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Jahnsite, $CaMn^{2+}Mg_2(H_2O)_8Fe^{3+}_2(OH)_2[PO_4]_4$: A Novel Stereoisomerism of Ligands about Octahedral Corner-Chains

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Abstract

Jahnsite, $CaMn^{2+}Mg_2(H_2O)_8Fe^{3+}_2(OH)_2[PO_4]_4$, *a* 14.94(2) Å, *b* 7.14(1) Å, *c* 9.93(1) Å, *β* 110.16(8)°, *P*2/*a*, *Z* = 2, is one of the 7 Å octahedral corner-linked chain structures allied to laueite, pseudolaueite, childrenite, *etc.* *R*(*hkl*) = 0.09 for 2292 independent non-zero reflections.

The structure is based on a backbone of corner-linked ... Fe^{3+}-OH-Fe^{3+} ... octahedra with a novel arrangement of $[PO_4]$ tetrahedra about these chains. The structure possesses dense slabs of $[CaMn^{2+}Fe^{3+}_2(OH)_2[PO_4]_4]^{4-}$ oriented parallel to {001} which are bridged by PO_4 corner-sharing to $Mg(O,H_2O)_6$ octahedra.

Polyhedral interatomic averages are ^{VI}Fe(1)-O 1.973 Å, ^{VI}Fe(2)-O 1.973, ^{VI}Ca-O 2.418, $^{VI}Mn^{2+}$-O 2.190, ^{VI}Mg(1)-O 2.088, ^{VI}Mg(2)-O 2.089, ^{IV}P(1)-O 1.543, and ^{IV}P(2)-O 1.533.

Introduction

Jahnsite is one of several new mineral species described by Moore (1974) which occur as late-stage hydrothermal products of the decomposition of triphylite-lithiophilite in pegmatites. A rather frequently found mineral, it occurs in a paragenesis with laueite, strunzite, and stewartite, suggesting that these minerals have a closely-related structural principle. The jahnsite structure type provides a range of compositions from an aluminum analogue $Ca(Fe,Mn)^{2+}Mg_2(H_2O)_8Al^{3+}_2(OH)_2[PO_4]_4$ to highly oxidized large-cation deficient material $(Ca,Mn^{2+})_{<1}(Fe^{3+},Mg)_{<2}(OH,H_2O)_8Fe^{3+}_2(OH)_2[PO_4]_4$. A closely related structure apparently occurs in segelerite, $CaMg(H_2O)_4Fe^{3+}(OH)[PO_4]_2$ (Moore, 1974).

Our laboratory has been much interested in the systematics of transition-metal phosphate structures, especially with respect to polynuclear clustering of the transition metals and with problems of ligand stereoisomerisms about these clusters. Additionally, we seriously doubt if, without a detailed structure analysis, sensible formulae can be applied to these complex structures wherein the role of (H_2O) is often manifold.

Experimental

The crystal cell parameters for jahnsite are *a* 14.94(2) Å, *b* 7.14(1) Å, *c* 9.93(1) Å, *β* 110.16(8)°, *Z* = 2, with formula unit $CaMn^{2+}Mg_2(H_2O)_8Fe^{3+}_2(OH)_2[PO_4]_4$ derived from the study of Moore (1974). Weak $0k0$ reflections with $k \neq 2n$ and the systematic absence $h = 2n$ for $h0l$ established the space group as *P*2/*a* or *Pa*. The centric group, *P*2/*a*, was chosen on the basis of the observed morphological holosymmetry.

A suitable single crystal nearly equant in shape and 0.2 mm in mean dimension was selected from the type specimen collected by P.B.M. at the Tip Top pegmatite, near Custer, South Dakota.

With [010] as the rotation axis, reflections to $2\theta = 65°$ were gathered on a PAILRED diffractometer utilizing a graphite monochromator and Mo*Kα* radiation. Twenty-second background counts were taken on each side of the peak. The scan rate was 2.5°/minute with half-scan interval of 2.0°, widening to 2.8° at high levels. *ω*-scans revealed low absorption anisotropy, so a correction was not applied. Symmetry-equivalent reflections were averaged and the data were processed by conventional computational procedures to obtain |F(obs)|.

Solution and Refinement

A three-dimensional Patterson synthesis, *P*(*uvw*), revealed strong concentrations of vectors at 0, ½, 0; ½, 0, 0; ¼, 0, 0; ¼, ½, 0 and immediately led to a model based on octahedral chains. Unfortunately, a pronounced substructure, discussed further on, led to ambiguities in the *y*-coordinates for the $[PO_4]$ tetrahedra and the $Mg(O,H_2O)_6$ octahedra. Approximate location of the atoms in the dense slabs parallel to {001} was achieved through the β- and γ'-syntheses of Ramachandran and Srinivasan (1970). Correct locations for the y-coordinates of the phosphorus and magnesium atoms were achieved through a careful inspection of the bond distances in the partly determined structure.

When all atoms were located, refinement of atomic coordinates and isotropic thermal vibration parameters proceeded from the scattering curves of Cromer and Mann (1968) for Ca^{1+}, Mn^{2+}, Fe^{2+}, Mg^{1+}, P^0 and O^{1-}. The full-matrix refinement, on IBM-360 computer, and using a local, unpublished program modified from the ORFLS program of Busing, Martin, and Levy (1962) converged, for different structure factor magnitudes, to the values of $R(hkl)$ given in Table 1. Table 2 provides the final atomic coordinates and isotropic thermal vibration parameters and Table 3 is the list of structure factors.

Description of the Structure

General Structural Features and Principles

Moore (1970a) outlined the general problems associated with the "7 Å octahedral corner-linked chain structures," which include a large number of discrete structure types. The dominating motif of these structures is an infinitely extending octahedral chain which involves $Me^{3+}(=Al^{3+},Fe^{3+})$ cations and opposing apical corner-links of $(OH)^-$ anions. This structural backbone is featured in Figure 1. We shall find it convenient to refer to a structural prototype, that is, the simplest arrangement which affords such a corner-linked chain. This is evidently the structure of $Fe^{3+}(OH)[SO_4]$ (and isostructural $In^{3+}(OH)[SO_4]$), described by Johansson (1962). It possesses the octahedral chains parallel to the a-axis which link laterally by $[SO_4]$ tetrahedra to form an indefinitely extending network of octahedra and tetrahedra.

Baur (1969) has noted that, in the 7 Å chain structures he investigated, the octahedral backbone is linked laterally by tetrahedra to similar backbones, forming dense slabs. Between these slabs are more weakly linked bridging groups, usually consisting of insular $Me^{2+}(O,H_2O)_6$ octahedra.

TABLE 1. Dependence of $R(hkl)$ on $|F(hkl)|$ for Jahnsite

$$\underline{R}(hkl) = \frac{\Sigma||F(obs)| - |F(calc)||}{\Sigma|F(obs)|}$$

$\underline{F}$(hkl)	Number	$\underline{R}$(hkl)
Above 0.0	3234	0.12
" 6.0	2292	0.09
" 18.0	1207	0.06
" 36.0	415	0.05
" 61.0	147	0.04

TABLE 2. Jahnsite. Atomic Coordinates and Isotropic Thermal Vibration Parameters*

Atom	x	y	z	B(Å^2)
Fe(1)	0.0000	0.0000	0.0000	1.58(3)
Fe(2)	.0000	.5000	.0000	1.70(3)
Mg(1)	.5000	.0000	.5000	1.21(7)
Mg(2)	.2500	.4963(3)	.5000	0.96(7)
Ca	.2500	-.0249(3)	.0000	1.69(3)
Mn	.2500	.4775(2)	.0000	1.12(3)
P(1)	.1830(1)	.2615(2)	.1881(2)	.92(2)
O(1)	.2758(4)	.2345(7)	.1512(6)	1.83(8)
O(2)	.2041(4)	.2956(7)	.3462(6)	1.65(8)
O(3)	.1229(4)	.0827(7)	.1399(6)	1.57(8)
O(4)	.1369(3)	.4352(6)	.0941(5)	1.15(7)
P(2)	.0813(1)	.7476(2)	.7978(2)	.87(2)
O(5)	.1890(4)	.6984(7)	.8553(6)	1.52(8)
O(6)	.0497(3)	.7802(7)	.6381(5)	1.47(8)
O(7)	.0747(3)	.9293(6)	.8791(5)	1.29(7)
O(8)	.0245(3)	.5881(6)	.8314(5)	1.29(7)
OH	.0256(3)	.7509(6)	.0935(5)	1.06(6)
OW(1)	.2231(4)	.7185(8)	.3445(6)	2.09(9)
OW(2)	.4497(4)	.2130(8)	.3452(6)	2.37(9)
OW(3)	.6307(4)	-.0066(8)	.4629(6)	2.18(9)
OW(4)	.3917(4)	.5131(7)	.5115(5)	1.72(9)

*Estimated standard errors refer to the last digit.

Moore (1970a) has singled out two kinds of isomerism which explain the unusual diversity of the 7 Å chain structures. The first kind involves the arrangements of the $[PO_4]$ and (H_2O) ligands about the backbone, of which seven types of isomerisms which permit the formation of slabs were discerned. In addition, the bridging Me^{2+}-(O,H_2O) octahedral species between the slabs can exhibit *cis* or *trans* stereoisomerism. Jahnsite and segelerite (based on a preliminary structure analysis) belong to arrangement VI (see Moore, 1970a) of tetrahedra about the backbone, an arrangement postulated on stereochemical grounds and heretofore unknown in mineral structures. The distinction between jahnsite and segelerite apparently occurs in the conformation of the bridging octahedral species and locations of the $[PO_4]$ tetrahedra.

The idealized jahnsite slab (Fig. 2) is formed by the coupling of octahedral backbones by infinitely extending columns of $Me^{2+}O_6$ edge-sharing octahedra. The large Me^{2+} cations, such as Ca^{2+} and Mn^{2+}, form six- to eight-fold coordinated polyhedra (see Fig. 3). In the ideal structure these polyhedra each share two edges with the $Me^{3+}O_6$ octahedra at the same level, two edges with the $[PO_4]^{3-}$

TABLE 3. Jahnsite. Structure Factors

h	k	l	F_{obs}	F_{calc}
0	0	2	177.1	174.6
0	0	3	40.1	37.0
0	0	4	28.9	43.4
0	0	5	36.6	44.2
0	0	6	239.5	235.1
0	0	7	6.3	11.3
0	0	8	76.4	71.6
0	0	9	33.7	37.6
0	0	10	87.3	82.1
0	0	11	64.0	59.8
0	0	12	47.5	43.7
0	0	13	5.3	2.5
0	0	14	45.5	39.3
2	0	1	15.4	23.4
2	0	2	20.7	22.4
2	0	3	39.4	30.1
2	0	4	6.3	7.2
2	0	5	23.5	24.9
2	0	6	8.3	7.6
2	0	7	25.4	32.4
2	0	8	18.4	21.1
2	0	9	17.4	13.9
2	0	10	31.5	34.2
2	0	11	11.1	9.8
2	0	12	14.7	10.4
2	0	13	13.4	17.5
2	0	-2	20.6	32.3
2	0	-3	46.0	47.8
2	0	-4	13.8	21.6
2	0	-5	28.2	33.8
2	0	-6	82.5	53.8
2	0	-7	9.3	1.2
2	0	-8	4.7	2.1
2	0	-9	10.5	12.3
2	0	-10	4.7	7.2
2	0	-11	4.9	1.1
2	0	-12	5.2	2.4
2	0	-13	28.3	23.1
2	0	-14	5.5	4.7
4	0	0	173.7	174.4
4	0	1	278.6	284.3
4	0	2	87.2	103.3
4	0	3	129.3	135.8
4	0	4	61.5	72.9
4	0	5	31.0	35.6
4	0	6	137.4	150.1
4	0	7	86.2	81.3
4	0	8	34.1	43.2
4	0	9	4.7	5.5
4	0	10	29.6	30.1
4	0	11	45.6	45.9
4	0	12	52.0	55.2
4	0	13	14.3	17.0
4	0	-1	32.8	36.8
4	0	-2	182.3	191.9
4	0	-3	224.3	214.0
4	0	-4	128.6	142.4
4	0	-5	167.0	162.4
4	0	-6	71.6	74.0
4	0	-7	17.5	23.6
4	0	-8	156.5	151.8
4	0	-9	76.3	71.1
4	0	-10	59.6	60.7
4	0	-11	19.5	20.5
4	0	-12	29.7	30.6
4	0	-13	33.1	35.5
4	0	-14	76.8	64.7
6	0	0	21.9	9.7
6	0	1	75.7	71.5
6	0	2	47.3	52.0
6	0	3	32.1	39.4
6	0	4	74.6	71.9
6	0	5	33.0	11.4
6	0	6	77.1	73.1
6	0	7	10.3	15.4
6	0	8	4.7	1.3
6	0	9	13.3	12.3
6	0	10	5.1	1.6
6	0	11	10.5	12.8
6	0	12	3.4	0.6
6	0	-1	22.0	10.0
6	0	-2	30.4	29.2
6	0	-3	46.7	36.8
6	0	-4	38.2	39.1
6	0	-5	28.0	35.2
6	0	-6	41.1	41.4
6	0	-7	29.4	28.7
6	0	-8	33.9	37.5
6	0	-9	54.3	56.5
6	0	-10	4.7	0.8
6	0	-11	27.0	25.9
6	0	-12	49.3	43.9
6	0	-13	21.7	16.9
6	0	-14	27.7	26.0
6	0	-15	11.1	23.4
8	0	0	56.4	138.9
8	0	1	40.4	47.0
8	0	2	106.3	112.5
8	0	3	67.5	69.8
8	0	4	143.7	142.8
8	0	5	20.6	17.5
8	0	6	48.2	51.4
8	0	7	67.5	62.9
8	0	8	91.8	93.5
8	0	9	45.7	47.9
8	0	10	36.7	30.1
8	0	11	5.4	7.5
8	0	-1	91.5	86.6
8	0	-2	270.7	276.9
8	0	-3	73.8	77.5
8	0	-4	130.9	136.3
8	0	-5	32.6	39.8
8	0	-6	71.6	75.7
8	0	-7	65.7	72.6
8	0	-8	114.5	115.8
8	0	-9	4.6	3.3
8	0	-10	62.7	64.9
8	0	-11	49.4	49.0
8	0	-12	76.6	75.7
8	0	-13	48.6	40.7
8	0	-14	36.8	36.2
8	0	-15	8.9	2.6
10	0	0	28.1	31.1
10	0	1	12.2	12.7
10	0	2	21.7	17.5
10	0	3	56.9	54.8
10	0	4	4.6	1.4
10	0	5	11.1	12.1
10	0	6	29.2	30.5
10	0	7	16.2	15.3
10	0	8	13.7	18.0
10	0	9	10.4	7.7
10	0	10	5.3	7.0
10	0	-1	42.5	48.9
10	0	-2	4.2	1.5
10	0	-3	4.2	2.3
10	0	-4	48.1	51.1
10	0	-5	37.7	35.3
10	0	-6	16.4	11.4
10	0	-7	22.2	21.7
10	0	-8	64.6	60.5
10	0	-9	4.7	4.8
10	0	-10	41.6	38.7
10	0	-11	21.6	15.8
10	0	-12	5.1	4.6
10	0	-13	20.8	24.3
10	0	-14	5.6	6.4
10	0	-15	33.7	26.1
12	0	0	81.3	80.6
12	0	1	40.9	44.1
12	0	2	45.3	46.3
12	0	3	15.8	18.9
12	0	4	105.1	104.9
12	0	5	69.1	67.2
12	0	6	36.7	36.5
12	0	7	12.0	10.3
12	0	8	33.1	32.0
12	0	9	31.7	29.8
12	0	-1	99.1	105.8
12	0	-2	83.9	90.1
12	0	-3	11.5	19.3
12	0	-4	139.8	120.2
12	0	-5	84.1	86.4
12	0	-6	101.7	100.9
12	0	-7	50.2	51.7
12	0	-8	42.2	38.1
12	0	-9	23.7	24.6
12	0	-10	90.0	94.2
12	0	-11	45.5	44.6
12	0	-12	43.1	45.2
12	0	-13	5.4	9.0
12	0	-14	21.3	20.5
14	0	0	8.3	1.4
14	0	1	32.6	25.4
14	0	2	29.5	30.4
14	0	3	4.9	3.8
14	0	4	27.9	33.3
14	0	5	5.2	5.6
14	0	6	5.3	4.8
14	0	7	12.8	12.6
14	0	9	5.4	3.6
14	0	-1	18.0	21.5
14	0	-2	26.4	32.3
14	0	-3	33.9	35.2
14	0	-4	39.4	41.4
14	0	-5	4.6	6.0
14	0	-6	18.0	19.4
14	0	-7	20.0	23.2
14	0	-8	15.7	9.6
14	0	-9	53.4	46.5
14	0	-10	5.0	1.1
14	0	-11	18.6	22.9
14	0	-12	12.9	15.4
14	0	-13	9.0	5.0
14	0	-14	25.4	17.5
16	0	0	74.8	74.4
16	0	1	50.5	49.8
16	0	2	70.8	73.4
16	0	3	5.7	5.4
16	0	4	12.3	13.9
16	0	5	31.5	27.1
16	0	6	54.3	50.8
16	0	-1	21.3	21.7
16	0	-2	40.0	35.6
16	0	-3	44.2	44.4
16	0	-4	102.7	106.4
16	0	-5	41.7	40.6
16	0	-6	53.7	60.5
16	0	-7	18.7	21.6
16	0	-8	52.2	50.7
16	0	-9	44.0	46.4
16	0	-10	49.2	48.4
16	0	-11	5.3	5.6
16	0	-12	26.3	31.6
16	0	-13	27.3	21.8
18	0	0	22.2	25.1
18	0	1	25.1	28.9
18	0	2	12.1	7.8
18	0	3	23.4	22.9
18	0	4	10.7	8.1
18	0	-1	10.8	12.6
18	0	-2	22.4	19.5
18	0	-3	29.2	27.7
18	0	-4	5.0	9.6
18	0	-5	5.1	12.9
18	0	-6	23.1	17.5
18	0	-7	28.4	21.6
18	0	-8	17.5	19.0
18	0	-9	16.7	18.5
18	0	-10	30.9	38.9
18	0	-11	5.4	10.2
18	0	-12	22.8	19.0
20	0	0	10.6	12.8
20	0	1	5.4	2.4
20	0	2	44.3	48.8
20	0	-1	5.4	3.8
20	0	-2	52.6	51.4
20	0	-3	48.3	52.5
20	0	-4	47.6	49.9
20	0	-5	12.1	11.7
20	0	-6	37.1	41.0
20	0	-7	17.8	20.3
20	0	-8	52.6	55.8
20	0	-9	27.1	29.5
20	0	-10	32.2	33.5
20	0	-11	11.5	13.9
22	0	-2	5.5	2.0
22	0	-3	15.4	18.4
22	0	-4	13.1	16.2
22	0	-5	30.5	30.0
22	0	-6	23.4	20.1
22	0	-7	11.9	1.2
22	0	-8	12.8	19.0
22	0	-9	5.5	16.5
0	1	2	8.4	6.9
0	1	3	6.5	6.0
0	1	4	27.2	25.4
0	1	5	9.0	9.2
0	1	6	18.4	18.2
0	1	7	16.5	15.9
0	1	8	4.3	3.4
0	1	9	4.4	9.4
0	1	10	17.4	17.2
0	1	11	10.7	10.4
0	1	12	17.7	20.8
0	1	13	6.1	1.0
0	1	14	6.1	2.4
1	1	2	37.7	36.7
1	1	3	46.7	49.4
1	1	4	78.5	77.4
1	1	5	14.2	13.2
1	1	6	54.1	52.7
1	1	7	24.0	27.0
1	1	8	18.2	16.7
1	1	9	25.2	24.2
1	1	10	4.6	2.1
1	1	11	35.8	30.5
1	1	12	19.7	18.9
1	1	13	22.9	18.0
1	1	-2	67.2	67.8
1	1	-3	3.4	2.3
1	1	-4	69.7	67.5
1	1	-5	43.9	39.8
1	1	-6	14.5	14.9
1	1	-7	23.9	20.5
1	1	-8	14.1	14.3
1	1	-9	4.4	1.2
1	1	-10	9.3	6.9
1	1	-11	4.8	4.8
1	1	-12	5.1	0.8
1	1	-13	5.3	8.3
1	1	-14	5.4	3.8
2	1	1	21.5	24.2
2	1	2	50.9	55.4
2	1	3	13.1	10.3
2	1	4	58.9	57.9
2	1	5	32.9	33.7
2	1	6	38.2	36.0
2	1	7	34.4	35.4
2	1	8	16.9	18.7
2	1	9	8.1	9.3
2	1	10	15.2	13.4
2	1	11	4.9	2.7
2	1	12	20.8	17.2
2	1	13	5.1	2.3
2	1	-2	44.8	44.6
2	1	-3	13.8	17.8
2	1	-4	22.1	19.6
2	1	-5	39.3	37.2
2	1	-6	28.7	25.2
2	1	-7	4.3	4.6
2	1	-8	60.2	58.1
2	1	-9	9.5	10.3
2	1	-10	23.9	22.1
2	1	-11	13.5	17.0
2	1	-12	5.9	3.4
2	1	-13	6.3	17.5
2	1	-14	16.8	17.0
3	1	0	83.5	89.7
3	1	1	102.6	101.7
3	1	2	20.5	16.4
3	1	3	41.5	43.4
3	1	4	7.3	7.2
3	1	5	25.9	27.4
3	1	6	18.9	15.9
3	1	7	4.5	11.8
3	1	8	30.5	28.7
3	1	9	17.4	16.9
3	1	10	15.7	16.5
3	1	11	19.2	16.4
3	1	12	5.1	0.6
3	1	13	5.2	4.2
3	1	-1	28.9	30.7
3	1	-2	107.5	105.4
3	1	-3	99.7	91.0
3	1	-4	3.6	9.2
3	1	-5	67.0	66.1
3	1	-6	9.7	9.9
3	1	-7	41.7	39.1
3	1	-8	4.5	5.5
3	1	-9	25.9	23.9
3	1	-10	39.0	36.1
3	1	-11	9.7	0.3
3	1	-12	33.1	31.8
3	1	-13	19.9	19.7
3	1	-14	10.8	11.8
4	1	0	37.2	36.6
4	1	1	12.2	12.2
4	1	2	12.7	11.9
4	1	3	24.0	22.8
4	1	4	8.1	9.0
4	1	5	21.2	21.7
4	1	6	29.7	32.9
4	1	7	31.0	32.3
4	1	8	4.5	4.6
4	1	9	9.6	4.0
4	1	10	5.7	15.1
4	1	11	5.9	3.4
4	1	12	5.1	1.2
4	1	-1	18.0	17.9
4	1	-2	7.4	9.2
4	1	-3	3.5	3.3
4	1	-4	7.3	9.8
4	1	-5	27.4	27.1
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4	1	-7	23.3	24.8
4	1	-8	10.2	1.3
4	1	-9	22.0	19.4
4	1	-10	4.5	6.4
4	1	-11	10.3	9.7
4	1	-12	4.9	7.0
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4	1	-14	5.3	2.4
5	1	0	78.9	79.6
5	1	1	29.3	30.3
5	1	2	3.8	5.6
5	1	3	16.6	15.8
5	1	4	4.0	1.2
5	1	5	34.5	33.8
5	1	6	4.4	1.7
5	1	7	42.6	44.7
5	1	8	32.3	31.7
5	1	9	4.7	1.2
5	1	10	31.3	31.8
5	1	11	26.9	26.2
5	1	12	14.1	11.1
5	1	-1	17.7	19.3
5	1	-2	47.3	46.2
5	1	-3	44.5	44.6
5	1	-4	37.0	35.8
5	1	-5	3.9	2.9
5	1	-6	3.9	3.0
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5	1	-8	4.5	2.7
5	1	-9	12.9	11.6
5	1	-10	12.3	10.7
5	1	-11	10.4	9.8
5	1	-12	5.8	3.0
5	1	-13	5.2	4.3
5	1	-14	11.2	4.8
6	1	0	19.5	18.0
6	1	1	57.4	54.6
6	1	2	34.4	35.8
6	1	3	7.9	5.9
6	1	4	55.6	58.8
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6	1	6	22.8	24.5
6	1	7	14.1	15.7
6	1	8	14.9	18.0
6	1	9	4.6	0.7
6	1	10	19.7	22.3
6	1	11	5.1	7.6
6	1	-1	90.4	84.8
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6	1	-3	20.0	20.1
6	1	-4	99.2	91.9
6	1	-5	11.3	11.0
6	1	-6	51.6	49.9
6	1	-7	35.2	37.6
6	1	-8	37.7	32.2
6	1	-9	30.5	35.5
6	1	-10	18.9	14.5
6	1	-11	4.9	11.8
6	1	-12	21.1	19.5
6	1	-13	16.5	6.3
6	1	-14	30.2	21.4
7	1	0	3.9	8.0
7	1	1	49.0	47.9
7	1	2	46.3	48.5
7	1	3	13.9	10.7
7	1	4	44.1	46.4
7	1	5	30.9	31.5
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7	1	7	32.5	30.8
7	1	8	11.0	12.7
7	1	9	20.7	19.0
7	1	10	18.3	15.5
7	1	11	5.1	7.5
7	1	-1	3.9	1.0
7	1	-2	24.9	26.7
7	1	-3	12.4	11.8
7	1	-4	12.3	13.3
7	1	-5	56.4	55.3
7	1	-6	57.3	60.6
7	1	-7	33.4	34.4
7	1	-8	68.2	65.0
7	1	-9	15.6	16.9
7	1	-10	24.0	23.5
7	1	-11	40.8	40.0
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7	1	-13	47.0	40.1
7	1	-14	22.3	22.2
8	1	0	10.6	14.1
8	1	1	26.4	29.1
8	1	2	15.7	16.3
8	1	3	14.3	13.9
8	1	4	4.5	8.0
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8	1	-9	7.4	3.6
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8	1	-11	9.1	6.8
8	1	-12	13.9	14.0
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8	1	-14	6.4	4.6
9	1	0	7.7	3.3
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9	1	-13	5.7	2.4
9	1	-14	14.6	13.2
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10	1	1	13.3	13.0
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10	1	-14	11.5	7.8
11	1	0	13.5	13.5
11	1	1	50.4	53.0
11	1	2	16.3	15.7
11	1	3	23.7	24.0
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11	1	8	5.1	9.8
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11	1	-1	69.1	69.6
11	1	-2	63.2	59.7
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12	1	1	7.7	11.6
12	1	2	18.6	22.5
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12	1	4	7.9	11.9
12	1	5	4.7	2.7
12	1	6	5.1	4.9
12	1	7	5.0	1.4
12	1	8	10.6	4.3
12	1	9	5.1	0.5
12	1	-1	17.9	19.4
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12	1	-4	15.4	8.5
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12	1	-11	11.0	9.5
12	1	-12	5.1	5.9
12	1	-13	13.4	7.9
12	1	-14	5.2	0.5
13	1	0	14.0	12.9
13	1	1	18.7	18.5
13	1	2	4.6	1.3
13	1	3	4.7	5.5
13	1	4	10.2	9.8
13	1	5	31.7	32.0
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13	1	7	5.1	8.2
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13	1	-1	4.4	2.2
13	1	-2	4.4	4.1
13	1	-3	12.2	13.5
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13	1	-6	4.4	1.4
13	1	-7	17.2	13.8
13	1	-8	20.2	16.7
13	1	-9	15.5	10.8
13	1	-10	3.8	7.7
13	1	-11	16.0	15.4
13	1	-12	6.0	6.0
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13	1	-14	6.3	1.9
14	1	0	37.3	34.7
14	1	1	15.7	16.3
14	1	2	25.1	25.4
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14	1	4	13.7	17.6
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14	1	7	5.1	2.7
14	1	-1	19.6	16.4
14	1	-2	29.7	28.1
14	1	-3	35.8	36.9
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14	1	-9	27.1	25.9
14	1	-10	11.6	11.6
14	1	-11	10.9	15.0
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14	1	-13	6.2	3.8
14	1	-14	16.5	11.7
15	1	0	37.1	41.5
15	1	1	9.6	2.0
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15	1	3	30.8	33.3
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15	1	-3	21.0	19.6
15	1	-4	17.0	14.3
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15	1	-9	12.7	17.8
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17	1	3	13.1	15.6
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18	1	0	13.7	19.3
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19	1	0	11.3	4.6
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5	2	0	11.6	10.7
5	2	1	53.9	53.9
5	2	2	54.7	54.4
5	2	3	18.6	19.2
5	2	4	4.0	7.0
5	2	5	17.7	17.7
5	2	6	4.9	1.0
5	2	7	21.9	22.8
5	2	8	26.9	27.0
5	2	9	14.4	15.0
5	2	10	4.9	2.7
5	2	11	5.2	5.1
5	2	12	5.1	4.9
5	2	-1	35.2	30.2
5	2	-2	15.0	13.6
5	2	-3	3.6	4.4
5	2	-4	37.0	38.5
5	2	-5	47.1	44.0
5	2	-6	25.8	26.1
5	2	-7	14.2	14.6
5	2	-8	16.5	15.0
5	2	-9	4.6	1.7
5	2	-10	5.4	1.9
5	2	-11	4.7	0.7
5	2	-12	6.1	1.8
5	2	-13	5.2	6.8
5	2	-14	6.4	11.5
6	2	0	11.6	17.0
6	2	1	19.3	27.5
6	2	2	4.0	10.6
6	2	3	33.9	42.8
6	2	4	4.1	7.7
6	2	5	34.3	37.4
6	2	6	4.3	2.1
6	2	7	4.6	3.7
6	2	8	17.7	20.8
6	2	9	4.7	0.7
6	2	10	4.5	8.4
6	2	11	5.0	4.0
6	2	-1	38.9	31.6
6	2	-2	47.5	30.5
6	2	-3	6.4	5.3
6	2	-4	16.1	16.8
6	2	-5	19.3	19.4
6	2	-6	19.2	23.1
6	2	-7	27.8	25.8
6	2	-8	27.3	27.3
6	2	-9	42.6	38.5
6	2	-10	16.8	14.9
6	2	-11	4.7	10.2
6	2	-12	27.1	23.8
6	2	-13	5.2	12.1
6	2	-14	24.7	18.5
7	2	0	17.8	16.2
7	2	1	20.3	20.7
7	2	2	3.9	0.8
7	2	3	4.1	4.7
7	2	4	4.2	2.4
7	2	5	4.3	5.2
7	2	6	5.3	10.8
7	2	7	16.5	19.3
7	2	8	3.0	9.5
7	2	9	11.8	7.7
7	2	10	9.7	5.6
7	2	11	6.2	1.1
7	2	-1	34.9	31.3
7	2	-2	30.9	28.2
7	2	-3	21.3	19.5
7	2	-4	21.3	20.0
7	2	-5	15.5	17.6
7	2	-6	10.7	8.8
7	2	-7	8.5	5.7
7	2	-8	4.3	1.3
7	2	-9	4.5	2.3
7	2	-10	5.4	4.1
7	2	-11	4.6	12.2
7	2	-12	11.4	17.5
7	2	-13	12.7	13.9
7	2	-14	6.7	4.6
8	2	0	237.2	235.5
8	2	1	73.8	76.2
8	2	2	141.6	148.1
8	2	3	4.2	3.4
8	2	4	45.6	49.6
8	2	5	78.5	80.2
8	2	6	112.2	112.6
8	2	7	18.1	19.9
8	2	8	40.5	37.2
8	2	9	4.9	4.7
8	2	10	44.7	44.2
8	2	-1	34.0	42.6
8	2	-2	32.7	35.9
8	2	-3	36.6	44.7
8	2	-4	185.3	179.1
8	2	-5	77.7	82.4
8	2	-6	147.4	151.2
8	2	-7	4.4	4.3
8	2	-8	52.7	56.3
8	2	-9	72.4	70.7
8	2	-10	96.9	90.4
8	2	-11	35.9	33.8
8	2	-12	45.7	45.2
8	2	-13	5.2	7.0
8	2	-14	43.7	42.4
9	2	0	4.0	4.6
9	2	1	7.9	5.7
9	2	2	19.0	19.8
9	2	3	15.3	19.1
9	2	4	17.0	18.5
9	2	5	4.5	4.8
9	2	6	4.5	3.1
9	2	7	4.6	1.6
9	2	8	9.2	5.7
9	2	9	5.0	5.4
9	2	10	5.2	7.1
9	2	-1	14.3	16.1
9	2	-2	28.7	27.2
9	2	-3	22.4	22.0
9	2	-4	20.4	20.7
9	2	-5	4.1	0.7
9	2	-6	9.6	10.7
9	2	-7	4.4	9.5
9	2	-8	8.2	11.5
9	2	-9	4.5	11.7
9	2	-10	12.6	15.8
9	2	-11	4.8	4.8
9	2	-12	5.0	3.7
9	2	-13	6.1	9.3
9	2	-14	6.3	4.3
10	2	0	14.2	12.4
10	2	1	17.8	12.5
10	2	2	12.2	14.9
10	2	3	20.1	18.6
10	2	4	14.6	17.7
10	2	5	4.5	8.1
10	2	6	11.8	16.3
10	2	7	4.8	7.2
10	2	8	5.0	4.2
10	2	9	5.1	0.1
10	2	-1	24.4	22.1
10	2	-2	42.5	47.0
10	2	-3	48.9	53.0
10	2	-4	11.2	9.2
10	2	-5	12.6	12.7
10	2	-6	26.0	23.5
10	2	-7	17.3	14.4
10	2	-8	56.3	49.7
10	2	-9	13.5	11.5
10	2	-10	19.0	21.5
10	2	-11	4.7	6.2
10	2	-12	5.0	4.8

TABLE 3, Continued

h	k	l	Fobs	Fcalc
10	2	-13	23.8	15.7
10	2	-14	5.3	4.2
11	2	0	30.5	31.0
11	2	1	18.6	17.5
11	2	2	11.5	10.3
11	2	3	4.4	6.7
11	2	4	8.1	6.0
11	2	5	12.0	9.7
11	2	6	17.5	8.0
11	2	7	11.7	8.2
11	2	8	9.2	4.8
11	2	9	5.1	2.4
11	2	-1	28.3	31.1
11	2	-2	4.3	6.1
11	2	-3	17.9	22.3
11	2	-4	16.1	14.8
11	2	-5	4.4	3.0
11	2	-6	24.2	23.3
11	2	-7	31.3	32.8
11	2	-8	19.6	22.7
11	2	-9	4.7	8.3
11	2	-10	4.7	3.7
11	2	-11	4.3	0.4
11	2	-12	6.0	2.0
11	2	-13	5.3	0.8
11	2	-14	6.3	1.0
12	2	0	64.9	69.9
12	2	1	64.7	66.2
12	2	2	108.6	110.9
12	2	3	74.0	75.7
12	2	4	27.6	24.7
12	2	5	4.7	3.1
12	2	6	65.2	63.0
12	2	7	43.1	41.7
12	2	8	46.1	48.8
12	2	-1	4.3	3.2
12	2	-2	77.0	81.0
12	2	-3	96.5	101.4
12	2	-4	81.2	81.2
12	2	-5	27.3	30.0
12	2	-6	61.1	63.3
12	2	-7	37.4	35.4
12	2	-8	111.7	112.9
12	2	-9	66.1	65.2
12	2	-10	51.7	49.3
12	2	-11	19.2	19.4
12	2	-12	43.0	38.9
12	2	-13	25.0	18.7
12	2	-14	37.5	36.0
13	2	0	4.4	0.5
13	2	1	4.5	4.4
13	2	2	4.6	4.1
13	2	3	4.6	6.6
13	2	4	13.3	11.6
13	2	5	11.3	13.2
13	2	6	5.0	6.5
13	2	7	5.1	4.7
13	2	8	5.2	4.5
13	2	-1	11.6	13.4
13	2	-2	11.6	11.9
13	2	-3	13.5	12.9
13	2	-4	17.1	15.8
13	2	-5	4.3	1.9
13	2	-6	11.4	9.6
13	2	-7	8.5	14.5
13	2	-8	4.7	5.9
13	2	-9	9.3	8.5
13	2	-10	4.8	6.6
13	2	-11	5.9	2.4
13	2	-12	5.7	4.8
13	2	-13	5.2	4.9
13	2	-14	6.3	7.6
14	2	0	13.3	11.9
14	2	1	12.0	13.6
14	2	2	4.6	7.7
14	2	3	22.7	19.7
14	2	4	14.6	10.6
14	2	5	5.0	3.8
14	2	6	13.0	20.9
14	2	7	5.1	5.6
14	2	-1	28.3	27.4
14	2	-2	17.0	18.5
14	2	-3	29.9	34.9
14	2	-4	36.3	39.0
14	2	-5	9.5	8.9
14	2	-6	25.8	21.3
14	2	-7	33.8	27.7
14	2	-8	4.6	0.3
14	2	-9	16.3	23.2
14	2	-10	16.2	10.3
14	2	-11	38.2	34.1
14	2	-12	14.4	7.5
14	2	-13	5.1	7.5
15	2	0	4.6	4.0
15	2	1	4.6	3.7
15	2	2	8.5	3.6
15	2	3	5.0	5.1
15	2	4	5.1	4.0
15	2	5	11.0	10.2
15	2	6	11.1	4.4
15	2	-1	4.6	1.8
15	2	-2	4.6	4.6
15	2	-3	11.1	10.8
15	2	-4	23.9	24.6
15	2	-5	23.4	23.6
15	2	-6	14.1	15.7
15	2	-7	4.7	2.2
15	2	-8	19.2	13.7
15	2	-9	4.9	4.2
15	2	-10	5.1	7.4
15	2	-11	6.1	12.2
15	2	-12	9.3	11.3
15	2	-13	6.2	9.5
16	2	0	56.9	59.5
16	2	1	19.4	16.8
16	2	2	44.7	43.8
16	2	3	46.2	48.4
16	2	4	58.7	58.7
16	2	5	5.1	3.1
16	2	-1	43.3	47.0
16	2	-2	89.2	93.3
16	2	-3	21.0	21.3
16	2	-4	34.0	31.7
16	2	-5	25.9	25.0
16	2	-6	69.4	67.5
16	2	-7	46.0	46.9
16	2	-8	56.4	60.5
16	2	-9	16.0	11.6
16	2	-10	43.2	42.0
16	2	-11	34.1	35.0
16	2	-12	48.8	45.1
16	2	-13	20.0	21.7
17	2	0	4.9	9.8
17	2	1	4.9	0.8
17	2	2	5.1	4.6
17	2	3	9.2	3.2
17	2	4	5.1	3.1
17	2	-1	11.0	13.4
17	2	-2	8.8	11.5
17	2	-3	9.2	13.0
17	2	-4	4.7	4.5
17	2	-5	4.7	7.5
17	2	-6	4.7	0.5
17	2	-7	4.8	0.4
17	2	-8	5.0	6.4
17	2	-9	11.1	16.1
17	2	-10	6.1	10.1
17	2	-11	5.2	3.6
17	2	-12	5.3	5.2
18	2	0	16.0	12.7
18	2	1	18.5	16.6
18	2	2	5.1	2.7
18	2	3	13.1	17.8
18	2	-1	4.9	0.5
18	2	-2	13.9	16.1
18	2	-3	9.5	15.6
18	2	-4	27.3	24.7
18	2	-5	27.6	23.4
18	2	-6	4.9	9.8
18	2	-7	16.7	19.7
18	2	-8	5.1	12.3
18	2	-9	22.9	15.4
18	2	-10	38.5	35.2
18	2	-11	5.2	4.6
18	2	-12	16.2	22.4
19	2	0	9.2	9.9
19	2	1	10.6	8.3
19	2	2	5.2	9.5
19	2	-1	5.1	0.9
19	2	-2	5.1	0.8
19	2	-3	5.1	6.3
19	2	-4	9.3	7.2
19	2	-5	5.1	4.2
19	2	-6	5.9	4.0
19	2	-7	8.5	1.3
19	2	-8	5.2	3.4
19	2	-9	5.2	10.2
19	2	-10	6.3	10.7
19	2	-11	5.4	5.9
20	2	0	49.9	47.8
20	2	1	31.5	30.1
20	2	-1	29.3	26.9
20	2	-2	29.9	33.9
20	2	-3	5.1	3.3
20	2	-4	43.4	47.3
20	2	-5	32.5	33.7
20	2	-6	48.3	43.6
20	2	-7	16.6	14.5
20	2	-8	31.0	31.2
20	2	-9	17.3	16.5
20	2	-10	42.9	47.5
21	2	-1	5.2	1.9
21	2	-2	5.2	3.4
21	2	-3	5.1	1.9
21	2	-4	5.2	1.1
21	2	-5	12.7	8.3
21	2	-6	11.4	15.3
21	2	-7	10.4	10.1
21	2	-8	5.2	7.4
21	2	-9	5.3	1.3
22	2	-4	19.0	16.7
22	2	-5	16.0	21.4
22	2	-6	25.4	32.0
0	3	2	25.4	25.9
0	3	3	20.4	21.0
0	3	4	17.4	20.1
0	3	5	4.0	3.6
0	3	6	4.1	1.5
0	3	7	4.2	5.7
0	3	8	18.6	16.7
0	3	9	4.5	3.4
0	3	10	8.7	12.3
0	3	11	5.6	0.5
0	3	12	5.9	8.3
0	3	13	9.0	2.9
1	3	2	66.5	64.1
1	3	3	80.6	81.2
1	3	4	41.3	40.1
1	3	5	34.7	31.9
1	3	6	72.4	73.3
1	3	7	30.0	30.5
1	3	8	26.0	24.4
1	3	9	30.1	32.8
1	3	10	5.4	5.4
1	3	11	27.4	24.1
1	3	12	15.0	10.8
1	3	13	24.2	22.3
1	3	-2	30.2	29.2
1	3	-3	41.8	40.8
1	3	-4	46.5	45.6
1	3	-5	4.1	2.1
1	3	-6	36.8	35.9
1	3	-7	24.4	23.5
1	3	-8	8.1	7.4
1	3	-9	4.5	1.4
1	3	-10	5.4	3.3
1	3	-11	10.4	10.5
1	3	-12	5.2	3.7
1	3	-13	5.2	5.8
2	3	1	13.8	14.5
2	3	2	55.6	53.7
2	3	3	45.4	43.6
2	3	4	52.5	57.8
2	3	5	14.6	15.3
2	3	6	4.1	1.3
2	3	7	11.4	12.7
2	3	8	30.7	29.2
2	3	9	16.2	15.2
2	3	10	29.3	27.4
2	3	11	5.0	6.6
2	3	12	5.0	4.9
2	3	-2	13.8	14.0
2	3	-3	53.1	48.4
2	3	-4	68.5	62.2
2	3	-5	22.2	24.4
2	3	-6	20.5	22.3
2	3	-7	13.4	14.0
2	3	-8	15.4	14.0
2	3	-9	13.8	13.6
2	3	-10	28.3	25.4
2	3	-11	16.0	15.9
2	3	-12	18.5	20.2
2	3	-13	6.2	1.7
3	3	0	52.3	54.1
3	3	1	68.2	67.0
3	3	2	3.7	5.8
3	3	3	55.4	54.7
3	3	4	31.1	32.2
3	3	5	18.8	19.7
3	3	6	19.2	17.2
3	3	7	4.2	1.4
3	3	8	23.8	22.3
3	3	9	17.8	17.6
3	3	10	8.8	4.1
3	3	11	11.7	11.9
3	3	12	5.0	1.5
3	3	-1	9.1	9.8
3	3	-2	65.6	67.5
3	3	-3	30.2	30.0
3	3	-4	30.9	27.6
3	3	-5	54.9	51.1
3	3	-6	19.2	20.7
3	3	-7	60.4	55.6
3	3	-8	28.2	25.7
3	3	-9	23.4	24.2
3	3	-10	36.9	34.9
3	3	-11	8.1	8.9
3	3	-12	31.3	30.2
3	3	-13	13.1	16.5
3	3	-14	5.5	11.1
4	3	0	3.0	3.0
4	3	1	8.1	6.7
4	3	2	6.4	8.5
4	3	3	4.0	8.0
4	3	4	8.0	13.1
4	3	5	4.1	10.4
4	3	6	4.1	1.6
4	3	7	4.3	5.1
4	3	8	4.5	6.0
4	3	9	11.3	11.3
4	3	10	5.6	1.4
4	3	11	5.1	2.1
4	3	12	5.1	6.4
4	3	-1	11.7	12.4
4	3	-2	7.4	5.3
4	3	-3	7.7	5.3
4	3	-4	3.8	1.9
4	3	-5	25.2	25.8
4	3	-6	4.0	4.4
4	3	-7	30.4	29.0
4	3	-8	4.2	8.0
4	3	-9	4.4	0.7
4	3	-10	4.6	3.8
4	3	-11	5.6	11.0
4	3	-12	5.8	0.9
4	3	-13	6.3	11.3
4	3	-14	6.2	5.2
5	3	0	5.5	0.7
5	3	1	21.6	21.4
5	3	2	23.0	21.3
5	3	3	4.0	1.9
5	3	4	22.0	24.5
5	3	5	47.7	40.0
5	3	6	16.1	17.0
5	3	7	27.8	29.0
5	3	8	24.8	26.3
5	3	9	4.7	3.7
5	3	10	21.5	19.3
5	3	11	15.0	15.6
5	3	-1	20.3	20.8
5	3	-2	3.3	4.9
5	3	-3	38.0	33.4
5	3	-4	41.1	36.3
5	3	-5	27.0	24.5
5	3	-6	12.6	14.6
5	3	-7	42.4	43.1
5	3	-8	7.9	5.3
5	3	-9	16.4	13.2
5	3	-10	24.7	24.3
5	3	-11	14.5	13.9
5	3	-12	5.9	3.1
5	3	-13	10.9	9.8
5	3	-14	5.3	2.7
6	3	0	65.8	68.2
6	3	1	45.4	51.6
6	3	2	58.2	60.7
6	3	3	35.5	34.5
6	3	4	4.2	15.2
6	3	5	4.1	3.9
6	3	6	20.9	21.0
6	3	7	14.0	13.3
6	3	8	29.5	29.7
6	3	9	16.6	13.1
6	3	10	9.8	14.7
6	3	11	5.1	2.3
6	3	-1	8.8	7.3
6	3	-2	17.6	16.2
6	3	-3	41.4	38.7
6	3	-4	67.2	65.8
6	3	-5	46.3	45.3
6	3	-6	75.6	72.6
6	3	-7	8.1	13.7
6	3	-8	13.7	11.4
6	3	-9	15.5	16.6
6	3	-10	21.7	15.6
6	3	-11	5.7	13.4
6	3	-12	31.9	26.9
6	3	-13	6.1	2.7
6	3	-14	6.2	8.7
7	3	0	45.3	48.0
7	3	1	25.5	23.0
7	3	2	64.5	63.6
7	3	3	19.9	21.5
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7	3	7	18.4	18.8
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7	3	9	17.1	17.8
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10	4	8	10.2	13.8
10	4	9	11.8	4.1
10	4	-1	25.9	28.4
10	4	-2	11.0	9.6
10	4	-3	14.5	14.1
10	4	-4	25.5	25.6
10	4	-5	41.0	39.3
10	4	-6	28.5	26.0
10	4	-7	4.2	1.5
10	4	-8	35.1	36.9
10	4	-9	4.5	2.7
10	4	-10	27.6	24.4
10	4	-11	19.4	15.3
10	4	-12	5.1	1.8
10	4	-13	5.1	13.0
11	4	0	37.7	39.2
11	4	1	35.1	34.5
11	4	2	23.7	22.6
11	4	3	12.8	11.7
11	4	4	9.2	4.0
11	4	5	4.7	2.1
11	4	6	19.7	19.8
11	4	7	4.9	7.8
11	4	8	10.1	5.2
11	4	-1	4.1	2.6
11	4	-2	4.0	3.0
11	4	-3	4.0	2.3
11	4	-4	4.1	6.4
11	4	-5	20.0	18.4
11	4	-6	21.1	23.1
11	4	-7	16.6	16.1
11	4	-8	25.0	26.2
11	4	-9	19.4	20.6
11	4	-10	12.7	15.2
11	4	-11	5.9	5.4
11	4	-12	6.0	1.6
11	4	-13	5.3	0.5
12	4	0	79.0	79.9
12	4	1	22.9	22.6
12	4	2	19.3	15.8
12	4	3	12.4	9.2
12	4	4	79.2	78.1
12	4	5	55.9	55.1
12	4	6	34.2	33.4
12	4	7	4.9	2.1
12	4	8	26.3	21.6
12	4	-1	86.0	88.6
12	4	-2	71.0	72.8
12	4	-3	13.5	7.7
12	4	-4	62.2	63.6
12	4	-5	57.5	55.6
12	4	-6	87.4	86.7
12	4	-7	39.5	41.2
12	4	-8	34.9	31.9
12	4	-9	10.9	9.2
12	4	-10	57.4	54.9
12	4	-11	32.3	29.8
12	4	-12	43.7	40.3
12	4	-13	19.4	16.1
13	4	0	4.3	4.9
13	4	1	14.5	11.6
13	4	2	10.8	12.9
13	4	3	15.9	18.3
13	4	4	10.4	11.6
13	4	5	4.9	5.7
13	4	6	9.3	10.4
13	4	7	13.8	14.0
13	4	-1	4.3	3.7
13	4	-2	19.8	10.7
13	4	-3	21.0	22.7
13	4	-4	14.9	17.2
13	4	-5	19.9	23.8
13	4	-6	13.9	13.9
13	4	-7	4.4	7.1
13	4	-8	24.9	23.0
13	4	-9	4.8	9.1
13	4	-10	4.8	7.5
13	4	-11	5.0	8.7
13	4	-12	5.1	2.7
13	4	-13	6.1	8.3
14	4	0	4.4	1.1
14	4	1	14.7	13.3
14	4	2	11.9	8.5
14	4	3	8.0	3.7
14	4	4	10.5	16.2
14	4	5	14.4	12.1
14	4	6	13.2	9.5
14	4	-1	4.4	6.9
14	4	-2	4.4	9.6
14	4	-3	33.1	32.5
14	4	-4	37.8	36.5
14	4	-5	9.1	2.4
14	4	-6	4.5	11.2
14	4	-7	4.5	9.5
14	4	-8	14.5	10.4
14	4	-9	32.5	29.3
14	4	-10	5.0	5.7
14	4	-11	17.3	21.0
14	4	-12	5.1	8.6
14	4	-13	16.3	14.7
15	4	0	4.6	1.6
15	4	1	12.6	15.5
15	4	2	10.9	11.2
15	4	3	11.6	13.9
15	4	4	9.6	9.4
15	4	5	5.1	1.3

TABLE 3, Continued

h	k	l	Fobs	Fcalc
15	4	-1	4.5	6.1
15	4	-2	13.7	14.4
15	4	-3	15.3	17.1
15	4	-4	20.0	20.8
15	4	-5	23.2	16.0
15	4	-6	14.5	15.0
15	4	-7	14.9	9.7
15	4	-8	4.9	5.7
15	4	-9	5.0	3.9
15	4	-10	5.9	1.8
15	4	-11	5.1	3.4
15	4	-12	13.8	14.5
16	4	0	53.4	50.8
16	4	1	33.0	30.9
16	4	2	49.9	47.4
16	4	3	5.0	2.9
16	4	4	24.0	21.7
16	4	-1	15.0	10.5
16	4	-2	37.5	33.2
16	4	-3	38.0	36.1
16	4	-4	79.3	81.1
16	4	-5	36.3	33.1
16	4	-6	41.7	41.3
16	4	-7	10.6	10.1
16	4	-8	44.6	39.7
16	4	-9	35.3	37.8
16	4	-10	41.7	41.5
16	4	-11	14.9	10.5
16	4	-12	27.6	26.9
17	4	0	9.1	13.2
17	4	1	5.0	8.1
17	4	2	5.0	2.5
17	4	3	5.1	4.4
17	4	-1	20.4	22.9
17	4	-2	26.9	30.3
17	4	-3	11.5	7.8
17	4	-4	4.8	2.3
17	4	-5	4.9	2.6
17	4	-6	4.9	3.1
17	4	-7	16.2	14.3
17	4	-8	23.1	25.6
17	4	-9	5.0	0.9
17	4	-10	5.1	10.5
17	4	-11	9.8	5.6
18	4	0	5.0	5.8
18	4	1	5.1	15.1
18	4	2	13.2	6.8
18	4	-1	9.7	2.6
18	4	-2	24.0	18.3
18	4	-3	21.7	16.8
18	4	-4	8.5	13.8
18	4	-5	5.0	13.3
18	4	-6	20.8	16.9
18	4	-7	30.2	25.1
18	4	-8	22.2	16.2
18	4	-9	5.2	15.8
18	4	-10	21.7	28.4
19	4	0	9.4	5.7
19	4	1	5.1	9.0
19	4	-1	14.2	10.8
19	4	-2	15.1	15.0
19	4	-3	5.0	0.8
19	4	-4	5.0	7.5
19	4	-5	5.0	3.4
19	4	-6	5.1	5.5
19	4	-7	5.1	11.0
19	4	-8	9.8	12.5
19	4	-9	5.2	7.9
19	4	-10	17.7	14.1
20	4	-1	11.9	9.0
20	4	-2	42.6	45.1
20	4	-3	30.4	30.3
20	4	-4	34.9	33.8
20	4	-5	12.0	12.1
20	4	-6	35.0	37.5
20	4	-7	24.8	21.5
20	4	-8	43.3	42.1
21	4	-4	13.2	6.9
21	4	-5	5.2	11.4
21	4	-6	5.3	11.8
0	5	2	5.3	2.7
0	5	3	11.1	10.0
0	5	4	3.5	0.6
0	5	5	8.7	0.7
0	5	6	18.5	19.7
0	5	7	7.2	4.6
0	5	8	11.2	10.3
0	5	9	4.4	5.7
0	5	10	8.1	7.2
0	5	11	5.9	9.0
0	5	12	5.9	0.5
1	5	2	23.6	26.8
1	5	3	35.4	34.2
1	5	4	39.7	42.8
1	5	5	7.7	3.4
1	5	6	38.2	36.3
1	5	7	20.1	24.8
1	5	8	13.6	13.9
1	5	9	24.1	22.1
1	5	10	4.7	2.5
1	5	11	26.3	25.4
1	5	12	22.5	18.2
1	5	-2	27.1	29.9
1	5	-3	3.2	6.6
1	5	-4	30.5	31.2
1	5	-5	20.8	19.9
1	5	-6	5.8	8.4
1	5	-7	7.0	4.0
1	5	-8	4.3	0.7
1	5	-9	8.8	5.0
1	5	-10	8.5	3.3
1	5	-11	5.0	4.7
1	5	-12	5.1	1.0
2	5	1	10.8	11.5
2	5	2	5.6	2.5
2	5	3	9.4	10.2
2	5	4	6.2	6.5
2	5	5	26.5	23.7
2	5	6	61.5	61.7
2	5	7	14.9	11.7
2	5	8	8.9	14.1
2	5	9	4.6	5.3
2	5	10	5.5	0.9
2	5	11	5.8	2.3
2	5	-2	22.9	26.5
2	5	-3	5.9	4.2
2	5	-4	7.4	3.9
2	5	-5	19.0	18.3
2	5	-6	38.8	35.8
2	5	-7	37.2	36.3
2	5	-8	16.7	16.3
2	5	-9	9.4	12.9
2	5	-10	8.4	9.3
2	5	-11	5.0	7.7
2	5	-12	6.3	14.9
3	5	0	50.7	57.1
3	5	1	42.0	45.7
3	5	2	9.7	8.8
3	5	3	33.2	32.6
3	5	4	3.8	1.9
3	5	5	25.5	28.6
3	5	6	21.5	22.4
3	5	7	7.8	8.4
3	5	8	19.7	18.9
3	5	9	16.3	16.0
3	5	10	5.8	11.4
3	5	11	11.5	12.2
3	5	-1	5.8	3.9
3	5	-2	52.1	52.1
3	5	-3	47.2	47.9
3	5	-4	13.9	11.1
3	5	-5	31.3	29.1
3	5	-6	8.1	10.8
3	5	-7	20.1	21.3
3	5	-8	5.2	2.5
3	5	-9	26.4	27.9
3	5	-10	35.7	33.7
3	5	-11	4.5	1.0
3	5	-12	26.0	25.8
4	5	0	10.8	7.4
4	5	1	7.8	4.7
4	5	2	13.5	16.1
4	5	3	18.5	15.7
4	5	4	11.6	9.1
4	5	5	6.3	2.9
4	5	6	6.1	1.7
4	5	7	4.2	0.7
4	5	8	4.5	6.6
4	5	9	4.6	3.4
4	5	10	5.8	5.8
4	5	11	6.8	11.3
4	5	-1	5.1	9.4
4	5	-2	11.8	10.3
4	5	-3	40.0	40.4
4	5	-4	14.5	12.4
4	5	-5	3.5	1.6
4	5	-6	13.6	16.3
4	5	-7	7.5	7.2
4	5	-8	4.2	3.0
4	5	-9	28.3	29.4
4	5	-10	4.7	1.2
4	5	-11	4.5	4.5
4	5	-12	6.0	6.7
4	5	-13	6.7	3.3
5	5	0	48.8	48.7
5	5	1	35.3	37.3
5	5	2	3.7	3.9
5	5	3	14.9	15.0
5	5	4	5.6	9.9
5	5	5	10.0	7.9
5	5	6	4.1	7.2
5	5	7	27.7	31.3
5	5	8	21.6	25.5
5	5	9	4.7	5.9
5	5	10	24.5	24.3
5	5	-1	3.2	1.4
5	5	-2	38.8	39.6
5	5	-3	39.6	40.8
5	5	-4	28.8	26.8
5	5	-5	3.7	3.7
5	5	-6	3.7	1.6
5	5	-7	11.0	7.5
5	5	-8	4.8	1.5
5	5	-9	4.4	7.1
5	5	-10	5.5	3.4
5	5	-11	4.9	7.2
5	5	-12	5.8	5.2
5	5	-13	4.2	2.3
6	5	0	33.4	33.4
6	5	1	2.8	4.3
6	5	2	7.4	12.1
6	5	3	10.8	12.2
6	5	4	32.5	31.6
6	5	5	32.0	32.3
6	5	6	26.7	30.4
6	5	7	4.4	2.2
6	5	8	4.8	8.3
6	5	9	4.9	5.0
6	5	10	10.9	9.6
6	5	-1	46.2	48.5
6	5	-2	65.0	70.4
6	5	-3	25.3	27.2
6	5	-4	24.8	27.2
6	5	-5	9.4	11.3
6	5	-6	3.8	1.8
6	5	-7	30.8	31.6
6	5	-8	45.1	45.9
6	5	-9	4.4	5.9
6	5	-10	32.5	30.7
6	5	-11	5.7	0.5
6	5	-12	5.1	2.5
6	5	-13	12.6	10.2
7	5	0	15.2	13.3
7	5	1	21.2	22.7
7	5	2	36.7	38.0
7	5	3	8.6	6.4
7	5	4	30.1	30.2
7	5	5	21.9	27.0
7	5	6	7.4	5.5
7	5	7	18.5	19.7
7	5	8	8.3	10.0
7	5	9	9.2	9.4
7	5	10	10.7	7.0
7	5	-1	14.6	12.3
7	5	-2	18.0	18.4
7	5	-3	41.4	41.8
7	5	-4	12.2	7.9
7	5	-5	35.1	36.3
7	5	-6	38.5	42.8
7	5	-7	11.7	13.1
7	5	-8	42.5	42.0
7	5	-9	21.8	22.7
7	5	-10	12.9	16.9
7	5	-11	26.0	26.7
7	5	-12	5.0	0.5
7	5	-13	33.7	28.9
8	5	0	11.3	11.1
8	5	1	11.6	11.1
8	5	2	3.8	0.9
8	5	3	24.2	26.1
8	5	4	12.7	14.6
8	5	5	4.2	2.4
8	5	6	4.4	2.2
8	5	7	4.7	1.4
8	5	8	4.8	5.3
8	5	9	4.9	4.0
8	5	-1	3.9	5.8
8	5	-2	21.0	21.6
8	5	-3	24.2	22.7
8	5	-4	3.9	1.3
8	5	-5	3.8	4.7
8	5	-6	8.9	9.8
8	5	-7	4.1	3.5
8	5	-8	26.3	25.1
8	5	-9	4.4	4.4
8	5	-10	4.7	2.3
8	5	-11	4.9	2.9
8	5	-12	5.0	7.7
8	5	-13	6.1	0.8
9	5	0	11.9	14.2
9	5	1	16.3	16.0
9	5	2	10.5	10.1
9	5	3	4.1	2.7
9	5	4	27.4	20.2
9	5	5	4.4	11.1
9	5	6	10.8	10.2
9	5	7	15.3	11.1
9	5	8	4.9	8.1
9	5	9	13.1	15.7
9	5	-1	25.2	27.7
9	5	-2	10.0	11.5
9	5	-3	7.0	7.7
9	5	-4	8.9	6.1
9	5	-5	3.9	9.4
9	5	-6	4.0	7.5
9	5	-7	10.9	7.1
9	5	-8	8.9	5.9
9	5	-9	13.1	12.0
9	5	-10	4.7	3.1
9	5	-11	4.9	5.5
9	5	-12	5.9	5.0
9	5	-13	5.1	0.4
10	5	0	12.3	11.4
10	5	1	10.6	12.0
10	5	2	30.6	32.3
10	5	3	4.2	4.9
10	5	4	26.4	27.5
10	5	5	23.4	22.9
10	5	6	4.8	3.3
10	5	7	4.8	1.9
10	5	8	14.9	14.5
10	5	-1	20.5	19.2
10	5	-2	11.3	14.5
10	5	-3	15.2	19.5
10	5	-4	37.7	37.2
10	5	-5	21.2	17.9
10	5	-6	12.7	10.3
10	5	-7	4.3	4.5
10	5	-8	11.2	3.3
10	5	-9	20.1	26.1
10	5	-10	15.9	14.6
10	5	-11	5.8	2.7
10	5	-12	16.8	17.4
10	5	-13	5.2	4.6
11	5	0	8.5	8.2
11	5	1	34.1	35.7
11	5	2	4.2	3.2
11	5	3	30.4	30.1
11	5	4	29.9	31.0
11	5	5	4.7	2.9
11	5	6	25.7	21.6
11	5	7	13.3	15.0
11	5	-1	30.1	32.9
11	5	-2	40.9	42.9
11	5	-3	6.8	7.9
11	5	-4	32.3	33.1
11	5	-5	25.2	29.2
11	5	-6	25.7	23.8
11	5	-7	33.5	31.5
11	5	-8	4.4	2.2
11	5	-9	26.9	27.2
11	5	-10	4.8	4.2
11	5	-11	19.8	18.0
11	5	-12	36.6	31.8
12	5	0	10.5	12.0
12	5	1	4.2	0.4
12	5	2	4.7	5.7
12	5	3	4.5	0.4
12	5	4	9.3	12.5
12	5	5	4.8	0.5
12	5	6	4.9	1.2
12	5	7	5.0	5.2
12	5	-1	9.5	6.7
12	5	-2	15.7	16.9
12	5	-3	4.1	3.5
12	5	-4	4.1	8.5
12	5	-5	17.2	15.7
12	5	-6	4.2	1.2
12	5	-7	7.6	7.0
12	5	-8	4.5	2.9
12	5	-9	4.7	6.9
12	5	-10	4.8	1.7
12	5	-11	21.1	19.5
12	5	-12	5.2	3.6
13	5	0	7.5	5.3
13	5	1	4.4	2.6
13	5	2	4.6	2.3
13	5	3	4.7	2.7
13	5	4	4.8	6.6
13	5	5	17.8	20.4
13	5	6	10.5	12.0
13	5	-1	9.5	9.6
13	5	-2	8.9	9.7
13	5	-3	8.7	7.7
13	5	-4	4.3	7.1
13	5	-5	4.3	3.9
13	5	-6	14.8	11.0
13	5	-7	16.1	12.2
13	5	-8	18.0	14.8
13	5	-9	4.8	3.4
13	5	-10	5.0	10.9
13	5	-11	5.1	12.0
13	5	-12	6.0	1.3
14	5	0	20.3	21.1
14	5	1	12.5	10.0
14	5	2	25.0	26.0
14	5	3	18.2	18.5
14	5	4	11.4	14.1
14	5	5	4.9	1.5
14	5	-1	8.6	3.2
14	5	-2	11.7	14.4
14	5	-3	26.4	27.2
14	5	-4	33.9	33.8
14	5	-5	11.9	17.1
14	5	-6	29.3	27.9
14	5	-7	5.2	5.4
14	5	-8	4.8	5.6
14	5	-9	17.2	17.9
14	5	-10	23.4	23.4
14	5	-11	6.0	4.1
14	5	-12	22.6	17.6
15	5	0	32.7	36.9
15	5	1	4.8	4.9
15	5	2	28.0	29.5
15	5	3	25.9	29.0
15	5	4	4.5	1.5
15	5	-1	27.2	29.3
15	5	-2	9.7	10.7
15	5	-3	15.1	16.4
15	5	-4	9.9	7.3
15	5	-5	25.9	25.1
15	5	-6	10.4	9.6
15	5	-7	20.1	21.4
15	5	-8	27.1	32.0
15	5	-9	5.0	5.5
15	5	-10	28.9	26.1
15	5	-11	17.8	17.3
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16	5	1	19.2	21.3
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7	7	1	7.4	8.9
7	7	2	33.7	23.4
7	7	3	3.8	3.7
7	7	4	15.1	22.8
7	7	5	13.7	15.9
7	7	6	4.4	3.1
7	7	7	4.7	7.7
7	7	8	4.7	1.9
7	7	-1	18.6	22.1
7	7	-2	6.2	6.0
7	7	-3	24.6	23.8
7	7	-4	3.8	1.1
7	7	-5	38.3	35.5
7	7	-6	34.0	32.9
7	7	-7	4.1	0.7
7	7	-8	28.1	32.3
7	7	-9	18.6	18.7
7	7	-10	12.1	17.9
7	7	-11	26.3	24.0
8	7	0	3.5	5.9
8	7	1	6.3	4.7
8	7	2	5.5	8.3
8	7	3	10.1	11.6
8	7	4	4.3	6.2
8	7	5	16.1	19.1
8	7	6	14.4	15.0
8	7	7	5.6	9.1
8	7	-1	11.9	12.4
8	7	-2	3.7	4.3
8	7	-3	12.8	13.6
8	7	-4	10.0	9.9
8	7	-5	3.8	3.6
8	7	-6	13.9	12.9
8	7	-7	8.1	8.5
8	7	-8	4.5	2.6
8	7	-9	4.6	3.5
8	7	-10	10.2	9.9
8	7	-11	5.2	11.3
9	7	0	11.8	10.9
9	7	1	15.4	21.7
9	7	2	11.9	17.0
9	7	3	4.3	5.9
9	7	4	17.1	13.6
9	7	5	11.7	11.8
9	7	6	5.0	11.5
9	7	7	11.8	13.9
9	7	-1	1.7	4.1
9	7	-2	7.9	7.7
9	7	-3	3.7	0.6
9	7	-4	3.8	1.6
9	7	-5	3.9	3.1
9	7	-6	4.2	4.7
9	7	-7	7.4	2.2
9	7	-8	4.6	4.4
9	7	-9	4.7	0.4
9	7	-10	4.9	5.2
9	7	-11	17.4	11.1
10	7	0	26.8	27.2
11	7	1	4.1	6.6

TABLE 3, Continued

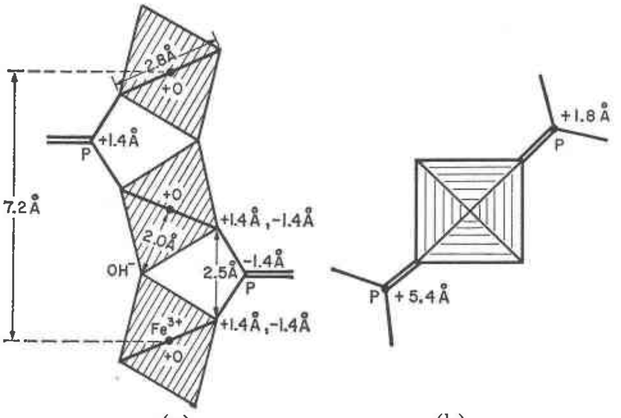
h	k	l	F_{obs}	F_{calc}
10	7	2	16.6	15.7
10	7	3	4.3	3.3
10	7	4	6.6	4.9
10	7	5	4.7	2.5
10	7	6	18.3	19.7
10	7	-1	16.6	16.4
10	7	-2	10.5	10.0
10	7	-3	3.8	4.3
10	7	-4	15.1	14.7
10	7	-5	7.4	8.0
10	7	-6	27.0	26.9
10	7	-7	8.9	15.7
10	7	-8	4.6	3.4
10	7	-9	5.6	0.7
10	7	-10	5.7	3.8
11	7	0	8.0	10.8
11	7	1	23.1	25.4
11	7	2	10.5	12.9
11	7	3	18.8	17.4
11	7	4	13.5	9.9
11	7	5	8.5	10.7
11	7	-1	22.9	24.4
11	7	-2	22.5	22.5
11	7	-3	4.1	2.5
11	7	-4	36.5	37.7
11	7	-5	16.0	15.3
11	7	-6	12.4	9.1
11	7	-7	19.9	20.2
11	7	-8	12.3	11.7
11	7	-9	25.2	24.1
11	7	-10	19.1	16.4
12	7	0	4.4	2.7
12	7	1	4.5	5.9
12	7	2	4.5	5.1
12	7	3	9.2	8.0
12	7	4	4.8	3.2
12	7	-1	10.9	11.6
12	7	-2	10.7	11.2
12	7	-3	15.8	17.6
12	7	-4	4.3	7.4
12	7	-5	14.7	16.7
12	7	-6	11.2	14.5
12	7	-7	4.6	3.7
12	7	-8	4.7	0.4
12	7	-9	20.4	21.1
12	7	-10	5.0	3.5
13	7	0	4.5	2.9
13	7	1	4.6	3.9
13	7	2	9.4	2.0
13	7	3	4.8	4.0
13	7	-1	4.8	11.1
13	7	-2	5.7	5.4
13	7	-3	4.4	3.1
13	7	-4	8.3	1.4
13	7	-5	11.7	8.5
13	7	-6	4.6	4.0
13	7	-7	4.7	0.6
13	7	-8	4.8	5.0
13	7	-9	4.9	1.9
14	7	0	10.8	12.3
14	7	1	9.0	10.2
14	7	2	4.8	11.9
14	7	-1	15.7	23.0
14	7	-2	26.9	25.7
14	7	-3	4.6	4.9
14	7	-4	15.8	16.2
14	7	-5	17.5	16.5
14	7	-6	4.6	0.7
14	7	-7	27.8	23.1
14	7	-8	23.0	25.6
14	7	-9	4.8	4.1
15	7	0	23.7	25.9
15	7	1	11.3	7.1
15	7	-1	11.0	11.0
15	7	-2	16.7	17.1
15	7	-3	25.1	26.8
15	7	-4	8.6	1.5
15	7	-5	17.8	18.1
15	7	-6	4.8	8.1
15	7	-7	18.2	19.0
15	7	-8	24.2	27.8
16	7	0	4.5	0.2
16	7	-1	4.9	2.7
16	7	-2	7.8	1.9
16	7	-3	4.8	3.0
16	7	-4	4.8	7.4
16	7	-5	4.5	7.1
16	7	-6	11.7	14.3
16	7	-7	10.4	8.4
17	7	-3	5.4	5.2
17	7	-4	11.0	12.4
17	7	-5	4.9	1.1
0	8	2	28.0	31.0
0	8	3	9.2	11.8
0	8	4	66.8	65.5
0	8	5	49.4	45.2
0	8	6	47.7	47.5
0	8	7	4.5	8.6
0	8	8	5.8	5.6
0	8	9	10.1	8.4
1	8	1	10.9	16.1
1	8	2	16.1	16.0
1	8	3	27.3	26.3
1	8	4	21.4	22.5
1	8	5	11.5	12.1
1	8	6	10.9	14.1
1	8	7	15.3	12.3
1	8	8	21.6	20.9
1	8	9	20.0	19.7
1	8	-2	22.8	23.2
1	8	-3	17.5	16.7
1	8	-4	7.6	4.7
1	8	-5	14.4	11.5
1	8	-6	24.9	21.4
1	8	-7	38.7	35.8
1	8	-8	20.0	21.1
1	8	-9	6.0	6.9
2	8	0	15.7	20.0
2	8	1	18.5	20.3
2	8	2	18.3	19.1
2	8	3	12.7	13.4
2	8	4	18.8	17.5
2	8	5	10.8	10.2
2	8	6	15.9	14.5
2	8	7	4.4	3.6
2	8	8	13.8	4.3
2	8	9	6.1	8.1
2	8	-1	9.0	12.7
2	8	-2	17.1	16.5
2	8	-3	27.1	27.9
2	8	-4	15.9	11.9
2	8	-5	8.1	6.7
2	8	-6	4.1	8.2
2	8	-7	3.7	8.0
2	8	-8	20.7	18.7
2	8	-9	26.7	24.5
3	8	0	20.5	24.3
3	8	1	9.6	6.4
3	8	2	27.4	27.0
3	8	3	23.6	21.7
3	8	4	24.1	23.8
3	8	5	11.3	10.0
3	8	6	5.1	10.4
3	8	7	13.6	9.3
3	8	8	31.1	24.6
3	8	-1	17.2	21.5
3	8	-2	26.7	32.0
3	8	-3	23.7	21.3
3	8	-4	13.3	12.0
3	8	-5	11.9	5.7
3	8	-6	22.6	22.9
3	8	-7	19.0	18.8
3	8	-8	9.0	20.5
3	8	-9	5.4	10.0
3	8	-10	7.3	6.8
4	8	0	41.7	42.8
4	8	1	50.6	55.0
4	8	2	61.5	63.3
4	8	3	3.6	2.3
4	8	4	6.8	9.1
4	8	5	9.3	1.7
4	8	6	44.2	43.8
4	8	7	36.0	37.7
4	8	8	36.3	32.4
4	8	-1	17.0	13.4
4	8	-2	35.8	36.1
4	8	-3	46.8	47.6
4	8	-4	61.5	59.9
4	8	-5	3.8	2.4
4	8	-6	4.0	2.1
4	8	-7	4.4	2.1
4	8	-8	43.0	40.6
4	8	-9	34.8	32.0
5	8	0	31.1	30.6
5	8	1	3.3	3.6
5	8	2	6.7	1.4
5	8	3	17.8	9.6
5	8	4	31.4	30.8
5	8	5	32.8	31.9
5	8	6	27.3	22.2
5	8	7	4.7	4.7
5	8	-1	35.2	35.2
5	8	-2	34.3	37.7
5	8	-3	13.6	12.3
5	8	-4	12.0	12.6
5	8	-5	11.7	7.5
5	8	-6	28.6	24.6
5	8	-7	14.7	17.9
5	8	-8	8.1	13.3
5	8	-9	11.2	13.4
5	8	-10	10.5	11.7
6	8	0	13.3	7.4
6	8	1	11.0	3.6
6	8	2	8.5	7.2
6	8	3	11.0	12.5
6	8	4	9.3	4.4
6	8	5	8.7	9.1
6	8	6	7.8	7.0
6	8	7	21.2	15.4
6	8	-1	33.4	29.3
6	8	-2	45.7	43.5
6	8	-3	26.9	25.9
6	8	-4	9.6	5.2
6	8	-5	3.8	2.4
6	8	-6	13.7	9.5
6	8	-7	16.3	14.1
6	8	-8	11.3	11.5
6	8	-9	4.8	4.3
6	8	-10	5.5	2.5
7	8	0	28.8	28.0
7	8	1	13.6	16.8
7	8	2	9.2	7.4
7	8	3	19.2	17.9
7	8	4	13.5	15.8
7	8	5	25.5	23.7
7	8	6	18.3	16.0
7	8	-1	25.3	24.3
7	8	-2	18.0	16.4
7	8	-3	14.6	14.2
7	8	-4	7.5	13.1
7	8	-5	23.2	23.1
7	8	-6	19.0	21.0
7	8	-7	13.8	12.4
7	8	-8	12.7	14.2
7	8	-9	13.1	13.8
7	8	-10	16.4	17.6
8	8	0	29.7	26.6
8	8	1	9.6	15.6
8	8	2	45.5	44.7
8	8	3	34.4	31.7
8	8	4	49.3	43.0
8	8	5	4.5	4.9
8	8	6	17.0	17.0
8	8	-1	25.4	23.5
8	8	-2	65.5	70.7
8	8	-3	23.7	22.4
8	8	-4	22.3	19.9
8	8	-5	11.1	12.7
8	8	-6	50.6	46.9
8	8	-7	42.4	37.1
8	8	-8	45.5	43.5
8	8	-9	4.9	2.0
9	8	0	29.8	29.4
9	8	1	25.1	23.6
9	8	2	16.2	17.6
9	8	3	4.3	4.2
9	8	4	4.2	7.3
9	8	5	14.4	14.0
9	8	-1	16.8	16.5
9	8	-2	3.0	8.7
9	8	-3	11.5	12.6
9	8	-4	13.7	14.8
9	8	-5	23.8	23.2
9	8	-6	24.6	24.3
9	8	-7	11.9	5.9
9	8	-8	11.1	10.6
9	8	-9	17.9	14.4
10	8	0	26.9	22.2
10	8	1	20.2	17.4
10	8	2	15.7	12.0
10	8	3	3.2	5.6
10	8	4	14.5	14.1
10	8	-1	17.4	13.7
10	8	-2	7.8	7.3
10	8	-3	4.1	5.1
10	8	-4	17.4	14.3
10	8	-5	36.6	33.7
10	8	-6	25.5	21.0
10	8	-7	8.3	1.8
10	8	-8	4.7	17.9
10	8	-9	4.9	1.6
11	8	0	16.4	12.9
11	8	1	15.7	13.1
11	8	2	20.7	19.4
11	8	3	14.3	15.3
11	8	4	14.6	13.5
11	8	-1	4.3	3.7
11	8	-2	15.2	17.4
11	8	-3	24.4	23.3
11	8	-4	31.9	31.4
11	8	-5	22.3	20.3
11	8	-6	4.6	4.8
11	8	-7	4.6	1.9
11	8	-8	14.5	14.6
11	8	-9	16.1	17.3
12	8	0	47.5	46.4
12	8	1	4.5	2.0
12	8	2	4.6	4.4
12	8	3	5.2	2.1
12	8	-1	37.6	36.9
12	8	-2	36.4	34.0
12	8	-3	12.3	5.1
12	8	-4	27.2	22.2
12	8	-5	78.8	75.3
12	8	-6	44.5	42.1
12	8	-7	11.2	5.2
12	8	-8	13.6	11.3
13	8	0	13.7	12.9
13	8	1	12.9	16.0
13	8	2	14.9	15.5
13	8	-1	4.6	5.5
13	8	-2	13.5	15.9
13	8	-3	18.5	17.7
13	8	-4	13.3	15.0
13	8	-5	17.3	15.9
13	8	-6	8.9	10.5
13	8	-7	8.2	5.6
13	8	-8	14.5	18.9
14	8	0	4.8	1.0
14	8	-1	4.7	4.5
14	8	-2	4.7	0.9
14	8	-3	21.8	22.5
14	8	-4	36.4	32.7
14	8	-5	21.2	17.1
14	8	-6	4.8	2.0
14	8	-7	6.1	1.4
15	8	-2	25.1	25.4
15	8	-3	18.4	16.0
15	8	-4	8.6	7.4
15	8	-5	6.0	0.9
0	9	2	5.0	7.9
0	9	3	7.9	10.4
0	9	4	1.6	6.1
0	9	5	10.4	8.8
0	9	6	4.7	17.0
0	9	7	5.0	1.5
1	9	1	4.2	12.8
1	9	2	5.5	4.4
1	9	3	25.0	27.0
1	9	4	12.6	14.3
1	9	5	10.4	14.0
1	9	6	28.0	30.9
1	9	7	14.5	22.3
1	9	-2	5.1	6.4
1	9	-3	12.8	12.5
1	9	-4	15.0	18.6
1	9	-5	3.0	1.1
1	9	-6	9.4	10.2
1	9	-7	4.5	1.6
2	9	0	15.2	21.4
2	9	1	6.7	9.5
2	9	2	2.8	1.2
2	9	3	3.3	5.6
2	9	4	3.6	4.7
2	9	5	5.7	9.1
2	9	6	24.4	26.8
2	9	7	4.6	6.3
2	9	-1	10.1	20.2
2	9	-2	12.1	14.6
2	9	-3	7.1	6.7
2	9	-4	9.2	12.1
2	9	-5	3.8	4.9
2	9	-6	4.1	8.7
2	9	-7	23.7	24.1
2	9	-8	8.8	5.4
3	9	0	29.1	29.4
3	9	1	13.4	12.1
3	9	2	6.8	0.8
3	9	3	19.8	20.3
3	9	4	3.7	3.1
3	9	5	15.6	15.9
3	9	6	15.3	17.4
3	9	-1	2.4	3.5
3	9	-2	15.0	16.9
3	9	-3	13.0	12.7
3	9	-4	18.5	19.4
3	9	-5	10.9	12.8
3	9	-6	4.1	1.7
3	9	-7	14.8	17.3
3	9	-8	7.9	3.6
4	9	0	5.2	3.0
4	9	1	12.2	11.9
4	9	2	14.5	16.5
4	9	3	3.6	0.3
4	9	4	11.3	10.4
4	9	5	4.1	6.2
4	9	6	4.3	1.1
4	9	-1	2.8	0.4
4	9	-2	8.2	8.6
4	9	-3	7.1	10.9
4	9	-4	12.4	11.3
4	9	-5	3.8	7.1
4	9	-6	4.1	6.2
4	9	-7	4.4	7.0
4	9	-8	4.6	2.4
5	9	0	3.1	4.1
5	9	1	7.3	6.7
5	9	2	6.9	10.9
5	9	3	7.3	9.8
5	9	4	4.0	0.6
5	9	5	10.1	7.7
5	9	-1	8.4	10.5
5	9	-2	13.9	15.6
5	9	-3	3.3	5.0
5	9	-4	3.6	4.0
5	9	-5	7.1	10.2
5	9	-6	8.6	9.2
5	9	-7	14.2	15.7
5	9	-8	5.5	10.1
6	9	0	8.2	10.3
6	9	1	3.5	4.4
6	9	2	11.4	15.1
6	9	3	3.9	0.6
6	9	4	14.1	17.5
6	9	5	19.3	21.3
6	9	-1	22.6	24.1
6	9	-2	24.5	24.7
6	9	-3	10.5	2.8
6	9	-4	12.3	12.6
6	9	-5	8.3	9.9
6	9	-6	4.1	1.0
6	9	-7	13.1	11.0
6	9	-8	25.7	25.1
7	9	0	17.6	18.2
7	9	1	6.6	8.9
7	9	2	24.2	25.6
7	9	3	15.1	17.0
7	9	4	4.3	8.5
7	9	-1	20.2	18.2
7	9	-2	3.6	6.9
7	9	-3	33.6	35.4
7	9	-4	12.8	14.5
7	9	-5	20.8	18.4
7	9	-6	25.3	26.2
7	9	-7	9.0	2.3
7	9	-8	19.6	21.5
8	9	0	3.9	9.9
8	9	1	10.8	7.6
8	9	2	8.1	4.0
8	9	3	15.3	16.5
8	9	4	4.5	5.0
8	9	-1	6.4	5.0
8	9	-2	6.1	5.7
8	9	-3	15.8	12.3
8	9	-4	3.9	0.6
8	9	-5	4.1	1.8
8	9	-6	4.3	6.3
8	9	-7	4.5	1.5
9	9	0	4.0	2.6
9	9	1	17.9	17.4
9	9	2	9.8	9.5
9	9	3	4.4	5.5
9	9	-1	3.9	3.0
9	9	-2	7.9	3.8
9	9	-3	7.9	2.3
9	9	-4	9.5	8.4
9	9	-5	10.7	11.2
9	9	-6	19.0	13.8
9	9	-7	4.5	0.6
10	9	0	4.2	4.9
10	9	1	4.3	4.0
10	9	2	4.4	0.0
10	9	-1	8.1	2.3
10	9	-2	15.8	16.8
10	9	-3	4.1	6.9
10	9	-4	9.2	10.1
10	9	-5	7.4	1.9
10	9	-6	4.4	6.9
11	9	0	4.4	2.4
11	9	1	16.9	16.5
11	9	-1	14.4	18.3
11	9	-2	28.0	30.3
11	9	-3	4.3	1.5
11	9	-4	20.8	20.0
11	9	-5	18.7	17.2
11	9	-6	13.2	13.6
12	9	-1	4.5	6.0
12	9	-2	11.3	9.5
12	9	-3	8.0	4.6
12	9	-4	10.7	9.3
0	10	2	34.0	40.6
0	10	3	24.4	24.9
0	10	4	18.6	19.1
0	10	5	3.9	8.5
1	10	1	13.5	20.8
1	10	2	13.3	16.4
1	10	3	8.1	7.0
1	10	4	10.9	12.7
1	10	5	19.1	19.6
1	10	-2	5.4	2.6
1	10	-3	9.7	12.3
1	10	-4	18.5	20.2
1	10	-5	35.4	35.6
2	10	0	7.6	10.0
2	10	1	6.5	9.9
2	10	2	15.6	16.2
2	10	3	16.2	15.5
2	10	4	21.5	13.9
2	10	-1	10.5	15.2
2	10	-2	11.7	9.2
2	10	-3	8.1	5.8
2	10	-4	7.8	8.0
2	10	-5	23.7	21.7
3	10	0	17.3	23.4
3	10	1	21.4	24.8
3	10	2	22.4	21.8
3	10	3	3.4	2.6
3	10	4	14.4	7.4
3	10	-1	4.9	6.4
3	10	-2	10.2	11.4
3	10	-3	14.3	12.9
3	10	-4	29.7	31.5
3	10	-5	15.9	18.3
4	10	0	26.6	29.8
4	10	1	3.0	4.3
4	10	2	3.3	3.9
4	10	3	21.4	18.2
4	10	-1	21.5	26.3
4	10	-2	29.0	32.7
4	10	-3	3.1	4.1
4	10	-4	3.5	1.5
4	10	-5	21.9	17.7
5	10	0	11.7	11.0
5	10	1	12.6	11.2
5	10	2	21.8	22.0
5	10	3	15.5	15.8
5	10	-1	11.3	7.9
5	10	-2	21.4	21.1
5	10	-3	20.4	21.3
5	10	-4	21.4	21.8
5	10	-5	4.0	6.6
6	10	0	19.8	17.6
6	10	1	24.4	22.0
6	10	2	16.8	11.7
6	10	-1	10.4	5.2
6	10	-2	7.9	5.8
6	10	-3	6.3	6.0
6	10	-4	27.7	23.0
6	10	-5	26.9	22.3
7	10	0	10.1	1.0
7	10	1	18.9	17.7
7	10	-1	9.0	6.8
7	10	-2	12.7	9.8
7	10	-3	21.1	19.7
7	10	-4	18.4	18.8
8	10	0	16.1	13.2
8	10	-1	3.4	11.0
8	10	-2	7.1	3.4
8	10	-3	8.8	10.3

tetrahedra and two edges above and below with the complementary polyhedron. In jahnsite and segelerite, the idealized slab has approximate plane cell dimensions 15.0 Å × 7.2 Å. The slab has formal composition $[Me^{2+}Me^{3+}(OH)[PO_4]_2]^{2-}$, where $2Me^{2+} = Ca^{2+} + Mn^{2+}$ in jahnsite and $2Ca^{2+}$ in segelerite, and $Me^{3+} = Fe^{3+}$ in both compounds.

In jahnsite, identical slabs are bridged by $Mg^{2+}(H_2O)_4(O_P)_2$ octahedra, where O_P are the corners of PO_4 tetrahedra which point away from the slabs. The actual structural distortion of jahnsite, as shown in a polyhedral diagram in Figure 3, is a result of Ca^{2+}-Mn^{2+} ordering along the edge-sharing chains and the perturbations resulting from the hydrogen bonding scheme about the Mg^{2+}-O bridging octahedra, to be discussed later.

Twinning of Jahnsite

Twinning by reflection on {001} is the rule rather than the exception for jahnsite. Without burdening the literature further, it will only be stated that several compositions are now recognized for the jahnsite structure type. Define $c' = 2c + a/2$



(a) (b)

FIG. 1. The $\cdots Fe^{3+}$-OH-$Fe^{3+}\cdots$ octahedral corner-linked chain which is called the backbone in this study. (a) Parallel to the chain (idealized). (b) Down the chain (idealized).

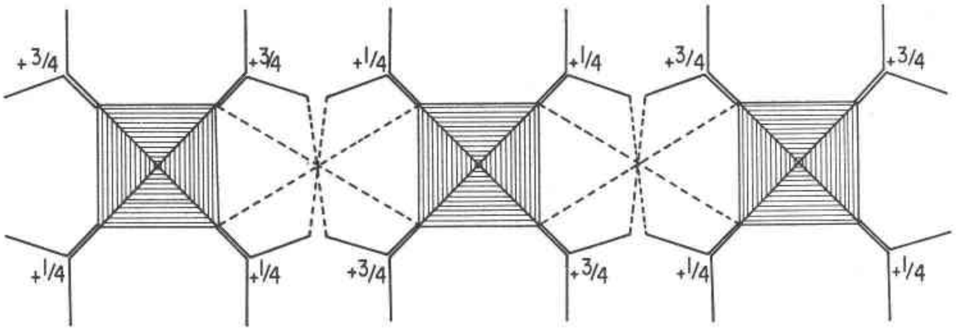

+3/4
+3/4
+1/4
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FIG. 2. Idealization of the slab with composition $[Me^{2+}_2Me^{3+}_2(OH)_2[PO_4]_4]^{4-}$ found in the crystal structure of jahnsite.

and $\cos \beta' = (a^2/4 + c'^2 - 4c^2)/ac'$. This provides a pseudo-orthogonal cell with dimensions a, b, c', $\beta' \sim 90°$. It is observed that as β' approaches 90° for certain compositions, the frequency of twinning increases. These pseudo-orthogonal coordinates are a 14.94 Å, c' 18.65 Å, and β' 88°06′ for the jahnsite used in this study.

A projection of the metals down [010] in Figure 4 shows why jahnsite twins. We observe a profound substructure, with subcell $a(\text{sub}) = a/4$ and $c(\text{sub}) = c'/2$ on the projection. Thus, *h0l* photographs of jahnsite can be easily mistaken as possessing an "orthogonal" cell. We observe, however, that when the heights in y are included (Fig. 4), the three-dimensional pseudo-orthogonality ceases to exist. We also note that a, b, and c' approximate segelerite in dimension, which has a 14.83 Å, b 18.75 Å, c 7.31 Å, *Pcca*. A preliminary structure analysis of segelerite shows that it *cannot* be continuously transformed into the jahnsite structure by mere distortions of the polyhedra. For this reason, jahnsite and segelerite represent two separate (but related) structure types, separated by the barrier of the relative locations of the [PO$_4$] tetrahedra.

Bond Distances

Table 4 provides a list of the individual polyhedral bond distances for jahnsite. The most extreme distortions are found for the CaO$_6$ and MnO$_6$ octahedra since they share edges with [PO$_4$] tetrahedra and with each other. We note that the short O(5)-O(7) distance, 2.442 Å, is the edge shared between

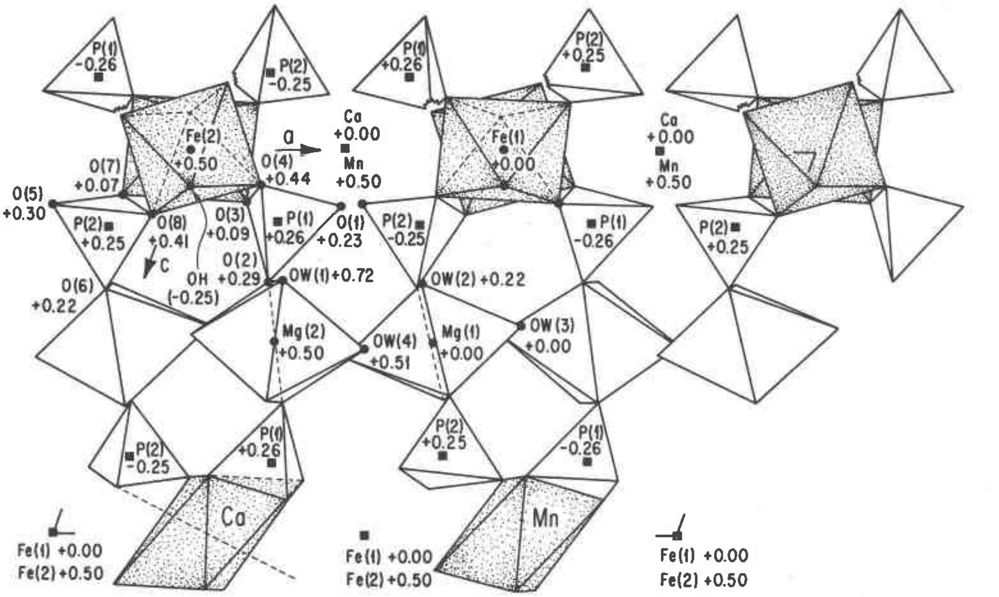
P(1) -0.26
P(2) -0.25
P(1) +0.26
P(2) +0.25
Fe(2) +0.50
a
Ca +0.00
Mn +0.50
Fe(1) +0.00
Ca +0.00
Mn +0.50
O(7) +0.07
O(4) +0.44
O(5) +0.30
P(2) +0.25
O(8) +0.41
O(3) +0.09
P(1) +0.26
O(1) +0.23
P(2) -0.25
P(1) -0.26
P(2) +0.25
c
O(2) OH +0.29
OH (-0.25)
OW(1) +0.72
OW(2) +0.22
O(6) +0.22
Mg(2) +0.50
OW(4) +0.51
Mg(1) +0.00
OW(3) +0.00
P(2) -0.25
P(1) +0.26
P(2) +0.25
P(1) -0.26
Ca
Mn
Fe(1) +0.00
Fe(2) +0.50
Fe(1) +0.00
Fe(2) +0.50
Fe(1) +0.00
Fe(2) +0.50

FIG. 3. Polyhedral diagram of the actual jahnsite structure. Some atoms have been left out to improve visualization. Heights are fractional coordinates in y.

CaO_6 and $P(2)O_4$. It is also the shortest edge distance for that tetrahedron. Likewise, O(1)-O(4), which equals 2.422 Å, is the edge shared between MnO_6 and $P(1)O_4$ and is that tetrahedron's shortest edge as well. Finally, O(5)-O(5)″ 2.822 Å and O(1)-O(1)″ 2.830 Å are edges shared between CaO_6 and MnO_6 polyhedra and are next in rank of shortness for their polyhedra. All of these distortions are consistent with the repulsion of cations across shared edges. In addition, the CaO_6 octahedron is more distorted and considerably larger than the MnO_6 octahedron, providing evidence that these cations are ordered.

The remaining polyhedra do not share topological elements other than corners and, consequently, their range of distortion is less. The polyhedral averages in the abstract and in Table 4 are all consistent with grand averages found for these cations in such oxygen coordination. The $Mg(O,H_2O)_6$ octahedra are substantially distorted. Since no elements other than corners are shared, these distortions result from deviations from local electrostatic neutrality and from hydrogen-bond formation.

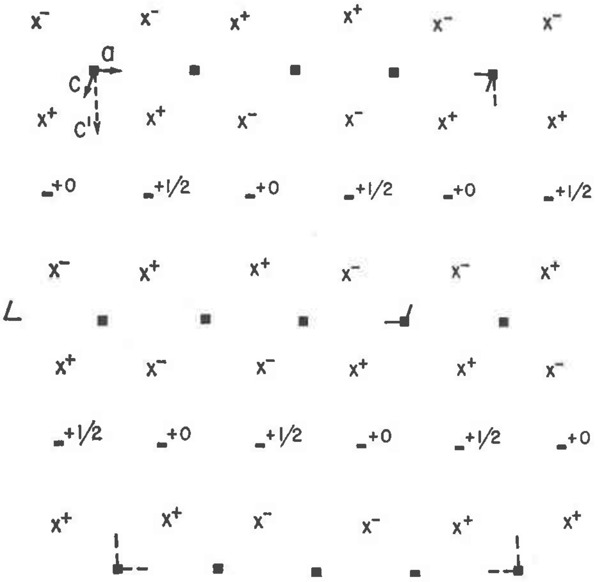

FIG. 4. Pseudo-orthogonal cell *a* × *c′* found in jahnsite. The structure cell used in this study is also outlined. Interpretation of symbols: solid squares = Me^{2+} and Me^{3+} at y = 0, 1/2; crosses are P atoms, and solid bars are Mg atoms.

TABLE 4. Jahnsite. Polyhedral Interatomic Distances†

Fe(1)		Ca		Mg(1)		P(1)	
2 Fe(1)-O(7)	1.966 Å	2 Ca -O(1)	2.331 Å	2 Mg(1) -O(6)^{ii}	2.047 Å	1 P(1)-O(2)	1.510 Å
2 " -O(3)	1.973	2 " -O(5)	2.427	2 " -OW(2)	2.108	1 " -O(3)	1.539
2 " -OH	1.981	2 " -O(7)	2.497	2 " -OW(3)	2.108	1 " -O(1)	1.562
average	1.973	average	2.418	average	2.088	1 " -O(4)	1.562
						average	1.543
2 O(3) -O(7)	2.671	2 O(5)-O(7)	2.442**	2 OW(2)^{i}-O(6)^{ii}	2.774	1 O(1)-O(4)	2.422**
2 O(3) -OH	2.733	1 O(5)-O(5)^{ii}	2.822*	2 OW(3)^{i}-O(6)^{ii}	2.924	1 O(1)-O(3)	2.494
2 O(7) -OH	2.787	1 O(1)-O(1)^{ii}	2.830*	2 OW(3) -O(6)^{ii}	2.953	1 O(2)-O(3)	2.503
2 OH -O(7)^{i}	2.794	2 O(1)-O(7)^{ii}	3.207	2 OW(2) -OW(3)^{i}	2.970	1 O(1)-O(2)	2.552
2 OH -O(3)^{i}	2.856	2 O(1)-O(5)^{ii}	3.865	2 OW(2) -OW(3)	2.992	1 O(2)-O(4)	2.556
2 O(3) -O(7)^{i}	2.894	2 O(1)-O(7)	3.933	2 OW(2) -O(6)^{ii}	3.093	1 O(3)-O(4)	2.577
average	2.789	2 O(5)-O(7)^{ii}	3.964	average	2.951	average	2.517
		average	3.373				

Fe(2)		Mn		Mg(2)		P(2)	
2 Fe(2)-O(8)	1.938	2 Mn -O(5)	2.116	2 Mg(2) -O(2)	2.033	1 P(2)-O(6)	1.508
2 " -O(4)	1.988	2 " -O(4)	2.215	2 " -OW(4)	2.083	1 " -O(8)	1.523
2 " -OH	1.993	2 " -O(1)	2.238	2 " -OW(1)	2.152	1 " -O(7)	1.548
average	1.973	average	2.190	average	2.089	1 " -O(5)	1.551
						average	1.533
2 OH -O(8)^{i}	2.712	2 O(1)-O(4)	2.422**	2 O(2) -OW(4)^{ii}	2.801	1 O(5)-O(7)	2.442**
2 O(4) -O(8)^{i}	2.760	1 O(5)-O(5)^{ii}	2.822*	1 O(2) -O(2)^{ii}	2.884	1 O(6)-O(8)	2.490
2 O(4) -O(8)	2.791	1 O(1)-O(1)^{ii}	2.830*	2 OW(1) -OW(4)	2.892	1 O(5)-O(6)	2.495
2 OH -O(4)	2.799	2 O(4)-O(5)^{ii}	3.105	1 OW(1) -OW(1)^{ii}	2.910	1 O(5)-O(8)	2.512
2 OH -O(4)^{i}	2.830	2 O(4)-O(5)	3.321	2 OW(1) -OW(4)^{ii}	2.970	1 O(6)-O(7)	2.526
2 OH -O(8)	2.844	2 O(1)-O(5)^{ii}	3.356	2 OW(1) -O(2)	3.032	1 O(7)-O(8)	2.544
average	2.789	2 O(1)-O(4)^{ii}	3.446	2 O(2) -OW(4)	3.128	average	2.502
		average	3.079	average	2.953		

†Estimated standard errors: Me-O ± 0.006 Å, O-O′ ± 0.009 Å.

*Ca-Mn shared edges, **Me^{2+}-P shared edges.

^{i}= -x, -y, -z; ^{ii}= 1/2-x, y, -z; ^{iii}= 1/2+x, -y, z applied to the coordinates in Table 2.

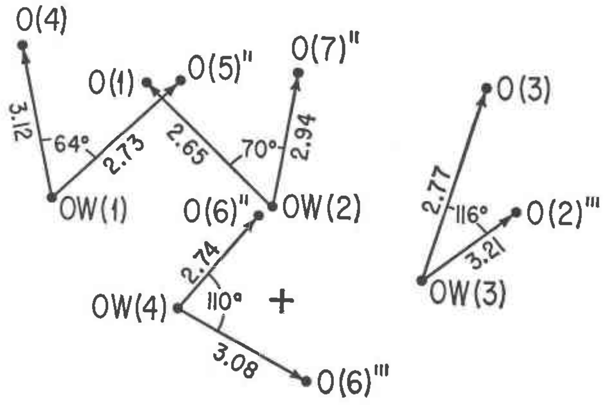

FIG. 5. Proposed hydrogen bonding scheme in one asymmetric unit for jahnsite down [010]. The cross is at $x = 1/2$, $z = 1/2$.

Hydrogen Bonds and Electrostatic Valence Balances

It was not possible to ascertain locations of the hydrogen atoms directly, but the geometrical restrictions are severe enough to warrant proposal of a hydrogen-bond model. The structure consists of the dense slabs $[CaMnFe^{3+}_2(OH)_2[PO_4]_4]^{4-}$ oriented parallel to {001} and weakly linked by the $Mg(O,H_2O)_6$ octahedra. Hydrogen bonds from OW(1), OW(2), OW(3), and OW(4) connect to the O_P oxygens in these slabs resulting in a herringbone pattern for these bonds. Distances and angles for the proposed model are featured as an asymmetric unit in Figure 5. They can be divided into short bonds OW(1) . . . O(5)″ 2.73 Å, OW(2) . . . O(1) 2.65, OW(3) . . . O(3) 2.77 Å, and OW(4) . . . O(6)″ 2.74; and long, more weakly linked bonds OW(1) . . . O(4) 3.12 Å, OW(2) . . . O(7)″ 2.94, OW(3) . . . O(2)‴ 3.21 and OW(4) . . . O(6)‴ 3.08 Å. Owing to its geometrical separation, $(OH)^-$ does not appear to form a strong bond since the only distances less than 3.0 Å are along polyhedral edges.

TABLE 5. Jahnsite. Electrostatic Valence Balances of Cations about Anions†

Anions	Coordinating cations	Bond strengths	ΔΣ
O(1)	P(1)+Mn+Ca+H(short)	5/4+2/6+2/6+1/6	+0.08
O(2)	P(1)+Mg(2)+H(short)	5/4+2/6+1/6	-0.17
O(3)	P(1)+Fe(1)+H(short)	5/4+3/6+1/6	-0.08
O(4)	P(1)+Fe(2)+Mn+H(long)	5/4+3/6+2/6+1/6	+0.23
O(5)	P(2)+Mn+Ca+H(short)	5/4+2/6+2/6+1/6	+0.08
O(6)	P(2)+Mg(1)+H(short)+H(long)	5/4+2/6+1/6+1/6	-0.08
O(7)	P(2)+Fe(1)+Ca+H(average)	5/4+3/6+2/6+1/6	+0.23
O(8)	P(2)+Fe(2)	5/4+3/6	-0.25
OH	Fe(1)+Fe(2)	3/6+3/6	0.00
OW(1)	Mg(2)-2H	2/6-2/6	0.00
OW(2)	Mg(1)-2H	2/6-2/6	0.00
OW(3)	Mg(1)-2H	2/6-2/6	0.00
OW(4)	Mg(2)-2H	2/6-2/6	0.00

†H(short) are bonds less than 2.8 Å, H(long) are bonds longer than 2.9 Å ΔΣ is the deviation from neutrality (Σ = 2.00 for O^{2-}; 1.00 for OH^- and 0.00 for H_2O).

From this model, a tabulation of electrostatic balances of cations about anions is offered (Table 5). Hydrogen bond receptors are given $\xi = +1/6$, as suggested by Baur (1970). The resulting undersaturated anions, O(2) and O(8), reveal polyhedral distances shorter than average, and the oversaturated anions O(4) and O(7) show a tendency toward longer-than-average polyhedral bond distances. The remaining anions are sufficiently close to neutrality to show no such correlation with their polyhedral distances.

Properties of the 7 Å Chain Structures

The resulting structures possess key features of benefit to the crystal chemist who is concerned with physical properties as well: the distance between slabs usually corresponds to the strongest low-angle intensities on powder and single crystal photographs and is, in addition, the plane of perfect cleavage. These relationships are also preserved in the "5 Å fiber axis" structures of basic ferrous-ferric phosphates, as noted by Moore (1970b) in a general review of the problem, although in these structures, the slabs are based on a different structural principle. A perplexing result for the mineralogist is an uncanny physical similarity among compounds within each structural group: the 7 Å structures involving Fe^{3+}-O octahedral chains are yellow to orange in color, and the 5 Å structures involving Fe^{3+}-Fe^{2+}-Fe^{3+} face-sharing trimers are all deep greenish-black and fibrous. We have found by experience that the most faithful means of distinguishing species within a group by visual means only is careful examination of their crystal morphology. To illustrate how frequent these structural principles are manifest in natural compounds, we note that among the phosphates laueite, gordonite, paravauxite, metavauxite, wavellite, pseudolaueite, childrenite, eosphorite, tavorite, strunzite, amblygonite, stewartite, jahnsite, overite, and segelerite are known to belong to the 7 Å chain structures; and dufrenite, rockbridgeite, laubmannite, "mineral A," beraunite, lipscombite, barbosalite, and souzalite are known to belong to the 5 Å fiber structures. This accounts for over 40 percent of the known basic Me^{3+} phosphate species! Since some of these species form under narrow conditions of T, pO_2 and pH and since practically no synthetic work has been done on these systems, the list of as yet unknown compounds belonging to this group is probably much larger.

Acknowledgments

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References

BAUR, W. H. (1969) A comparison of the crystal structures of pseudolaueite and laueite. *Am. Mineral.* **54,** 1312–1323.

——— (1970) Bond length variation and distorted coordination polyhedra in inorganic crystals. *Trans. Am. Crystallogr. Assoc.* **6,** 129–155.

BUSING, W. R., K. O. MARTIN, AND H. A. LEVY (1962) ORFLS, a Fortran crystallographic least-squares program. *U.S. Oak Ridge Nat. Lab.* ORNL-TM-**305.**

CROMER, D. T., AND J. B. MANN (1968). X-ray scattering factors computed from numerical Hartree-Fock wavefunctions. *Acta Crystallogr.* **A24,** 321–324.

JOHANSSON, G. (1962) On the crystal structures of $FeOHSO_4$ and $InOHSO_4$. *Acta Chem. Scand.* **16,** 1234–1244.

MOORE, P. B. (1970a). Structural hierarchies among minerals containing octahedrally coordinating oxygen: I. Stereoisomerism among corner-sharing octahedral and tetrahedral chains. *Neues Jahrb. Mineral. Monatsh.* **1970,** 163–173.

——— (1970b) Crystal chemistry of the basic iron phosphates. *Am. Mineral.* **55,** 135–170.

——— (1974) I. Jahnsite, segelerite, and robertsite, three new transition metal phosphate species. *Am. Mineral.* **59,** 48–59.

RAMACHANDRAN, G. N., AND R. SRINIVASAN (1970) *Fourier Methods in Crystallography.* Wiley-Interscience, New York, p. 96–119.

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