6	51.0
		5	53.8	53.3
		6	5.3	4.8
		7	5.1	1.4
		8	65.3	75.8
		9	49.4	59.9
		10	53.4	67.7
		11	39.1	67.4
		$\bar{1}$	148.4	146.3
		$\bar{2}$	55.6	53.1
		$\bar{3}$	44.4	39.9
		$\bar{4}$	78.5	74.1
		$\bar{5}$	19.0	16.8
		$\bar{6}$	3.8	5.4
		$\bar{7}$	70.9	70.6
		$\bar{8}$	33.6	33.2
		$\bar{9}$	4.2	1.9
		$\overline{10}$	25.1	28.0
		$\overline{11}$	5.6	7.6
2	4	0	5.3	3.7
		1	11.0	9.0
		2	20.6	17.6
		3	29.0	26.5
		4	31.8	29.9
		5	44.0	43.0
		6	48.3	50.8
		7	27.4	30.1
		8	36.0	40.5
		9	16.4	20.5
		10	9.4	11.5
		$\bar{1}$	28.9	26.2
		$\bar{2}$	60.1	55.1
		$\bar{3}$	32.3	30.3
		$\bar{4}$	64.3	59.9
		$\bar{5}$	56.1	56.3
		$\bar{6}$	32.3	30.2
		$\bar{7}$	43.0	42.5
		$\bar{8}$	7.2	6.6
		$\bar{9}$	6.9	8.2
		$\overline{10}$	3.2	3.0
		$\overline{11}$	8.7	12.6
3	4	0	75.5	72.0
		1	8.4	7.6
		2	4.5	3.4
		3	51.1	50.2
		4	18.0	17.6
		5	96.0	102.3
		6	84.5	94.6
		7	9.5	9.7
		8	31.1	38.3
		9	14.7	20.8
		10	14.0	25.9
		$\bar{1}$	46.5	42.7
		$\bar{2}$	7.8	6.8
		$\bar{3}$	15.2	11.4

Table 1. *(Continued)*

h	k	l	$\lvert F_o \rvert$	$\lvert F_c \rvert$	h	k	l	$\lvert F_o \rvert$	$\lvert F_c \rvert$	h	k	l	$\lvert F_o \rvert$	$\lvert F_c \rvert$	h	k	l	$\lvert F_o \rvert$	$\lvert F_c \rvert$
3	4	$\bar{4}$	70.9	72.8	5	4	$\bar{6}$	28.1	30.5	1	5	1	13.7	10.5	3	5	7	20.9	18.4
		$\bar{5}$	8.5	6.2			$\bar{7}$	4.1	1.9			2	7.5	4.0			$\bar{1}$	14.7	11.7
		$\bar{6}$	124.7	134.6			$\bar{8}$	40.5	48.3			3	55.8	53.9			$\bar{2}$	39.2	38.4
		$\bar{7}$	66.8	71.6			$\bar{9}$	46.3	69.5			4	17.4	16.5			$\bar{3}$	4.8	2.6
		$\bar{8}$	10.1	9.8	6	4	0	22.7	22.4			5	4.5	4.1			$\bar{4}$	10.0	8.7
		$\bar{9}$	23.9	25.1			1	6.9	9.0			6	39.4	36.5			$\bar{5}$	24.7	23.5
		$\overline{10}$	26.5	30.6			2	19.7	21.5			7	9.3	6.4			$\bar{6}$	16.6	14.8
4	4	0	47.2	44.8			3	14.2	17.0			8	10.8	9.2			$\bar{7}$	17.2	18.0
		1	29.1	26.4			4	20.0	25.9			$\bar{1}$	19.2	18.7			$\bar{8}$	3.5	2.6
		2	38.6	38.0			5	16.4	23.3			$\bar{2}$	10.7	8.1	4	5	0	74.9	67.6
		3	31.0	28.5			6	23.9	33.1			$\bar{3}$	26.3	19.8			1	14.0	11.6
		4	12.8	12.8			$\bar{1}$	44.8	49.6			$\bar{4}$	4.2	4.2			2	17.1	14.4
		5	28.2	29.3			$\bar{2}$	31.0	33.0			$\bar{5}$	22.7	21.7			3	70.3	64.5
		6	8.3	8.3			$\bar{3}$	38.2	41.6			$\bar{6}$	20.5	19.7			4	11.2	10.8
		7	5.1	3.5			$\bar{4}$	28.7	31.5			$\bar{7}$	10.0	10.6			5	12.8	13.3
		8	7.7	9.9			$\bar{5}$	15.5	16.9			$\bar{8}$	46.5	45.3			6	53.0	51.9
		9	10.7	17.9			$\bar{6}$	15.6	18.1			$\bar{9}$	29.3	29.1			$\bar{1}$	23.3	22.3
		$\bar{1}$	36.9	36.0			$\bar{7}$	9.4	11.2	2	5	0	88.5	82.5			$\bar{2}$	7.3	8.6
		$\bar{2}$	19.2	18.6			$\bar{8}$	2.8	2.6			1	61.0	55.1			$\bar{3}$	120.1	118.6
		$\bar{3}$	1.6	2.7	7	4	0	19.6	24.3			2	94.1	85.5			$\bar{4}$	9.5	10.9
		$\bar{4}$	7.8	7.3			1	3.9	5.6			3	96.2	88.4			$\bar{5}$	11.3	10.8
		$\bar{5}$	17.5	15.2			2	4.2	2.3			4	40.7	37.9			$\bar{6}$	10.6	10.9
		$\bar{6}$	15.7	15.2			3	17.2	21.2			5	7.0	3.6			$\bar{7}$	55.9	60.6
		$\bar{7}$	28.1	29.8			4	31.8	52.5			6	26.7	25.6	5	5	0	8.1	6.5
		$\bar{8}$	26.7	30.5			$\bar{1}$	42.9	52.6			7	15.1	13.4			1	18.5	15.4
		$\bar{9}$	14.0	16.6			$\bar{2}$	96.2	107.4			8	35.8	33.5			2	18.3	14.7
		$\overline{10}$	20.4	28.0			$\bar{3}$	24.9	30.7			$\bar{1}$	32.1	28.5			3	9.5	8.4
5	4	0	77.3	80.6			$\bar{4}$	24.6	29.3			$\bar{2}$	8.0	7.9			4	3.6	1.0
		1	66.3	67.4			$\bar{5}$	11.2	15.0			$\bar{3}$	20.8	19.8			$\bar{1}$	16.5	15.5
		2	9.2	6.7			$\bar{6}$	15.3	22.3			$\bar{4}$	84.3	81.0			$\bar{2}$	7.1	5.7
		3	87.8	98.8								$\bar{5}$	42.2	39.2			$\bar{3}$	14.5	12.3
		4	35.0	37.8	0	5	1	48.6	44.7			$\bar{6}$	8.5	7.6			$\bar{4}$	58.4	57.6
		5	5.1	7.6			2	65.8	60.3			$\bar{7}$	49.0	49.5			$\bar{5}$	6.5	5.8
		6	20.1	23.7			3	18.5	15.6			$\bar{8}$	18.9	19.4			$\bar{6}$	2.0	2.4
		7	32.9	43.4			4	90.2	84.4	3	5	0	6.9	3.7	6	5	0	77.6	74.8
		8	1.0	2.0			5	42.2	38.8			1	37.6	35.8			1	23.8	22.5
		$\bar{1}$	13.0	13.3			6	52.8	48.8			2	17.8	16.5			$\bar{1}$	13.2	12.2
		$\bar{2}$	17.6	16.9			7	93.5	93.1			3	10.5	7.6			$\bar{2}$	6.7	4.5
		$\bar{3}$	52.1	52.0			8	25.9	23.4			4	35.9	32.6			$\bar{3}$	14.4	15.3
		$\bar{4}$	5.9	3.2			9	6.1	3.9			5	3.5	5.1					
		$\bar{5}$	28.8	28.9	1	5	0	16.1	12.9			6	4.9	2.8					

Correction for anomalous dispersion of the Mn atom was then introduced with values for $\Delta f'$ and $\Delta f''$ obtained from the International Tables (1961). R dropped to 0.067. Careful examination of the Fourier and difference Fourier maps in the neighborhood of the two hydroxyl groups, $O_{(5)}$ and $O_{(6)}$, indicated the possible positions of the two H atoms. They were accordingly introduced into the structure-factor calculation (with a constant temperature factor 2.5) and, after six cycles of refinement, although they did not lower the value of R, they improved the agreement between F_o and F_c, especially for many weak reflections of low $\sin\theta$.

Table 1 gives the $|F_o|$ and the $|F_c|$ values for hodgkinsonite obtained from the final parameters listed in Table 2. In Table 3 are compared the final parameters with those obtained from the M_6 map. The agreement is, in many instances, striking.

Table 2. *Atomic coordinates and temperature factors for hodgkinsonite with their standard deviations*

	x	$\sigma(x)$	y	$\sigma(y)$	z	$\sigma(z)$	B	$\sigma(B)$
$\mathrm{Zn}_{(1)}$	0.2732	(0.0002)	0.0657	(0.0003)	0.0788	(0.0001)	0.864	(0.023)
$\mathrm{Zn}_{(2)}$	0.6084	(0.0002)	0.0623	(0.0003)	0.2491	(0.0001)	0.886	(0.023)
Mn	0.1063	(0.0002)	0.2420	(0.0003)	0.5482	(0.0001)	0.541	(0.028)
Si	0.0673	(0.0003)	0.0666	(0.0005)	0.8292	(0.0002)	0.137	(0.045)
$\mathrm{O}_{(1)}$	0.1067	(0.0009)	0.0810	(0.0014)	0.1911	(0.0006)	0.521	(0.119)
$\mathrm{O}_{(2)}$	0.1657	(0.0009)	0.0405	(0.0014)	0.7151	(0.0006)	0.395	(0.119)
$\mathrm{O}_{(3)}$	0.8193	(0.0009)	0.0702	(0.0015)	0.0660	(0.0006)	0.452	(0.118)
$\mathrm{O}_{(4)}$	0.5384	(0.0008)	0.1441	(0.0014)	0.8621	(0.0006)	0.256	(0.115)
$\mathrm{O}_{(5)}$	0.4902	(0.0009)	0.0892	(0.0015)	0.3836	(0.0006)	0.494	(0.110)
$\mathrm{O}_{(6)}$	0.8491	(0.0009)	0.0882	(0.0015)	0.5560	(0.0006)	0.564	(0.124)
$\mathrm{H}_{(1)}$	0.466	(0.027)	0.260	(0.040)	0.333	(0.018)	2.5	
$\mathrm{H}_{(2)}$	0.842	(0.027)	−0.83	(0.040)	0.600	(0.018)	2.5	

Table 3. *Comparison between coordinates obtained from the minimum function and those from the final least-squares cycle*

	x_{min}	x_{fin}	y_{min}	y_{fin}	z_{min}	z_{fin}
$\mathrm{Zn}_{(1)}$	0.275	0.2732	0.067	0.0657	0.085	0.0788
$\mathrm{Zn}_{(2)}$	0.613	0.6084	0.067	0.0623	0.250	0.2491
Mn	0.099	0.1063	0.250	0.2420	0.554	0.5482
Si	0.061	0.0673	0.067	0.0666	0.828	0.8292
$\mathrm{O}_{(1)}$	0.143	0.1067	0.100	0.0810	0.199	0.1911
$\mathrm{O}_{(2)}$	0.175	0.1657	0.067	0.0405	0.716	0.7151
$\mathrm{O}_{(3)}$	0.828	0.8193	0.067	0.0702	0.040	0.0660
$\mathrm{O}_{(4)}$	0.512	0.5384	0.067	0.1441	0.877	0.8621
$\mathrm{O}_{(5)}$	0.484	0.4902	0.067	0.0892	0.370	0.3836
$\mathrm{O}_{(6)}$	0.835	0.8491	0.075	0.0882	0.542	0.5560

The interatomic distances and angles, computed with the program ORXLS written by BUSING and LEVY (1959) are given in Tables 4 and 5. The coordination of the O atoms is shown in Table 6 together with the corresponding O—cation distances.

Description of the structure and discussion

Figure 6 shows the projection of the asymmetric unit on (010) as obtained from the final three-dimensional Fourier synthesis. Its resemblance with the M_6 map (Fig. 5) is obvious. Fig. 7 is a schematic representation of the structure viewed along the *b* axis. The coordination polyhedra with cation—anion distances are shown in Fig. 8.

The SiO_4 tetrahedron is almost regular with one shorter and one longer Si—O distance than the average, 1.626 Å. The longer distance,

Table 4. *Interatomic distances in hodgkinsonite*

SiO_4 tetrahedron

Si—$O_{(1)}$	1.622 Å	$O_{(1)}$—$O_{(2)}$	2.653 Å
$O_{(2)}$	1.632	$O_{(3)}$	2.655
$O_{(3)}$	1.642	$O_{(4)}$	2.656
$O_{(4)}$	1.608	$O_{(2)}$—$O_{(3)}$	2.633
Average Si—O	1.626 ± 0.007	$O_{(4)}$	2.649
		$O_{(3)}$—$O_{(4)}$	2.685
		Average O—O	2.655 ± 0.010

$Zn_{(1)}O_4$ tetrahedron

$Zn_{(1)}$—$O_{(1)}$	1.983 Å	$O_{(1)}$—$O_{(3)}$	3.239 Å
$O_{(3)}$	1.938	$O'_{(3)}$	3.015
$O'_{(3)}$	1.980	$O_{(4)}$	3.250
$O_{(4)}$	1.975	$O_{(3)}$—$O'_{(3)}$	3.230
Average $Zn_{(1)}$—O	1.969 ± 0.007	$O_{(4)}$	3.188
		$O'_{(3)}$—$O_{(4)}$	3.346
		Average O—O	3.211 ± 0.010

$Zn_{(2)}O_4$ tetrahedron

$Zn_{(2)}$—$O_{(1)}$	2.015 Å	$O_{(1)}$—$O_{(2)}$	3.204 Å
$O_{(4)}$	2.016	$O_{(4)}$	3.259
$O_{(2)}$	1.934	$O_{(5)}$	3.082
$O_{(5)}$	1.933	$O_{(2)}$—$O_{(4)}$	3.406
Average $Zn_{(2)}$—O	1.974 ± 0.007	$O_{(5)}$	3.213
		$O_{(4)}$—$O_{(5)}$	3.134
		Average O—O	3.216 ± 0.010

MnO_6 octahedron

Mn—$O_{(2)}$	2.250 Å	$O_{(2)}$—$O'_{(5)}$	3.348 Å
$O_{(5)}$	2.262	$O_{(6)}$	3.061
$O_{(6)}$	2.265	$O'_{(6)}$	3.187
$O'_{(5)}$	2.188	$O''_{(6)}$	3.252
$O'_{(6)}$	2.179	$O_{(5)}$—$O'_{(5)}$	2.888
$O''_{(6)}$	2.190	$O_{(6)}$	2.968
Average Mn—O	2.222 ± 0.007	$O'_{(6)}$	3.409
		$O''_{(6)}$	3.016
		$O'_{(5)}$—$O_{(6)}$	3.025
		$O'_{(6)}$	3.073
		$O_{(6)}$—$O''_{(6)}$	3.048
		$O'_{(6)}$—$O''_{(6)}$	3.321
		Average O—O	3.133 ± 0.010

OH groups

$O_{(5)}$—$H_{(1)}$	1.1 ± 0.2 Å	$O_{(6)}$—$H_{(2)}$	1.0_5 ± 0.2 Å

H bonding

$O_{(5)}$—$H_{(1)}$ . . . $O'_{(2)}$	1.1—1.9 Å	$O_{(5)}$—$O'_{(2)}$	= 2.908 Å

Table 5. *Bond angles in hodgkinsonite*

SiO$_4$ tetrahedron	
$O_{(1)}$—Si—$O_{(2)}$	109.20°
$O_{(3)}$	108.84
$O_{(4)}$	110.60
$O_{(2)}$—Si—$O_{(3)}$	107.03
$O_{(4)}$	111.92
$O_{(3)}$—Si—$O_{(4)}$	109.15
Average	109.45 ± 0.37

Zn$_{(1)}$O$_4$ tetrahedron	
$O_{(1)}$—Zn$_{(1)}$—$O_{(3)}$	111.37°
$O'_{(3)}$	99.06
$O_{(4)}$	110.42
$O_{(3)}$—Zn$_{(1)}$—$O'_{(3)}$	111.04
$O_{(4)}$	109.11
$O'_{(3)}$—Zn$_{(1)}$—$O_{(4)}$	115.54
Average	109.43 ± 0.31

Zn$_{(2)}$O$_4$ tetrahedron	
O_1—Zn$_2$—$O_{(2)}$	108.45°
$O_{(4)}$	107.89
$O_{(5)}$	102.65
O_2—Zn$_2$—$O_{(4)}$	119.12
$O_{(5)}$	112.40
$O_{(4)}$—Zn$_{(2)}$—$O_{(5)}$	105.01
Average	109.25 ± 0.31

MnO$_6$ octahedron	
$O_{(2)}$—Mn—$O_{(5)}$	97.93°
$O_{(6)}$	85.39
$O'_{(6)}$	92.16
$O''_{(6)}$	94.18
$O_{(5)}$—Mn—$O'_{(5)}$	80.91
$O_{(6)}$	81.94
$O'_{(6)}$	100.43
$O''_{(6)}$	85.26
$O'_{(5)}$—Mn—$O_{(6)}$	85.57
$O'_{(6)}$	89.56
$O_{(6)}$—Mn—$O''_{(6)}$	86.32
$O'_{(6)}$—Mn—$O''_{(6)}$	99.12
Average	89.89 ± 0.31

Hydrogen bond	
$O_{(5)}$—$H_{(1)}$—$O''_{(2)}$	152° ± 17°

Table 6. *Coordination of the O atoms and cation—O distances*

$O_{(1)}$—Si	1.622 Å	$O_{(4)}$—Si	1.608
Zn$_{(1)}$	1.983	Zn$_{(1)}$	1.975
Zn$_{(2)}$	2.015	Zn$_{(2)}$	2.016
$O_{(2)}$—Si	1.632	$O_{(5)}$—Zn$_{(2)}$	1.933
Zn$_{(2)}$	1.934	Mn	2.262
Mn	2.250	Mn	2.188
(H$_{(1)}$	1.89)	H$_{(1)}$	1.09
$O_{(3)}$—Si	1.642	$O_{(6)}$—Mn	2.265
Zn$_{(1)}$	1.938	Mn	2.179
Zn$_{(1)}$	1.980	Mn	2.190
		H$_{(2)}$	1.05

1.642 Å, corresponds to the oxygen atom $O_{(3)}$, which is bonded to two symmetry-equivalent Zn$_{(1)}$ atoms. It is of interest to note that this longer Si—O distance corresponds to the only short Zn$_{(1)}$—O distance of the $Zn_{(1)}O_4$ tetrahedron whose $Zn_{(1)}$ atom has the same y coordinate as Si. The shorter Si—O distance, 1.608 Å, is to $O_{(4)}$, bonded to $Zn_{(1)}$ and $Zn_{(2)}$, the distances to which are longer than the average in the corresponding ZnO_4 tetrahedra. Four O—O distances are almost equal to the average value, 2.655 Å. All three distances from $O_{(1)}$ are equal and the face $O_{(1)}$ $O_{(2)}$ $O_{(4)}$ is an equilateral triangle. The O—Si—O angles are close to the ideal value, 109.47°.

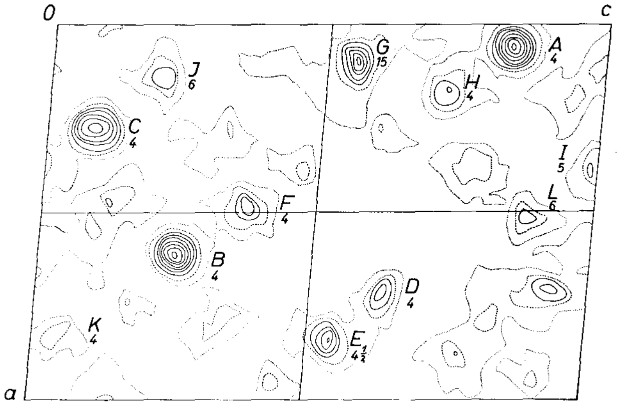

Fig. 5. Maxima of the minimum function M_6 projected parallel to b (asymmetric unit only). The numbers near the peaks indicate the y coordinate in 60ths along the b axis

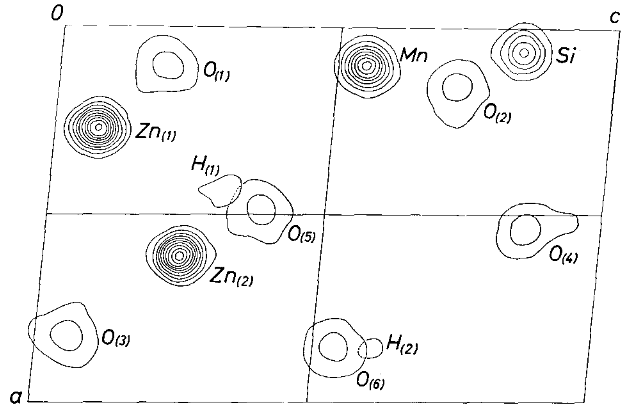

Fig. 6. Maxima in the asymmetric unit of the final three-dimensional Fourier synthesis projected parallel to b. Contours at 10 $e/Å^3$

Both the Zn atoms are tetrahedrally coordinated. $Zn_{(1)}$ is surrounded by four O atoms, whereas $Zn_{(2)}$ is surrounded by two "pure" O atoms, one OH group and one O bonded to an OH group through an H bridge. The average Zn—O distances in the two tetrahedra, 1.969 Å and 1.974 Å respectively, agree very well with the values 1.94—2.04 Å given for zincite, ZnO, (Strukturbericht I, 1931) and 1.79—2.03 Å given by Ito and West (1932) for hemimorphite, $Zn_4(OH)_2Si_2O_7 \cdot H_2O$. They are also very close to the value 2.02 Å found for the shorter Zn—O distances in a 4 + 2 coordination of the Zn atom (International Tables, 1962). Both the tetrahedra are distorted in a more or less similar way. In the $Zn_{(1)}O_4$ tetrahedron one $Zn_{(1)}$—O distance is short, 1.938 Å, the other three being larger than the average value and almost equal. In the $Zn_{(2)}O_4$ tetrahedron, however, there are two almost identical short $Zn_{(2)}$—O distances, 1.933 Å, and two, again almost identical long distances, 2.015 Å. The two shorter distances, which are almost equal to the short distance in the $Zn_{(1)}O_4$ tetrahedron, correspond to O atoms linked to Mn atoms (which are in octahedral coordination) whereas the longer distances correspond to atoms linked to Si and Zn atoms. The average O—O distances in the tetrahedra are very close to each other, 3.211 and 3.216 Å respectively, and are in agreement with those found for hemimorphite, 3.10 — 3.43 Å (Ito and

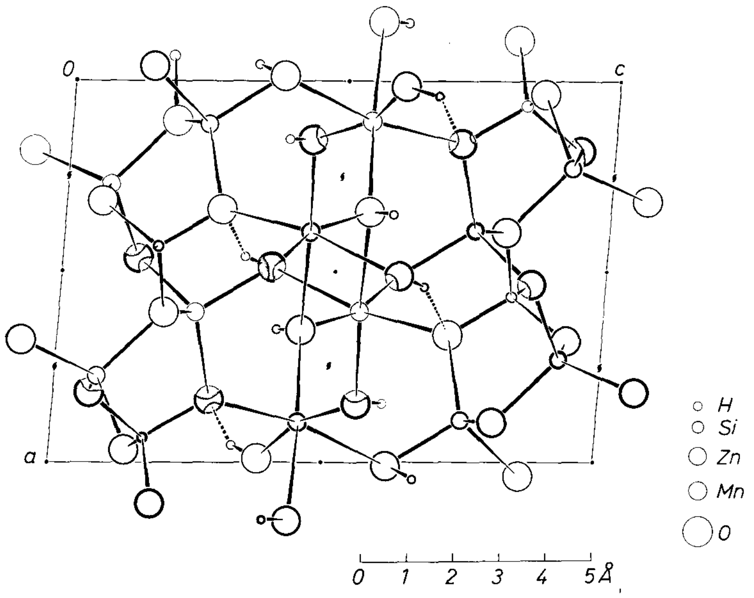

Fig. 7. Projection of the structure parallel to *b*. Atoms with greater *y* are indicated with heavier circles. In case of atoms differing by one *b* translation, the upper atom is shown cut and the lower shaded. The dashed lines show H bond

West, 1932). The average O—Zn—O angle is close to the ideal value, yet there is considerable deviation for two angles in each tetrahedron.

The Mn atom is surrounded by five OH groups and one O atom in the form of a distorted octahedron. Three Mn—O distances are shorter and three longer than the average value, 2.222 Å, which agrees very well with the value 2.21 Å given in the International Tables (1961) and with the values 2.203 Å and 2.245 Å reported recently by Peacor and Buerger (1962) for bustamite, $CaMnSi_2O_6$. Of particular interest are the two long distances $Mn—O_{(2)} = 2.250$ Å and $Mn—O_{(5)} = 2.262$ Å, because the corresponding O atoms participate in Si and Zn tetrahedra at much smaller Si—O and Zn—O distances, being therefore more strongly bonded to these cations than to the Mn. As indicated below, this may partly account for the perfect (001) cleavage of hodgkinsonite. $O_{(6)}$ is bonded only to Mn and $H_{(2)}$ atoms. The average O—O distance, 3.133 Å, does not differ very much from the O—O distance in the ZnO_4 tetrahedra. The average O—Mn—O angle is very close to 90°, but some angles deviate rather considerably from this value.

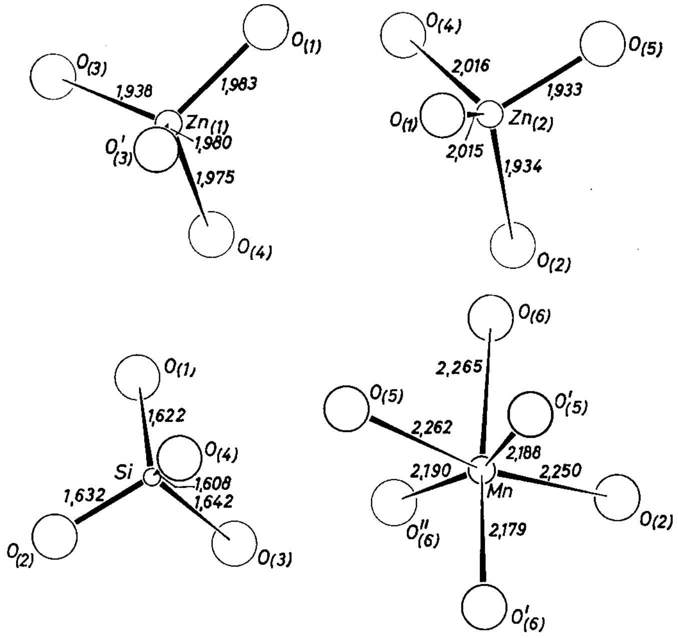

Fig. 8. Coordination polyhedra around the cations, with interatomic distances. The orientation of the polyhedra is for the cations in the asymmetric unit (see Fig. 7)

The O—H distances in the hydroxyl groups, 1.1 Å and 1.05 Å, lie within the range reported for inorganic substances. $H_{(1)}$ is of particular interest because it is very probably involved in a hydrogen bonding of $O_{(5)}$ to $O'_{(2)}$. This is supported by the fact that $O_{(5)}$—$H_{(1)}$ = 1.1 Å, $O'_{(2)}$— $H_{(1)}$ = 1.9 Å, $O_{(5)}$—$O'_{(2)}$ = 2.908 Å, and the angle $O_{(5)}$—$H_{(1)}$—$O'_{(2)}$ = 152°. It is worth noting that $O'_{(2)}$ belongs to the SiO_4 tetrahedron. $H_{(2)}$ seems to belong to $O_{(6)}$ only.

With the exception of the Mn and $H_{(1)}$ atoms all the other atoms in the asymmetric unit lie very near the plane defined by the two Zn and the Si atom, which is parallel to (010) at $y \approx 0.065$. In this way, we may visualize the unit cell as consisting of four layers of atoms parallel to (010) at heights $y \approx 0.065$, 0.435, 0.565 and 0.935, separated by two layers of Mn atoms at heights $y \approx 0.250$ and 0.750.

Considering the distribution of the coordination polyhedra we have the following picture (Fig. 7): The SiO_4 tetrahedra, while isolated from one another, share three corners with the ZnO_4 tetrahedra, whereas the fourth corner, $O_{(2)}$, is shared with the $Zn_{(2)}O_4$ tetrahedron and the MnO_6 octahedron. The $Zn_{(1)}O_4$ tetrahedron shares corners with four SiO_4 tetrahedra, two other $Zn_{(1)}O_4$ tetrahedra and two $Zn_{(2)}O_4$ tetrahedra. The $Zn_{(2)}O_4$ tetrahedron on the other hand shares corners with three SiO_4 and two $Zn_{(1)}O_4$ tetrahedra and two MnO_6 octahedra. The MnO_6 octahedron shares corners with one SiO_4 and three $Zn_{(2)}O_4$ tetrahedra and eight other MnO_6 octahedra. No coordination polyhedron shares an edge or a face with another. All the O atoms are bonded to three cations and, of course, those of the OH groups to an H atom as well (Table 6).

As a result of this arrangement the ZnO_4 and the SiO_4 tetrahedra form a network $(Zn_2SiO_4)_x$ extending in two dimensions along a and b. The structure within the network resembles in principle that of willemite, Zn_2SiO_4 (BRAGG and ZACHARIASEN, 1930), but as no accurate interatomic distances for the latter are available, no detailed comparison is possible. The MnO_6 octahedra also form a network extending in two dimensions along a and b. If we call A the $(Zn_2SiO_4)_x$ network and B the MnO_6 octahedra network, both of which are parallel to (100), then the structure can be described with the pattern . . . *ABAABA* . . . along the c axis.

This pattern explains very well the perfect (001) cleavage of hodgkinsonite. Owing to the greater valence of Si, the lower coordination around Si and Zn, and the shorter cation-anion distances in the A network, the bonding forces in it are much stronger than in B. Thus cleavage would preferably occur at the atoms connecting the two networks, leaving *A* complete. The cleavage surface would be parallel to (001).

The structural pattern . . . *ABAABA* . . . is reminiscent of a similar arrangement in the structure of norbergite (TAYLOR and WEST, 1928), the chemical formula of which, $Mg_3[(OH)_2|SiO_4]$ resembles that of hodgkinsonite. Here, however, the alternating Mg_2SiO_4 and $Mg(OH)_2$ slabs parallel to (001) are structurally different from *A* and *B* in hodgkinsonite and so the two minerals are not isotypic. Hodgkinsonite does not belong to the humite group but it constitutes a new silicate-structure type.

It can easily be seen from Fig. 7 that there is a pronounced O substructure with the O atoms forming roughly hexagonal closest-packed layers parallel to $(10\bar{2})$. The length of the *b* axis, 5.316 Å, is almost exactly equal to two oxygen diameters, but it is considerably greater than the O—O distance along *b* would be if the closest packing were ideal. In agreement with similar observations on structures with O atoms in closest-packed arrangement, the refractive indices of hodgkinsonite (1.724 — 1.746) are well over 1.71 (Strukturbericht, I, 1931).

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