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Crystal structure and hydrogen bonding of copiapite

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Auszug

Copiapit, $MgFe_4[(OH)_2|(SO_4)_6] \cdot 20H_2O$, ist triklin, Raumgruppe $P\bar{1}$, mit $a = 7{,}342$ Å, $b = 18{,}818$ Å, $c = 7{,}389$ Å, $\alpha = 91{,}45°$, $\beta = 102{,}15°$ und $\gamma = 98{,}85°$. In der Struktur sind $Fe(O,OH,H_2O)_6$-Koordinationsoktaeder und Sulfattetraeder zu eindimensional-unendlichen Komplexen parallel [101] verknüpft. $Mg(H_2O)_6$-Oktaeder und nicht an Kationen gebundene Wassermoleküle liegen zwischen den Komplexen. Die einzelnen Struktureinheiten sind nur über Wasserstoffbrücken miteinander verknüpft.

Abstract

The structure of copiapite, $MgFe_4[(OH)_2|(SO_4)_6] \cdot 20H_2O$, is triclinic, space group $P\bar{1}$, with $a = 7.342$ Å, $b = 18.818$ Å, $c = 7.389$ Å, $\alpha = 91.45°$, $\beta = 102.15°$, and $\gamma = 98.85°$. $Fe(O,OH,H_2O)_6$ octahedra and sulfate tetrahedra are connected to form one-dimensional infinite complexes along [101]. $Mg(H_2O)_6$ octahedra and water molecules not bound to cations lie between the complexes. These structural groups are interconnected only by hydrogen bonds.

Introduction

Copiapite, a greenish-yellow secondary mineral found in the oxidation zone of sulfidic iron-ore deposits, is the commonest of the natural ferric sulfates. It was first described by Rose (1833). Considered to be monoclinic by Linck (1889), it was later found to be triclinic by Palache *et al.* (1946). The general chemical formula (Berry, 1947) is $AB_4[(OH)_2|(SO_4)_6] \cdot 20H_2O$, where A is usually Fe^{2+}, Mg, Cu, Zn and B is Fe^{3+}, Al.

Experimental

The crystals used for this investigation are from Alcaparrosa, Chile. The cation chemistry was assumed to be $A = Mg$ and $B = Fe^{3+}$, which was later confirmed during the structure refinement.

Single-crystal x-ray photographs showed triclinic symmetry. The lattice constants were measured on NaCl-calibrated photographs and refined by the method of least squares. They are in good agreement with those determined earlier on crystals from other localities, as shown in Table 1.

The unit cell has a volume of 984.4 Å^3 and contains $1\times[MgFe_4(OH)_2(SO_4)_6\cdot 20H_2O]$. The calculated density is 2.05 g · cm^{-3}; the measured density is 2.04 g · cm^{-3}.

Table 1. *Cell constants of copiapites*

Cell dimensions	Chuquicamata, Chile, PALACHE *et al.* (1946)	Alaska, JOLLY and FOSTER (1967)	Alcaparrosa, Chile, this work
a	7.34 Å	7.251 Å	7.342 ± .007 Å
b	18.19	18.161	18.818 ± .010
c	7.28	7.267	7.389 ± .004
α	93° 51′	93° 59′ 35″	91.45 ± .04°
β	101° 30′	102° 17′ 16″	102.15 ± .11°
γ	99° 23′	97° 57′ 46″	98.85 ± .09°

Intensities were measured with an automated two-circle diffractometer on a square tabular crystal of dimensions 0.3 × 0.3 × 0.07 mm, rotated about the a axis. The reflected Zr-filtered Mo$K\alpha$ radiation was detected by a scintillation counter. Within the hemisphere out to $(\sin\theta)/\lambda = 0.55$ Å^{-1}, 2902 reflections were measured, of which 184 had intensities below the detectable limit and were assigned intensities of one-third the value of the weakest measurable reflection. The intensities were corrected for Lorentz, polarization, and absorption effects.

Structure determination and refinement

A three-dimensional Patterson synthesis was used to determine approximate positions of the two iron and three sulfur atoms. Through a subsequent structure-factor calculation yielding an R value of 46%, correct signs could be found for about two-thirds of the observed F's. They were used to compute a three-dimensional Fourier synthesis, which revealed the positions of all atoms except hydrogen. In the subsequent structure-factor calculation the R value dropped to 20%. A full-matrix, least-squares refinement with isotropic temperature

Table 2. *Atom parameters of copiapite*

Atom	x	y	z
Mg	0	0	0
Fe(1)	0.6861 (2)	0.3326 (1)	0.4944 (2)
Fe(2)	.6833 (2)	.6800 (1)	.8980 (2)
S(1)	.9461 (4)	.7338 (1)	.3113 (3)
S(2)	.7221 (4)	.4200 (1)	.1318 (3)
S(3)	.5945 (4)	.2057 (1)	.1675 (3)
O(1)	.774 (1)	.6993 (4)	.172 (1)
O(2)	.881 (1)	.7607 (4)	.469 (1)
O(3)	.944 (1)	.3248 (4)	.631 (1)
O(4)	.943 (1)	.2103 (4)	.771 (1)
O(5)	.551 (1)	.3702 (4)	.037 (1)
O(6)	.671 (1)	.4905 (4)	.166 (1)
O(7)	.807 (1)	.3917 (4)	.311 (1)
O(8)	.857 (1)	.4254 (4)	.011 (1)
O(9)	.580 (1)	.1272 (4)	.178 (1)
O(10)	.597 (1)	.7757 (4)	.893 (1)
O(11)	.712 (1)	.2317 (4)	.038 (1)
O(12)	.682 (1)	.2406 (4)	.357 (1)
O(13)	.567 (1)	.6562 (4)	.635 (1)
O(14)	.572 (1)	.2788 (4)	.694 (1)
O(15)	.706 (1)	.4262 (4)	.647 (1)
O(16)	.758 (1)	.9491 (5)	.076 (1)
O(17)	.778 (1)	.5834 (4)	.919 (1)
O(18)	.854 (1)	.9923 (5)	.728 (1)
O(19)	.919 (1)	.7206 (4)	.818 (1)
O(20)	.912 (1)	.0976 (5)	.035 (1)
O(21)	.725 (1)	.8934 (5)	.418 (1)
O(22)	.768 (1)	.5601 (4)	.509 (1)
O(23)	.657 (1)	.1007 (5)	.570 (1)

factors brought the R value down to 11%. Finally, anisotropic thermal parameters were varied in the least-squares refinement. This led to a final R value of 0.096 for all data. Table 2 lists the refined atom parameters and their standard deviations. Mg occupies the special position in the cell origin; all other atoms are in general positions. The thermal parameters and their standard deviations are given in Table 3. Table 4 lists the corresponding root-mean-square amplitudes along principal axes. The temperature factor is defined as $\exp[-\frac{1}{4}(B_{11}a^{*2}h^2 + B_{22}b^{*2}k^2 + B_{33}c^{*2}l^2 + 2B_{23}b^*c^*kl + 2B_{13}a^*c^*hl + 2B_{12}a^*b^*hk)]$. The equivalent isotropic temperature coefficients B_{iso} were computed from

Table 3. *Thermal parameters of atoms in copiapite*

Atom	B_{11}	B_{22}	B_{33}	B_{23}	B_{13}	B_{12}	B_{iso}
Mg	1.70(26) Å^2	2.19(22) Å^2	2.07(21) Å^2	0.34(17) Å^2	0.35(18) Å^2	0.52(18) Å^2	1.95 Å^2
Fe(1)	0.83(07)	1.47(06)	0.71(05)	0.22(04)	0.02(04)	0.21(05)	0.95
Fe(2)	0.48(07)	1.47(06)	1.00(05)	0.24(04)	−0.04(05)	0.18(05)	0.89
S(1)	0.89(12)	1.77(10)	0.93(09)	0.31(07)	0.13(08)	0.15(08)	1.13
S(2)	0.87(12)	1.57(10)	0.97(09)	0.32(07)	0.11(08)	0.11(08)	1.09
S(3)	0.77(12)	1.52(10)	1.20(09)	0.16(07)	0.09(08)	0.24(08)	1.12
O(1)	0.71(36)	2.81(36)	2.41(34)	0.27(27)	0.07(26)	0.01(27)	1.72
O(2)	2.87(42)	2.11(32)	1.18(28)	0.30(24)	0.72(27)	0.72(28)	1.81
O(3)	1.51(38)	1.56(31)	2.96(36)	0.54(26)	0.42(28)	0.64(26)	1.79
O(4)	1.76(40)	2.59(34)	1.76(31)	0.61(25)	0.58(27)	−0.35(28)	1.87
O(5)	0.39(34)	2.65(34)	1.04(27)	0.24(24)	−0.37(23)	−0.04(26)	0.90
O(6)	3.15(44)	1.06(30)	1.88(32)	0.06(24)	0.32(29)	0.44(28)	1.84
O(7)	1.26(37)	1.88(31)	1.06(28)	0.25(23)	0.02(25)	0.22(26)	1.37
O(8)	1.18(37)	3.06(36)	1.32(30)	1.06(26)	0.72(25)	0.15(28)	1.30
O(9)	1.57(39)	1.17(29)	2.69(35)	0.05(25)	0.13(28)	0.30(26)	1.72
O(10)	0.71(34)	1.95(30)	0.88(26)	0.01(22)	−0.07(23)	0.08(24)	1.09
O(11)	1.02(37)	2.61(35)	1.45(30)	0.26(25)	0.38(26)	0.29(27)	1.54
O(12)	1.75(39)	2.06(33)	1.15(28)	0.21(24)	0.14(26)	0.75(27)	1.55
O(13)	1.41(37)	2.00(31)	1.18(28)	0.31(23)	0.51(25)	−0.20(26)	1.41
O(14)	2.11(40)	2.30(33)	1.30(30)	−0.03(25)	0.76(27)	0.19(28)	1.74
O(15)	2.05(39)	2.22(33)	1.51(30)	0.41(25)	0.28(26)	0.52(27)	1.87
O(16)	2.02(43)	3.35(41)	2.87(38)	−0.07(31)	0.59(31)	−0.31(32)	2.69
O(17)	1.22(37)	1.84(31)	2.52(34)	0.76(26)	0.44(27)	0.60(26)	1.64
O(18)	4.49(55)	3.30(43)	2.88(40)	0.41(33)	0.30(37)	1.31(38)	3.42
O(19)	1.30(38)	2.62(35)	2.35(34)	0.63(27)	0.75(27)	−0.11(27)	1.85
O(20)	4.37(54)	2.07(36)	3.62(43)	0.25(31)	1.35(38)	0.96(34)	3.04
O(21)	3.43(49)	2.70(38)	3.09(40)	0.11(31)	0.51(35)	0.36(33)	3.10
O(22)	3.16(45)	1.91(33)	2.04(33)	0.35(26)	0.95(30)	0.35(29)	2.22
O(23)	3.70(52)	2.78(39)	3.37(42)	1.25(32)	0.51(36)	0.53(34)	3.11

Table 4. *Parameters for the ellipsoids of vibration*

Atoms	Root-mean-square amplitudes along the principal axes	Angles with the reciprocal lattice vectors		
		a*	b*	c*
Mg	.14 Å	29.4°	107.4°	67.9°
	.16	66.1	61.1	133.8
	.17	74.0	34.7	51.9
Fe(1)	.11	37.7	78.0	114.7
	.14	86.6	13.3	76.2
	.09	52.5	95.7	28.8
Fe(2)	.14	91.9	156.3	113.9
	.12	72.9	66.3	142.4
	.07	17.2	89.1	62.8
S(1)	.11	41.4	72.2	116.9
	.15	90.7	18.5	73.5
	.10	48.6	94.8	32.3
S(2)	.15	86.2	154.6	111.7
	.11	48.0	65.1	120.2
	.10	42.3	94.6	38.6
S(3)	.14	97.2	166.3	106.2
	.13	77.3	76.3	151.5
	.10	14.6	90.6	67.2
O(1)	.20	86.7	152.4	114.6
	.18	88.8	65.5	150.7
	.09	3.5	78.1	75.0
O(2)	.11	87.6	85.5	164.0
	.16	105.4	25.0	88.6
	.19	15.6	65.5	74.1
O(3)	.20	96.6	104.8	166.3
	.11	129.3	49.3	103.3
	.15	40.1	44.4	93.0
O(4)	.20	70.0	145.8	103.3
	.12	53.3	57.6	120.7
	.16	43.6	80.1	34.0

Table 4. *(Continued)*

Atoms	Root-mean-square amplitudes along the principal axes	Angles with the reciprocal lattice vectors		
		a*	b*	c*
O(5)	.13 Å	67.0°	74.5°	141.8°
	.19	94.5	17.7	78.9
	.05	23.5	81.6	54.0
O(6)	.20	16.4	82.9	93.8
	.11	87.7	7.2	87.2
	.15	73.8	88.8	4.7
O(7)	.14	37.4	69.2	111.8
	.16	94.7	21.3	74.1
	.11	53.0	94.1	27.5
O(8)	.21	93.3	158.0	112.9
	.07	58.2	68.8	113.5
	.14	32.0	95.5	50.2
O(9)	.19	80.6	87.8	158.0
	.12	96.6	16.0	90.4
	.14	11.5	74.2	68.0
O(10)	.12	60.4	85.6	137.9
	.16	91.3	10.7	89.9
	.09	29.6	80.2	47.9
O(11)	.11	19.4	83.8	96.7
	.18	85.2	7.3	82.0
	.13	71.3	93.8	10.5
O(12)	.14	57.0	119.8	118.2
	.12	120.9	76.6	151.7
	.17	48.5	33.3	88.0
O(13)	.17	67.5	147.3	93.6
	.10	58.7	66.1	130.6
	.14	40.2	69.0	40.8
O(14)	.11	74.7	93.5	151.7
	.18	121.1	43.2	108.6
	.16	35.5	47.0	69.5

Table 4. *(Continued)*

Atoms	Root-mean-square amplitudes along the principal axes	Angles with the reciprocal lattice vectors		
		a*	**b***	**c***
O(15)	.16	34.2	101.3	105.7
	.13	108.7	71.1	155.0
	.17	62.4	22.2	71.1
O(16)	.19	93.2	101.6	166.6
	.22	109.9	30.9	102.2
	.15	20.2	61.8	84.4
O(17)	.11	34.0	113.8	73.6
	.14	58.8	41.8	113.0
	.19	77.8	58.0	28.8
O(18)	.25	24.7	66.1	96.6
	.18	114.6	57.2	136.5
	.20	88.4	42.6	47.2
O(19)	.11	32.5	65.6	104.9
	.17	122.4	71.9	146.1
	.20	91.3	31.2	60.3
O(20)	.20	71.3	80.5	147.7
	.15	96.6	16.6	85.5
	.24	19.9	76.5	58.1
O(21)	.21	31.4	93.5	106.7
	.20	115.0	78.8	158.5
	.18	72.3	11.8	76.9
O(22)	.16	87.9	140.5	127.7
	.14	78.3	50.7	133.6
	.20	11.9	86.3	67.2
O(23)	.24	68.1	118.6	131.6
	.15	93.9	39.9	126.3
	.21	22.3	64.8	62.7

hypothetical spheres of vibration having the same volume as the corresponding ellipsoids. The observed and calculated structure factors are compiled in Table 5.

Table 5. *Observed and calculated structure factors of copiapite*

h k l	F_o	F_c	h k l	F_o	F_c	h k l	F_o	F_c	h k l	F_o	F_c	h k l	F_o	F_c
0 0 0		566.0	2 -16 0	10.5	- 6.2	5 -4 0	19.0	25.8	1 -18 1	13.9	12.5	4 14 1	16.4	15.8
1		-86.5	-17	1.7	- 4.8	-5	70.8	72.8	-19	2.8	1.1	15	10.2	8.0
2		-116.0	-18	5.3	5.5	-6	30.8	-32.3	-20	7.4	2.6	-1	25.3	32.0
3	116.0	100.2	-19	2.8	3.2	-7	13.1	- 9.4	-21	3.6	4.2	-2	49.2	-50.5
4	29.3	17.5	-20	2.5	4.5	-8	34.2	33.8	-22	2.2	5.6	-3	36.2	33.3
5	24.3	-14.3	-21	9.5	-10.0	-9	21.2	-21.4	2 0 1	5.8	- 6.1	-4		87.3
6	42.1	-34.9	-22	12.5	10.9	-10	3.6	0.3	1	74.7	83.8	-5	42.2	-53.1
7	21.4	12.5	3 0 0		104.2	-11	17.9	19.0	2	63.0	-70.4	-6	45.0	-44.2
8	33.7	-32.2	1	7.0	- 6.5	-12	38.5	-40.4	3	1.4	6.3	-7	69.8	72.0
9	124.7	117.4	2	17.5	-14.9	-13	14.7	13.4	4	10.2	- 8.7	-8	18.3	20.2
10	51.5	55.6	3	75.3	75.1	-14	19.6	18.6	5	7.0	- 7.9	-9	41.2	-40.7
11	66.6	-59.8	4	23.2	21.7	-15	10.7	11.1	6	23.9	-25.9	-10	14.6	14.9
12	67.3	62.8	5	84.3	-79.9	-16	4.9	- 5.2	7	7.2	7.6	-11	23.9	-24.9
13	44.5	-38.2	6	40.4	40.7	-17	6.7	- 5.7	8	4.8	1.7	-12	35.5	34.3
14		0.6	7	12.4	8.8	-18	2.7	- 4.6	9	4.6	- 0.1	-13	19.4	19.4
15	30.8	28.4	8	51.1	-48.5	-19	2.7	- 4.8	10	26.1	27.8	-14	2.8	4.0
16	12.7	3.9	9	31.9	26.8	6 0 0	8.8	-10.9	11	12.2	- 7.3	-15	28.8	-33.2
17	31.2	-30.3	10	11.8	11.2	1	34.6	-36.0	12	6.3	- 6.7	-16	8.0	11.5
18	26.3	26.6	11	13.4	8.1	2	40.0	43.2	13	61.3	70.6	-17	32.0	35.9
19	35.5	35.2	12	42.3	41.8	3	28.3	26.5	14	26.2	-24.1	-18	13.0	-13.7
1 0 0		-30.3	13	37.5	-35.9	4	4.1	- 2.0	15	9.9	-14.2	5 0 1	35.7	34.0
1		62.1	14	14.6	-16.2	5	49.1	-49.0	16	12.8	17.9	1	59.5	54.9
2		6.9	15	4.5	6.0	6	55.7	56.9	17	14.7	-14.1	2	50.9	-50.8
3	49.9	53.9	16	14.8	11.5	7	13.3	14.7	18	3.9	1.4	3	10.8	13.0
4	16.4	-17.6	17	21.3	-20.1	8	26.4	-28.5	19	5.5	9.9	4	51.4	49.4
5	5.5	1.8	18	10.3	1.1	9	15.7	14.6	20	2.7	2.5	5	10.0	-11.9
6	12.2	- 8.0	-1		-32.6	10	2.7	- 3.0	-1	78.5	-88.4	6	26.6	-27.6
7	22.0	23.3	-2		-105.5	11	15.2	9.7	-2	52.0	62.0	7	13.3	16.6
8	12.7	-12.1	-3	6.2	- 4.7	12	18.0	17.0	-3	56.5	64.3	8	2.8	1.9
9	35.6	-37.4	-4	5.2	0.6	13	20.3	23.2	-4	79.8	-80.8	9	7.6	10.7
10	23.9	22.3	-5	36.7	-34.8	14	16.0	-15.6	-5	57.3	-58.3	10	7.7	8.1
11	24.4	24.3	-6	61.7	60.7	-1	12.0	8.5	-6	26.9	26.6	11	13.1	-16.5
12	29.5	26.6	-7	62.0	-59.0	-2	15.2	-14.4	-7	12.2	-10.5	12	2.4	5.7
13	16.4	16.0	-8	14.4	-13.1	-3	55.7	52.4	-8	40.4	37.8	13	9.1	14.1
14	28.7	-27.8	-9	112.7	110.6	-4	24.5	-25.8	-9	42.5	40.4	14	2.7	2.2
15	31.6	36.5	-11	99.0	-99.7	-5	10.6	7.3	-10	73.0	-72.6	-1	12.4	-11.0
16	2.8	1.0	-12	59.3	56.2	-6	43.7	40.0	-11	99.1	100.2	-2	26.3	28.4
17	8.7	0.0	-13	22.2	16.8	-7	26.1	-25.0	-12	29.3	22.9	-3	17.8	17.2
18	2.8	2.5	-14	37.3	-35.9	-8	18.0	19.7	-13	61.5	-60.3	-4	45.1	-42.5
19	9.3	13.3	-15	47.2	43.6	-9	25.9	25.9	-14	18.9	-19.0	-5	27.8	26.7
20	5.1	-14.9	-16	2.9	- 6.2	-10	2.8	- 0.2	-15	20.8	19.7	-6	40.7	37.9
21	2.7	2.9	-17	36.6	-35.6	0 0 1		43.3	-16	29.9	-30.5	-7	11.4	-10.9
-1		- 3.2	-18	37.3	36.0	1	34.2	-35.8	-17	10.3	- 7.6	-8	23.5	22.5
-2		46.3	-19	35.9	32.6	2	65.6	61.1	-18	55.8	56.0	-9	26.3	27.9
-3	27.5	-26.4	-20	29.4	-30.3	3	51.9	-55.8	-19	39.3	-39.1	-10	21.2	-20.5
-4	148.1	137.5	-21	2.7	- 0.0	4	66.6	66.2	-20	2.7	1.9	-11	29.6	30.1
-5	34.6	22.6	4 0 0	12.9	5.0	5	83.9	80.3	-21	37.1	36.2	-12	12.6	10.9
-6	87.9	-82.2	1	22.9	-22.2	6	57.3	-52.0	-22	17.9	-20.7	-13	43.1	-44.2
-7	111.0	100.7	2	24.7	19.2	7	3.5	3.0	3 0 1	32.0	-33.7	-14	6.3	- 3.9
-8	56.3	53.9	3	52.2	54.1	8	6.7	6.2	1	46.7	43.9	-15	35.8	39.7
-9	33.0	-28.8	4	33.0	-31.9	9	16.2	-13.9	2	6.4	- 6.7	-16	9.3	0.3
-10	15.3	-14.2	5	7.7	9.4	10	6.8	6.7	3	13.1	-11.3	-17	6.2	- 2.5
-11	58.5	57.7	6	6.0	7.8	11	41.8	-41.6	4	50.5	48.8	-18	17.5	17.9
-12	11.1	4.5	7	46.0	47.9	12	8.8	4.9	5	2.9	0.3	6 0 1	2.8	- 2.1
-13	7.6	- 3.0	8	46.8	-51.1	13	4.0	10.2	6	35.5	35.0	1	2.8	- 2.4
-14	32.7	32.0	9	13.0	-16.4	14	33.5	33.1	7	5.9	- 2.5	2	2.2	0.9
-15	34.0	-31.8	10	33.4	35.6	15	27.5	-24.5	8	12.9	11.3	3	13.0	13.7
-16	6.8	6.0	11	40.2	-40.6	16	18.1	17.8	9	14.3	11.6	4	18.7	17.2
-17	14.6	9.7	12	10.5	8.8	17	5.7	- 6.1	10	3.1	2.6	5	40.5	-40.6
-18	2.8	3.4	13	12.7	12.2	18	24.0	-28.2	11	2.8	- 4.3	6	19.4	20.2
-19	2.8	0.2	14		- 0.0	19	28.6	31.3	12	2.8	4.4	7	39.4	40.8
-20	27.8	28.7	15	15.5	18.4	1 0 1	18.4	18.4	13	14.1	17.3	8	13.8	-15.9
-21	5.2	- 8.3	-1		-18.8	1	44.6	49.0	14	17.8	-20.1	9	16.1	-19.0
-22	5.6	- 7.7	-2		46.4	2	102.6	103.6	15	8.8	6.7	10	11.3	12.6
2 0 0		-89.3	-3	5.1	-12.3	3	49.1	-48.9	16	50.0	48.6	11	8.5	14.9
1		7.0	-4	2.0	4.0	4	137.8	-133.1	17	25.2	-25.3	12	6.7	9.7
2		-61.1	-5	6.6	4.7	5	34.7	43.2	-1	6.1	- 4.1	13	2.9	4.1
3		8.3	-6	38.4	-38.2	6	9.6	- 9.6	-2	9.6	8.4	-1	2.8	- 0.8
4	58.1	58.5	-7	18.2	16.4	7	48.0	-48.0	-3	60.5	-71.3	-2	16.6	-17.3
5	37.5	-34.3	-8	37.2	35.2	8	10.4	- 6.3	-4	21.6	21.4	-3	32.5	35.1
6	20.2	19.6	-9	11.9	- 9.3	9	9.7	6.5	-5	45.3	41.8	-4	22.2	23.2
7	9.3	9.3	-10	58.7	-59.9	10	8.9	5.8	-6	18.3	-18.7	-5	5.9	- 6.4
8	59.3	55.7	-11	42.1	46.0	11	31.1	33.0	-7	22.2	20.8	-6	20.5	20.1
9	67.3	-66.2	-12	21.3	14.3	12	30.7	32.3	-8	5.3	6.6	-7	6.8	3.0
10	13.4	10.4	-13	33.4	-34.1	13	51.9	-63.8	-9	19.3	-15.8	-8	22.9	22.8
11	75.8	74.0	-14	7.7	5.4	14	12.4	7.0	-10	32.6	33.1	-9	6.7	-11.1
12	75.5	-75.6	-15	36.2	-37.5	15	14.8	17.3	-11	6.4	- 6.8	0 1 -1	40.6	44.5
13	13.4	12.9	-16	35.5	38.3	16	18.5	-24.5	-12	44.4	-42.3	2	10.0	- 4.4
14	57.4	54.6	-17	26.5	25.4	17		41.7	-13	24.6	22.5	3	13.6	13.4
15	2.8	0.1	-18	25.4	-24.6	18	10.1	- 8.0	-14	19.6	18.5	4	21.2	-25.8
16	14.7	-13.7	-19	2.7	3.5	19	24.1	-23.4	-15	14.2	12.4	5	24.1	25.2
17	5.7	- 4.8	5 0 0	43.2	-45.0	20	30.5	33.1	-16	8.7	9.1	6	19.3	19.5
18	6.8	- 0.3	1	31.4	30.4	21	19.6	21.1	-17	15.2	-10.2	7	25.3	25.6
19	3.9	- 6.8	2	21.4	20.2	-1	18.0	-26.2	-18	15.5	-14.5	8	46.2	-45.5
20	18.4	19.7	3	41.8	-42.7	-2	13.9	-10.5	-19	22.6	26.8	9	33.2	-32.8
21	22.2	-25.7	4	6.3	1.0	-3	14.8	- 6.0	-20	2.7	1.2	10	105.9	103.4
-1		140.4	5	26.3	27.2	-4	101.1	100.8	4 0 1	5.1	- 4.8	12	53.5	-56.8
-2		-44.2	6	2.8	- 0.6	-5	62.4	-61.8	1	19.0	-20.2	13	31.4	32.5
-3		-63.4	7	2.0	5.3	-6	75.2	-68.9	2	95.0	90.3	14	28.1	26.6
-4	30.9	28.3	8	18.1	16.2	-7		62.2	3		- 7.1	15	11.6	-10.7
-5	62.9	55.9	9	41.1	-43.0	-8	56.6	50.1	4	13.9	- 8.3	16	17.5	19.0
-6	13.0	10.3	10	34.5	34.2	-9	47.0	-42.5	5	70.8	71.9	17	24.3	26.8
-8	94.9	86.2	11	40.6	43.0	-10	11.1	8.7	6	22.5	-21.3	18	24.3	-26.5
-9	10.8	-10.0	12	63.6	-68.2	-11	2.9	3.2	7	30.3	-30.0	19	31.8	37.2
-10	18.1	-14.5	13	2.7	1.8	-12	12.4	-14.3	8	67.2	70.3	20	13.1	- 7.6
-11	75.7	74.8	14	34.4	43.4	-13	14.4	13.0	9	16.2	-16.8	21	10.8	-15.8
-12	23.9	-21.4	15	2.7	- 0.3	-14	21.7	19.6	10	59.2	-62.1	22	23.2	26.1
-13	9.6	- 7.7	-1	33.0	41.0	-15	24.1	-22.5	11	48.2	50.2	1 0 -1		-43.3
-14	9.2	- 6.7	-2	12.4	19.0	-16	0.8	- 4.7	12	37.7	41.2	1	99.7	-95.0
-15	48.0	49.2	-3		-39.5	-17	2.4	- 5.7	13	38.4	-42.7	2	104.5	96.2

Table 5. *(Continued)*

h	k	l	F_o	F_c
1	3	-1	131.9	127.0
	4			-117.8
	5		37.4	33.3
	6		15.4	18.5
	7		47.9	-46.8
	8		25.2	22.7
	9		59.1	56.4
	10		56.6	-57.2
	11		48.0	48.9
	12		76.9	78.3
	13		35.1	-34.8
	14		31.6	35.5
	15		28.3	32.9
	16		60.1	-61.8
	17		20.1	16.6
	18		41.3	43.0
	19		23.1	-19.9
	20		7.2	- 8.1
	21		24.6	28.3
	-1			150.0
	-2		15.2	- 9.1
	-3		3.8	- 1.5
	-4		73.2	68.6
	-5		104.1	-99.5
	-6		64.2	61.5
	-7		135.7	122.9
	-8		95.6	-90.1
	-9		25.8	25.0
	-10		66.9	63.1
	-11		13.1	11.3
	-12		7.4	- 8.9
	-13		37.2	37.3
	-14		40.6	-41.0
	-15		19.9	-19.8
	-16		36.5	34.9
	-17		11.4	- 6.1
	-18		8.4	- 7.9
	-19		15.0	11.6
	-20		4.1	6.5
	-21		7.3	0.1
	-22		7.5	7.9
2	0	-1		16.0
	1		87.1	69.1
	2		50.2	60.8
	3		49.5	-49.5
	4		48.9	45.1
	5		34.0	29.9
	6		2.5	4.2
	7		8.8	- 8.7
	8		5.2	- 5.8
	9		41.7	39.1
	10		49.4	49.2
	11		12.2	14.6
	12		22.4	-18.4
	13		10.1	4.8
	14		43.4	42.9
	15		8.3	- 2.7
	16		6.1	- 1.3
	17		15.9	-17.2
	18		16.0	17.4
	19		14.0	-10.1
	20		4.9	0.7
	21		13.6	15.9
	-1			27.6
	-2			7.3
	-3		81.9	-66.7
	-4		61.7	-61.0
	-5		59.7	61.5
	-6		66.5	59.3
	-7			-51.8
	-8		99.9	93.7
	-9		62.1	60.4
	-10		19.6	-13.4
	-11			53.8
	-12		29.4	-25.4
	-13		19.2	-16.0
	-14		4.1	8.3
	-15		30.2	28.2
	-16		2.8	0.3
	-17		18.2	16.5
	-18		10.7	10.2
	-19		20.8	-21.2
	-20		35.6	35.6
	-21		8.2	8.3
	-22		31.4	-32.9
3	0	-1		15.5
	1		52.2	49.2
	2		30.1	-25.5
	3		6.8	4.4
	4		98.0	90.4
	5		16.2	-14.4
	6		17.7	17.6
	7		56.2	54.4
	8		31.4	-26.5
	9		21.4	-17.6
	10		48.7	46.6
	11		26.5	-23.3
	12		31.0	-29.3
	13		50.6	46.9
	14		6.0	- 1.6
3	15	-1	36.3	-35.9
	16		14.1	11.4
	17		32.5	31.9
	18		13.6	-12.5
	-1			-54.5
	-2			23.9
	-3			41.1
	-4		10.3	8.4
	-5		35.5	34.4
	-6		4.0	4.7
	-7		28.0	-28.3
	-8		25.0	26.2
	-9		8.5	- 0.4
	-10		9.8	6.8
	-11		13.3	- 9.9
	-12		30.0	26.5
	-13		28.8	26.2
	-14		25.3	24.8
	-15		12.7	-13.1
	-16		2.8	1.5
	-17		17.9	12.8
	-18		16.8	13.8
	-19		10.1	4.9
	-20		2.7	1.4
4	0	-1		21.9
	1		69.2	-66.0
	2		36.2	33.8
	3		53.8	54.1
	4		85.6	-85.4
	5		69.3	72.8
	6		32.9	31.5
	7		78.2	-80.4
	8		30.1	29.1
	9		21.7	21.6
	10		16.5	-17.3
	11		24.3	-23.4
	12		4.7	- 2.9
	13		13.0	14.9
	14		4.6	3.8
	15		24.2	25.7
	16		25.7	-28.6
	-1			89.9
	-2			-52.9
	-3			11.0
	-4		42.0	45.1
	-5		48.3	-49.1
	-6		26.1	26.8
	-7		75.5	76.4
	-8		83.0	-85.1
	-9		6.8	6.1
	-10		69.1	71.9
	-11		37.0	-39.7
	-12		23.3	-21.3
	-13		40.0	42.9
	-14		25.5	-26.4
	-15		16.1	-17.3
	-16		60.8	61.1
	-17		6.2	- 2.1
	-18		24.1	-25.2
	-19		23.3	25.6
5	0	-1		0.5
	1		35.8	35.3
	2		2.9	- 4.9
	3		3.0	3.2
	4		10.7	-11.7
	5		8.7	- 3.0
	6		47.3	45.2
	7		48.0	-46.9
	8		23.6	-26.6
	9		24.4	24.6
	10		2.8	4.3
	11		5.6	5.4
	12		10.3	12.9
	13		5.4	- 7.2
	14		2.7	2.4
	15		4.1	11.9
	-1			-26.5
	-2			-18.9
	-3			-19.1
	-4			26.5
	-5		46.6	46.9
	-6		2.9	- 4.3
	-7		2.2	-23.9
	-8		48.1	48.0
	-9		23.6	17.2
	-10		23.5	-24.2
	-11		16.8	-12.2
	-12		10.8	-13.3
	-13		4.1	2.0
	-14		19.3	21.9
	-15		8.8	17.0
	-16		39.0	-43.2
	-17		22.1	21.7
	-18		23.4	26.9
	-19		24.6	-26.4
6	0	-1	28.2	-27.9
	1		6.2	5.5
	2		2.8	3.3
	3		41.1	-40.3
	4		56.0	54.3
6	5	-1	14.0	-14.3
	6		22.3	-23.2
	7		51.8	51.4
	8		5.3	- 5.6
	9		10.4	9.2
	10		2.1	2.6
	11		14.8	-14.8
	12		2.7	- 2.3
	-1			-16.3
	-2			51.0
	-3			20.3
	-4			8.4
	-5		22.8	24.3
	-6		31.4	32.1
	-7		29.5	-31.7
	-8		6.8	6.5
	-9		7.1	0.8
	-10		6.7	3.8
	-11		3.4	4.8
0	0	2	37.8	49.7
	1		155.3	-149.3
	2		58.5	56.2
	3		32.8	37.0
	4		55.8	-50.9
	5		37.1	-37.5
	6		66.2	63.1
	7		20.8	-20.0
	8		19.7	-21.5
	9		131.7	129.3
	10		79.8	-80.6
	11		31.5	-31.9
	12		43.4	44.3
	13		8.8	- 7.1
	14		3.0	- 5.1
	15		22.2	-21.9
	16		6.9	- 5.5
	17		9.8	-12.8
	18		54.9	59.6
1	0	2	2.2	- 4.1
	1		42.5	45.2
	2		92.2	92.0
	3		73.2	-77.2
	4		25.1	23.2
	5		10.0	- 2.5
	6		21.7	-23.9
	7		43.4	43.7
	8		39.0	-42.9
	9		21.9	-22.3
	10		36.6	43.1
	11			17.9
	12			-20.5
	13		13.1	-20.5
	14			52.6
	15		16.1	-12.4
	16		10.7	9.5
	17		18.6	21.2
	18		21.8	-23.4
	19		10.2	6.8
	20		17.8	14.2
	-1		12.2	-14.5
	-2		87.9	93.3
	-3		71.2	-75.3
	-4		21.4	-18.7
	-5		76.6	76.5
	-6		42.8	-42.8
	-7		2.1	- 0.7
	-8		27.1	27.0
	-9		9.6	12.4
	-10		13.5	-11.9
	-11		8.5	- 4.8
	-12		6.3	- 7.2
	-13		37.8	-38.6
	-14		65.8	62.0
	-15		39.0	-37.0
	-16		18.0	-11.9
	-17		39.5	37.6
	-18		22.0	-17.7
	-19			-13.8
	-20		22.6	22.7
	-21		16.1	13.7
2	0	2		-91.6
	1		17.0	16.5
	2		22.8	30.5
	3			72.2
	4		27.4	-34.3
	5		14.8	17.2
	6		6.2	- 6.6
	7		5.1	2.8
	8		23.7	27.4
	9			-42.3
	10			39.7
	11		5.1	- 5.4
	12		13.0	15.7
	13			69.3
	14		22.0	-25.1
	15		14.5	-13.2
	16		6.3	5.3
	17		30.6	42.5
	18			-25.6
	19		2.7	- 3.9
2	20	2	14.1	21.2
	-1		22.6	31.1
	-2		36.9	45.8
	-3		11.2	-13.2
	-4		27.7	28.8
	-5		19.6	-19.6
	-6		84.0	90.4
	-7		2.9	- 1.2
	-8		19.0	-18.6
	-9		50.3	53.2
	-10		15.1	-13.8
	-11		12.7	-11.7
	-12		5.3	- 5.5
	-13		58.6	62.7
	-14		21.9	-16.6
	-15		54.7	-52.5
	-16		53.1	49.3
	-17		15.8	-13.1
	-18		13.8	12.6
	-19		7.0	1.2
	-20		21.9	-20.6
	-21		14.3	15.6
	-22		8.9	12.6
3	0	2	42.7	41.8
	1		38.4	-38.4
	2		6.0	- 1.7
	3		94.0	93.5
	4		75.5	-74.1
	5		15.6	- 7.6
	6		97.4	94.7
	7		76.2	-72.0
	8		21.7	21.8
	9		94.3	92.4
	10		22.7	-22.5
	11		19.8	-21.3
	12		42.5	41.0
	13		2.2	1.7
	14		16.3	-18.9
	15		35.1	35.8
	16		16.5	-16.2
	17		16.9	-16.7
	-1		81.6	82.4
	-2		34.6	-33.1
	-3		31.9	29.9
	-4		36.0	-35.7
	-5		62.2	-63.0
	-6		100.6	95.6
	-7		13.6	11.8
	-8		45.8	-43.1
	-9		38.9	38.2
	-10		77.8	77.0
	-11		2.8	3.5
	-12		21.2	-19.2
	-13		34.4	34.5
	-14		51.7	-51.0
	-15		42.1	41.8
	-16		18.5	14.8
	-17		20.1	-16.8
	-18		13.0	11.7
	-19		5.0	3.5
	-20		14.6	10.2
4	0	2	35.8	-31.2
	1		54.6	54.8
	2		83.2	84.9
	3		64.6	-66.8
	4		31.4	27.8
	5		41.8	47.7
	6		17.0	-17.2
	7		17.3	18.5
	8		11.3	-11.5
	9		2.8	1.3
	10		0.1	10.8
	11		6.5	4.6
	12		4.0	5.8
	13		2.7	- 2.1
	-1		50.0	-52.4
	-2		64.6	67.4
	-3		2.9	2.5
	-4		39.1	-41.3
	-5		57.4	60.0
	-6		14.2	-13.1
	-7		6.9	- 3.7
	-8		41.9	42.4
	-9		12.2	-12.6
	-10		16.4	15.6
	-11		2.8	- 3.7
	-12		3.8	4.3
	-13		3.9	- 0.3
	-14		51.6	50.8
	-15		10.1	-10.6
	-16		42.6	-43.2
	-17		57.2	58.7
	-18		9.4	5.6
5	0	2	10.2	- 9.8
	1		14.7	11.7
	2		16.2	-17.2
	3		7.6	7.2
	4		37.0	35.9
	5		12.5	14.9
	6		29.7	-30.5
5	7	2	12.4	14.8
	8		9.5	11.5
	9		10.8	- 6.3
	10		4.5	-10.7
	11		10.0	-17.5
	12		7.4	- 7.8
	13		25.8	29.9
	-1		22.6	-22.1
	-2		70.4	69.1
	-3		2.8	4.2
	-4		38.0	-35.8
	-5		19.9	23.8
	-6		32.2	28.9
	-7		24.9	25.4
	-8		34.1	-35.9
	-9		2.8	- 1.6
	-10		11.3	13.4
	-11		7.5	2.4
	-12		7.2	11.8
	-13		15.5	-15.8
	-14		3.8	4.6
	-15		2.7	1.4
	-16		22.7	25.5
	-17		2.7	2.5
6	0	2	26.1	24.1
	1		9.4	14.8
	2		13.5	-12.2
	3		9.3	8.0
	4		22.1	-22.8
	5		5.6	1.3
	6		42.0	40.8
	7		52.2	-52.6
	8		7.2	- 0.9
	9		31.1	34.8
	10		8.1	- 7.2
	11		2.7	- 2.2
	-1		6.9	7.3
	-2		71.0	-69.7
	-3		59.2	55.2
	-4		29.1	27.9
0	1	-2	114.5	109.2
	2		9.3	3.5
	3		49.6	49.7
	4		91.1	-80.8
	5		7.4	7.6
	6		50.6	-43.5
	7		47.0	-45.3
	8		43.9	-44.0
	9			24.5
	10		26.3	21.4
	11		25.9	-23.8
	12		60.3	58.7
	13		30.8	31.4
	14		53.9	-56.2
	15		10.6	- 7.0
	16		4.8	11.0
	17		16.3	20.2
	18		25.9	-31.1
	19		5.6	12.3
	20		13.2	16.7
	21		2.7	- 2.6
1	0	-2	40.4	-38.5
	1		14.7	17.6
	2		71.6	-67.4
	3		45.4	-38.0
	4		97.1	93.2
	5		49.1	-45.4
	6		24.8	-24.4
	7		17.4	13.1
	8		3.0	4.8
	9		50.7	49.8
	10		7.5	-10.0
	11		66.2	-68.9
	12		35.2	38.5
	13		73.3	75.0
	14		44.2	-43.5
	15		11.1	9.1
	16		26.9	26.9
	17		23.1	-24.2
	18		17.4	16.0
	19		2.7	2.7
	20		8.3	-12.9
	21		7.0	- 7.3
	-1		21.0	25.4
	-2		17.0	18.4
	-3		27.0	26.4
	-4		92.5	-86.6
	-5		19.8	14.3
	-6		22.8	25.6
	-7		2.1	- 1.4
	-8		20.3	19.0
	-9		14.0	-12.3
	-10		24.9	22.9
	-11		40.4	40.5
	-12		20.4	-24.9
	-13		6.8	- 2.3
	-14		17.7	-17.5
	-15		2.0	- 7.8
	-16		2.8	1.4
	-17		20.4	25.9

Table 5. *(Continued)*

h k l	F_o	F_c	h k l	F_o	F_c	h k l	F_o	F_c	h k l	F_o	F_c	h k l	F_o	F_c
1 -18 -2	4.6	-13.2	4 15 -2	36.0	42.0	1 5 3	40.3	47.8	3 -10 3	31.6	28.0	1 2 -3	20.5	16.4
-19	10.0	-14.3	-1	1.7	- 1.5	6	10.6	-13.3	-11	44.9	46.3	3	32.0	29.0
-20	20.6	17.2	-2	19.1	-16.8	7		- 9.4	-12	46.7	-44.3	4	65.2	-61.5
-21	7.4	- 0.8	-3	29.6	29.1	8	30.5	34.1	-13	27.4	25.0	5	30.0	28.5
2 0 -2	41.3	-36.3	-4	22.1	21.2	9	17.4	17.5	-14	8.6	4.1	6	27.7	25.4
1	12.2	13.5	-5		-22.1	10	12.2	13.7	-15	40.9	-38.9	7	44.7	-42.8
2	126.8	118.3	-6	75.2	74.5	11		7.0	-16	54.1	50.2	8	3.3	- 5.2
3	116.8	-110.7	-7	23.3	22.0	12		-22.4	-18	32.5	-30.0	9	31.1	31.0
4	19.6	16.0	-8	12.0	-10.6	13	23.1	-30.0	-19	5.7	0.3	10	10.0	9.2
5	111.8	102.6	-9	17.4	17.6	14		64.3	4 0 3	9.1	4.7	11	11.1	-10.3
6	50.6	-49.3	-10	13.6	-14.1	15	17.8	- 1.0	1	6.2	6.9	12	31.2	32.6
7	16.5	-11.2	-11	49.2	54.7	16		-18.7	2	37.0	40.2	13	19.5	-23.5
8	112.6	106.7	-12	42.2	-47.5	17	6.5	6.9	3	49.3	-51.3	14	16.3	17.8
9	36.1	-34.5	-13	19.3	-21.8	18	13.8	16.0	4	13.4	16.9	15	30.2	27.0
10	31.3	-29.6	-14	29.0	30.4	19	1.8	13.2	5	32.6	34.9	16	6.2	- 4.8
12	6.0	- 6.3	-15	28.3	26.1	-1	13.1	12.5	6	4.9	- 5.9	17	38.7	-38.5
13	51.3	-52.8	-16	6.4	3.4	-2	69.8	73.4	7	19.2	-17.4	18	16.4	10.5
14	46.9	40.4	-17	7.3	- 0.3	-3	3.8	2.7	8	12.7	9.3	19	10.2	12.7
15	13.1	-11.5	-18	11.2	10.9	-4	14.3	12.2	9	2.8	3.4	20	7.0	-10.1
16	14.2	14.6	5 1 -2	5.7	6.0	-5	7.6	- 1.2	10	9.2	12.4	-1	15.2	-11.4
17	20.1	19.2	2	91.3	88.9	-6	6.8	- 4.7	11	22.9	23.2	-2	51.4	-50.8
18	21.6	-23.0	3	99.3	-95.9	-7	10.2	7.9	12	28.1	-27.9	-3	16.0	16.3
19	5.4	- 5.6	4	20.8	19.0	-8	2.9	3.0	-1	39.8	39.8	-4	15.2	12.5
20	30.7	27.6	5		29.5	-9	21.9	18.3	-2	59.7	-59.4	-5	88.6	-87.2
21	2.7	3.0	6	13.0	- 9.4	-10	4.5	3.5	-3	27.2	-25.1	-6	75.6	72.1
-1	14.2	-12.2	7	2.8	- 2.6	-11	7.6	8.0	-4	19.5	17.2	-7	60.9	62.3
-2	4.3	- 0.1	8	36.4	37.3	-12	45.8	45.7	-5	46.1	46.2	-8	66.8	-65.3
-3	19.0	15.9	9	5.8	-11.0	-13	16.1	-19.5	-6	28.7	-28.1	-9	45.2	47.9
-4	27.7	-22.1	10	33.8	-33.2	-14	44.7	-43.3	-7	41.9	-45.0	-10	57.8	58.9
-5	12.6	8.3	11	59.8	65.3	-15	53.5	51.2	-8	57.1	60.3	-11	44.6	-43.1
-6	10.5	- 9.6	12	9.8	- 8.0	-16	15.2	16.9	-9	5.9	9.4	-12	17.1	18.4
-7		34.4	13	22.4	-24.6	-17	17.0	-12.7	-10	8.1	- 6.7	-13	19.6	19.6
-8	17.7	16.0	14	20.9	26.0	-18	3.5	- 5.3	-11	19.2	-20.4	-14	56.8	-62.0
-9	93.4	-89.4	15	6.1	- 6.4	-19	9.6	8.3	-12	2.8	2.3	-16	28.6	32.2
-10	99.3	96.1	-1		46.7	-20	13.2	11.9	-13	16.7	15.9	-17	44.6	-48.8
-11	2.9	1.4	-2	4.1	9.4	-21	10.6	15.1	-14	3.7	- 3.1	-18	3.7	2.6
-12	50.1	-47.9	-3	3.6	1.4	2 0 3		94.1	-15	22.0	23.7	-19	33.2	36.0
-13	31.0	30.0	-4	55.2	61.8	1	17.9	24.6	-16	12.9	-13.3	-20	8.6	-11.5
-14	48.7	47.0	-5	9.1	10.4	2		-64.8	5 0 3		32.9	2 0 -3	25.7	25.8
-15	10.2	-10.8	-6	65.1	-65.0	3		89.9	1	13.7	-14.2	1	25.7	-27.7
-16	23.0	-22.7	-7	63.5	65.3	4	5.4	- 8.8	2	16.2	-15.4	2	40.7	39.0
-17	20.8	22.0	-8	46.1	46.5	5		-82.7	3	54.6	53.0	3	98.1	94.1
-18	22.0	-19.4	-9	84.5	-88.1	6		38.8	4	3.2	4.6	4	15.1	-12.8
-19	2.7	4.0	-10	46.8	48.1	7		48.8	5	50.6	-49.9	5	49.7	-47.1
-20	14.9	13.5	-11	27.5	30.8	8		-54.6	6	18.3	19.5	6	40.2	41.2
-21	17.6	-14.1	-12	16.7	-14.5	9	5.6	5.6	7	34.8	33.9	7	31.8	26.5
-22	8.0	8.3	-13	15.1	18.4	10		61.3	8	27.8	-30.7	8	41.4	-40.4
3 0 -2	20.6	19.5	-14	19.9	23.3	11	22.8	-24.0	9	2.7	- 2.8	9	12.4	-12.1
1	52.3	46.4	-15	17.5	-16.9	12		21.4	10	10.6	13.4	10	31.6	-29.0
2	55.8	-55.0	-16	7.7	- 4.2	13	8.1	17.4	11	6.8	-15.7	11	41.8	38.0
3	125.6	120.7	-17	11.1	15.9	14		-33.6	-1	35.8	-35.3	12	60.8	58.3
4	63.5	61.4	-18	12.5	-15.6	15	13.9	20.0	-2	31.3	31.7	13	56.1	-47.4
5	3.4	- 0.7	-19	6.3	20.5	16	9.0	16.4	-3	45.6	44.5	14	16.6	-21.1
6	36.6	-31.4	6 0 -2	46.6	48.5	17	9.2	-10.2	-4	68.2	-65.1	15	35.4	31.6
7	31.5	29.0	1	53.0	-51.4	18	9.0	9.5	-5	6.2	6.7	16	9.7	3.5
8	15.5	15.0	2	11.2	-13.3	19	18.1	19.1	-6	40.3	38.7	17	27.2	-25.5
9	19.6	-18.2	3	5.9	5.6	-2	31.0	41.8	-7	40.9	-38.0	18	9.2	8.2
10	12.0	- 6.3	4	45.7	44.8	-3	40.9	50.0	-8	2.8	1.3	19	8.7	2.8
11	20.2	-20.1	5	8.7	8.8	-4	4.4	- 1.1	-9	23.0	21.0	20	27.1	-25.2
12	43.4	43.4	6	47.7	-47.0	-5	17.8	-19.7	-10	15.7	- 7.7	-1	97.7	-93.0
13	33.5	33.6	7	36.1	38.8	-6	63.4	74.5	-11	23.7	-23.3	-2	27.0	-24.9
14	9.9	-10.4	8	10.1	14.4	-7	33.7	-37.9	-12	50.2	52.7	-3	16.3	14.0
15	3.9	- 8.0	9	10.1	6.4	-8	7.8	- 8.2	-13	17.3	-17.5	-4	20.1	-16.7
16	9.9	- 5.2	10	14.3	-15.5	-9	92.1	99.8	-14	29.8	-31.2	-5	16.2	-14.7
17	18.9	20.9	11	2.7	2.7	-10	53.8	-56.6	-15	21.2	24.1	-6	2.7	- 1.2
-1	30.5	-35.5	12	8.5	6.4	-11	13.1	10.3	-16	8.7	-12.9	-7	31.2	32.4
-2	54.8	54.7	-1	5.1	3.8	-12	64.4	68.1	6 0 3		-14.5	-8	33.3	30.5
-3	17.7	-15.5	-2		-17.7	-14	9.4	12.7	1	3.9	7.9	-9	23.7	-23.0
-4	4.3	- 5.9	-3		23.6	-15	6.6	6.3	2	7.7	- 8.1	-10	15.5	-12.1
-5	17.0	-14.4	-4	39.4	-42.2	-16	8.5	- 1.0	3	5.9	2.8	-11	2.9	0.0
-6	61.5	61.1	-5	22.7	26.2	-17	28.1	-29.2	4	6.6	- 2.9	-12	11.1	8.4
-7	15.7	16.6	-6	19.2	21.7	-18	21.3	22.0	5	10.6	15.0	-13	23.7	-19.7
-8	30.9	-30.2	-7	2.9	5.1	-19	12.5	13.7	6	2.8	2.7	-14	30.0	28.4
-9	47.8	47.1	-8	10.9	-12.2	-20	5.6	0.5	7	5.1	- 1.2	-15	3.1	3.5
-10	12.3	-12.3	-9	3.2	- 2.9	-21	3.4	10.6	8	8.5	- 9.4	-16	15.5	-13.8
-11	3.6	- 4.9	-10	8.6	15.0	3 0 3	43.7	-45.1	9		- 1.2	-17	21.5	16.4
-12	23.8	22.1	0 0 3	34.2	-37.3	1	23.5	-21.9	10	24.1	23.9	-18	8.2	8.6
-13	18.1	-16.6	1	49.3	-46.9	2	3.0	- 1.5	0 1 -3	96.9	94.8	-19	5.7	4.0
-14	2.8	0.0	2	101.7	96.8	3	25.7	24.3	2	42.2	-40.9	-20	3.6	8.1
-15	21.1	19.8	3	55.3	55.6	4	33.5	35.2	3	14.8	-15.1	-21	17.9	-19.7
-16	10.8	-10.4	4	16.2	16.7	5	3.1	9.7	4	3.9	4.2	3 0 -3	41.3	-41.5
-17	3.4	1.2	5	32.2	32.5	6	30.1	-28.6	5	34.2	31.7	1	80.1	78.4
-18	57.1	60.2	6	50.9	-49.0	7	6.5	5.6	6	55.7	-55.4	2	50.3	-48.8
-19	14.4	-14.3	7	11.1	9.1	8	31.6	31.9	7	46.2	47.1	3	49.4	-46.9
-20	33.4	-31.5	8	71.3	68.8	9	18.5	-14.8	8	51.9	49.2	4	88.7	88.7
4 0 -2	57.3	60.7	9	18.5	-19.2	10	17.2	-15.3	9	77.0	-73.5	5	2.9	2.9
1	51.3	54.3	10	51.4	-47.2	11	18.4	18.0	10	19.3	19.1	6	56.2	-55.8
2	86.4	-87.3	11	69.9	69.8	12	2.8	- 2.9	11	35.5	34.2	7	39.9	37.5
3	58.4	59.5	12	19.4	19.2	13	26.8	26.1	12	16.5	-13.9	8	33.3	36.9
4	38.8	36.9	13	2.8	3.5	14	13.6	13.1	13	26.7	25.3	9	27.6	-25.6
5	26.5	-24.2	14	2.8	3.8	15	11.5	3.2	14	6.3	- 7.1	10	4.4	1.9
6	26.2	24.2	15	15.4	-18.0	-1	75.3	74.5	15	5.7	- 7.5	11	3.8	- 6.1
7	20.3	-19.5	16	2.8	- 3.8	-2	7.0	- 4.7	16	9.2	11.9	12	42.5	-42.0
8	9.4	9.4	17	3.5	6.8	-3	68.3	-68.3	17	19.5	24.3	13	40.6	40.0
9	17.6	16.3	18	14.9	13.4	-4	41.3	39.9	18	16.5	-20.3	14	10.1	11.1
10	4.5	9.5	1 0 3	46.7	49.2	-5	23.6	22.4	19	8.7	12.5	15	17.2	-20.0
11	22.9	-24.1	1	75.3	76.9	-6	23.0	-22.5	20	15.8	18.2	16	2.7	- 1.0
12	5.1	2.3	2	16.1	-17.1	-7	54.2	55.5	21	23.9	-28.6	17	22.2	23.4
13	27.3	27.1	3	42.8	-46.2	-8	12.6	11.6	1 0 -3	60.2	59.9	18	9.7	- 8.7
14	32.6	-34.2	4	26.6	27.7	-9	25.9	-25.1	1	40.6	-38.6	-1	33.8	35.4

Table 5. *(Continued)*

h k l	F_o	F_c	h k l	F_o	F_c	h k l	F_o	F_c	h k l	F_o	F_c	h k l	F_o	F_c
3 -2 -3	45.1	40.9	6 -5 -3	104.3	105.0	2 -20 4	31.4	-26.6	0 13 -4	37.3	36.7	3 -1 -4	48.9	47.4
-3	25.5	-24.3	-6	39.7	-42.9	3 0 4	14.5	-13.2	14	49.1	53.3	-2	16.8	-16.4
-4	3.0	4.3	-7	20.8	-23.2	1	5.9	- 6.2	15	7.7	- 4.9	-3	32.6	-28.8
-5	20.9	19.3	-8	27.4	31.7	2	26.9	-25.5	16	24.5	-28.4	-4	25.3	24.3
-6	49.9	-48.7	-9	9.7	13.7	3	57.1	56.2	17	4.6	1.3	-5	14.1	13.5
-7	6.3	- 8.1	0 0 4	23.1	-20.0	4	54.9	-56.3	18	29.9	35.7	-6	45.4	47.1
-8	34.8	35.8	1	12.4	12.7	5	8.4	1.7	19	20.0	-30.0	-7	36.7	-37.0
-9		- 2.5	2	33.7	30.6	6	19.7	19.7	20	6.5	6.4	-8	15.4	16.4
-10	53.1	-53.5	3		-15.1	7	25.5	-21.8	1 0 -4	79.6	77.0	-9		25.9
-11	44.1	45.2	4	9.8	- 3.6	8	42.7	39.0	1	34.4	31.9	-10	30.0	-29.6
-12	17.1	14.5	5	39.2	38.7	9	8.4	- 2.7	2	18.1	-16.0	-11	11.1	9.0
-13	31.4	-33.3	6	2.6	5.9	10	31.7	-27.7	3	18.4	-13.6	-12	26.9	-29.3
-14	1.7	2.1	7	6.3	5.7	11	20.5	18.8	4	67.5	68.7	-13	9.6	15.3
-15	11.2	-10.6	8	55.7	55.6	12	39.3	40.9	5	47.5	-48.1	-14	10.3	- 8.9
-16	10.0	10.0	9	23.1	22.1	13	24.9	-29.3	6	32.8	32.2	-15	24.2	23.5
-17	23.3	23.9	10	44.0	-44.1	-1	1.1	0.3	7	62.7	65.7	-16	3.4	5.8
-18	7.8	- 4.6	11	34.9	32.9	-2	21.4	21.8	8	70.5	-70.8	-17	5.8	3.8
-19	13.3	-15.7	12	34.1	29.2	-3	1.3	1.5	9	27.9	27.7	-18	18.8	18.2
4 0 -3	23.8	21.1	13	21.5	-19.7	-4	39.0	37.2	10	76.8	79.8	4 0 -4	30.2	-29.2
1	6.5	4.1	14	37.9	-41.1	-5	60.0	-60.9	11	21.6	-18.3	1	23.3	22.2
2	2.9	- 2.4	15	25.1	27.8	-6	7.5	4.5	12	15.1	-15.6	2	17.5	17.5
3	24.6	25.1	16	8.2	13.1	-7	39.4	41.0	13	16.1	12.5	3	14.2	-15.1
4	9.4	- 7.9	17	2.7	- 1.3	-8	22.5	-23.0	14	11.5	8.6	4	16.2	12.9
5	23.2	-22.5	18	10.5	12.2	-9		-16.2	15	7.6	- 7.2	5	43.1	-46.5
6	50.2	49.9	1 0 4	17.1	13.5	-10	3.1	9.3	16	34.6	35.8	6	44.9	48.9
7	24.2	-25.3	1		75.7	-11	43.3	42.0	17	16.5	-18.3	7	16.6	13.0
8	2.8	0.5	2	32.2	-38.3	-12	5.0	- 9.0	18	12.5	-11.7	8	43.8	-43.1
9	7.6	- 8.0	3	41.8	-48.7	-13	6.2	0.4	19	30.4	27.4	9	2.1	- 5.4
10	18.3	18.9	4	98.3	124.0	-14	6.3	5.2	-1	44.8	-44.0	10	22.8	20.6
11	14.7	14.2	5	8.9	-13.6	-15	14.8	-14.7	-2	8.5	- 6.2	11	8.8	5.8
12	11.2	- 8.9	6	42.9	-54.4	-16	2.7	- 2.0	-3	3.3	- 3.0	12	13.2	-14.2
13	2.3	5.6	7	24.3	27.4	-17	8.3	-10.8	-4	28.2	-23.6	13	37.7	39.5
14	3.9	- 5.6	8	2.8	- 1.7	4 0 4	7.5	10.7	-5	73.0	70.2	14	26.4	-29.2
15	23.1	25.1	9	5.5	5.8	1	50.8	49.7	-6	16.0	12.9	-1	50.2	-51.7
-1	27.2	27.0	10	7.1	- 0.4	2	51.6	-49.1	-7	37.6	-38.3	-2	31.8	31.0
-2	67.8	-68.8	11		- 5.1	3	32.6	-31.8	-8	30.8	30.6	-3	43.2	46.0
-3	44.6	46.1	12		-18.3	4	85.1	84.7	-9	71.2	69.6	-4	53.7	-57.9
-4	51.5	54.5	13	26.1	42.5	5	18.7	-18.5	-10	2.8	1.9	-5	45.3	47.0
-5	36.4	-37.8	14	2.8	4.3	6	19.4	-20.6	-11	38.3	-37.9	-6	59.9	61.4
-6	40.7	42.5	15	16.6	-31.8	7	26.4	28.7	-12	36.5	39.5	-7	72.3	-76.7
-7	2.9	- 2.9	16	5.3	23.5	8	4.6	- 1.3	-13	13.2	-14.8	-8	29.0	28.9
-8		9.1	17	6.4	-18.0	9	2.4	- 5.7	-14	24.1	28.3	-9	34.5	33.3
-9	13.8	11.9	18	5.1	- 8.1	10	20.0	21.1	-15	3.0	11.6	-10	20.6	-21.4
-10	12.7	-12.3	-1	16.7	-15.6	-1	16.8	17.2	-16	4.3	-12.1	-11	35.1	-37.1
-11	15.7	-13.4	-2	53.3	56.8	-2	35.3	-34.1	-17	20.7	19.0	-12	8.5	13.3
-12	2.8	3.9	-3	9.4	11.2	-3	10.8	-11.8	-18	6.2	-10.7	-13	25.1	23.2
-13	28.1	28.5	-4	76.9	-79.6	-4	9.2	- 1.7	-19	8.8	9.3	-14	2.5	- 5.8
-14	33.9	-39.1	-5	89.6	92.8	-5	24.9	27.1	2 0 -4	37.1	-37.8	-15	9.3	9.8
-15	22.3	24.3	-6	28.8	-26.4	-6	4.1	- 3.8	1	71.2	-67.6	-16	19.2	-21.3
-16	31.5	32.9	-7	43.5	-44.9	-7	46.9	-46.5	2	100.3	95.6	5 0 -4	18.7	-20.0
-17	44.9	-50.3	-8	56.7	55.1	-8	57.2	54.5	3	50.7	51.2	1	36.4	-36.4
5 0 -3	2.8	4.2	-9	10.3	-10.1	-9	6.0	2.5	4	82.5	-82.4	2		44.6
1	53.0	-53.9	-10	8.3	- 8.8	-10	23.7	-23.5	5	69.4	65.3	3		- 9.1
2	19.4	17.7	-11	48.5	46.0	-11	46.9	47.4	6	3.7	1.3	4	24.4	-24.7
3	54.0	51.1	-12	3.3	6.3	-12	22.2	-21.7	7	6.1	3.3	5	14.5	12.5
4	2.8	- 1.5	-13	30.1	-28.2	-13	32.9	-32.7	8	32.0	30.1	6	4.2	0.3
5	21.0	-20.6	-14	15.8	13.2	-14	21.1	19.2	9	15.7	-14.4	7	10.8	15.9
6	32.1	31.7	-15	23.7	20.9	5 0 4	7.9	14.6	10	13.2	-11.5	8	8.3	4.0
7	17.3	18.1	-16	35.2	-32.3	1	4.1	- 7.6	11	4.8	4.2	9	25.5	25.9
8	3.3	1.4	-17	32.1	33.3	2	47.2	46.5	12	33.2	30.4	10	12.5	-14.9
9	10.9	13.0	-18	20.0	16.3	3	6.4	- 6.8	13	8.8	-11.9	11	2.7	3.8
10	37.6	-39.8	-19	17.4	-18.5	4	7.5	14.1	14	6.0	4.0	12	9.6	10.2
11	15.0	14.5	-20	13.6	8.8	5	2.7	- 3.8	15	20.3	-15.3	13	2.7	- 2.2
12	43.6	51.2	2 0 4		73.2	6	9.1	9.6	16	21.5	-18.9	14	10.6	10.9
13	22.3	-22.7	1	2.9	- 3.4	7	10.4	18.7	17	54.5	50.7	-1	22.9	22.0
14	2.7	4.9	2	9.8	20.3	8	10.8	-17.0	18	27.4	-26.1	-2	30.7	31.9
-1	5.5	- 6.9	3	8.8	-12.6	-1	11.5	-15.1	19	2.4	- 5.7	-3	13.5	-11.4
-2	4.2	- 1.2	4		-28.4	-2	33.8	-33.3	-1	102.7	98.9	-4	13.6	-11.5
-3	47.7	50.0	5		43.1	-3	38.6	39.5	-2	2.9	2.9	-5	6.0	- 4.7
-4	5.2	- 6.6	6		-37.0	-4	24.1	23.1	-3	60.1	-58.2	-6	25.7	-28.5
-5		- 4.5	7	6.4	-20.8	-5	13.9	-12.1	-4	81.9	77.2	-7	70.2	74.1
-6	33.0	35.7	8	10.6	23.9	-6	28.6	-26.1	-5	7.1	- 6.7	-8	36.0	-37.3
-7	15.7	15.0	9	24.0	-25.2	-7	42.0	40.2	-6	63.9	-60.5	-9		-29.3
-8	21.3	19.2	10	13.3	14.0	-8	23.4	25.8	-7	48.4	46.0	-10	59.2	66.1
-9	11.9	-13.4	11	14.0	14.7	-9	33.5	-35.6	-8	4.9	- 4.8	-11	14.2	-17.0
-10	5.3	3.4	12	12.5	13.1	-10	8.0	11.1	-9	10.3	- 8.2	-12	9.6	- 3.2
-11	14.7	-14.3	13		-30.3	-11	22.8	-21.6	-10	38.6	40.0	-13		14.0
-12	33.8	38.2	14	4.6	3.7	-12	13.4	15.0	-11	13.0	-10.1	-14	5.0	- 1.5
-13	11.2	7.3	15		18.0	-13	22.1	20.5	-12	2.8	- 1.5	-15	31.3	-36.4
-14	20.0	-21.6	16	7.1	7.4	-14	12.4	-18.7	-13	65.2	59.1	-16	30.2	33.8
-15	7.0	12.7	17	9.6	- 1.4	6 0 4	32.5	31.8	-14	2.8	- 3.3	-17	17.1	22.0
-16	3.8	4.0	-1	17.1	-23.1	1	43.3	-42.6	-20	5.6	5.9	6 0 -4	4.2	0.6
-17	16.9	21.0	-2		-41.7	2	6.2	9.6	3 0 -4	37.4	-38.3	1	10.2	8.7
-18	6.7	1.3	-3	3.9	4.3	3	34.6	33.0	1	31.9	31.0	2	25.8	26.9
6 0 -3	20.3	22.1	-4		55.4	4	31.6	-32.8	2	1.9	3.1	3	5.8	- 9.1
1	7.7	4.8	-5	39.2	-49.3	5	19.5	21.1	3	11.5	11.2	4	36.1	-38.5
2	14.4	-16.5	-6	2.9	- 0.7	6	3.6	4.5	4	16.4	-14.8	5	66.8	70.2
3	18.2	-16.3	-7	71.7	84.1	7	19.0	-16.8	5	40.4	40.3	6	10.1	10.7
4	50.5	52.3	-8	48.5	-56.3	0 1 -4	32.2	32.7	6	31.1	30.9	7	34.5	-36.1
5	19.3	17.2	-9	6.7	5.9	2	3.0	1.3	7	56.7	-57.3	8	25.1	25.9
6	64.7	-66.6	-10	58.1	66.2	3	42.1	40.3	8	4.6	6.8	9	7.0	8.7
7	63.5	66.4	-11	39.7	-45.1	4	18.6	18.9	9	1.4	- 0.3	10	2.7	- 4.4
8	8.2	8.6	-12	18.5	-21.9	5	13.1	-12.1	10	9.5	- 3.7	11	6.2	6.2
9	19.5	-17.7	-13	3.4	2.0	6	31.6	31.3	11	9.3	- 8.6	-1	6.0	- 6.1
10	40.0	42.7	-14	21.4	21.1	7	21.5	-20.8	12	12.4	-13.4	-2	2.0	- 5.0
11	7.1	- 3.0	-15	2.8	- 4.7	8	6.9	- 2.9	13	8.3	- 5.0	-3	2.8	4.8
-1	14.8	11.1	-16	16.5	20.2	9	9.2	- 6.7	14	22.4	24.0	-4	19.7	19.1
-2	41.8	40.2	-17	27.7	-27.4	10	11.5	11.2	15	32.3	34.3	-5	5.8	- 4.0
-3	61.2	-58.9	-18	8.9	- 5.9	11	41.8	44.5	16	37.8	-38.5	-6	8.9	9.2
-4	20.2	-22.0	-19	58.0	54.8	12	30.5	-28.9	17	14.8	11.7	-7	11.5	11.9

Table 5. *(Continued)*

h k l	F_o	F_c	h k l	F_o	F_c	h k l	F_o	F_c	h k l	F_o	F_c	h k l	F_o	F_c
0 0 5	56.2	-55.6	3 -4 5	23.5	21.5	1 -16 -5	7.2	- 7.6	5 0 -5	36.9	33.3	2 -5 6	6.4	- 2.6
1		61.4	-5	22.8	20.7	-17	14.8	-15.4	1	17.8	-20.0	-6	12.7	-13.2
2	58.4	55.1	-6	45.1	-44.8	-18	18.5	19.9	2	33.4	-30.6	-7	29.7	38.3
3	70.0	67.9	-7	35.0	35.6	2 0 -5	41.2	40.5	3	24.9	25.1	-8	6.7	- 7.0
4	23.5	-18.7	-8	45.4	46.6	1	36.0	-34.2	4	4.4	- 5.8	-9	17.6	-22.1
5	31.2	30.4	-9	24.0	-22.3	2	11.3	- 5.9	5	9.2	6.3	-10	30.9	36.9
6	3.9	3.0	-10	2.8	- 1.1	3	99.5	96.2	6	25.7	27.6	-11	7.2	7.6
7	17.1	-16.5	-11	10.8	10.8	4	29.0	-26.4	7	9.6	- 0.5	-12	2.7	0.7
8	20.1	19.4	-12	14.0	-13.6	5	31.1	27.7	8	19.4	-24.3	-13	2.7	- 0.9
9	21.0	-17.9	-13	9.6	10.7	6	43.1	43.9	9	45.9	51.6	-14	21.4	-23.3
10	36.4	33.8	-14	30.4	30.3	7	16.0	-15.6	10	8.6	- 6.3	-15	2.3	5.6
11	41.2	40.1	-15	45.6	-47.0	8	16.0	-17.3	11	35.5	-39.2	-16	22.4	24.8
12	46.2	-43.6	4 0 5	5.5	- 4.7	9	51.6	48.7	12	26.7	29.2	3 0 6	15.6	12.9
13	1.5	- 1.2	1	14.0	14.8	10	18.9	-18.0	-1	14.8	-14.0	1	9.5	- 2.7
14	13.2	13.2	2	18.6	-20.8	11	68.2	-59.9	-2	19.3	-19.5	2	19.9	19.9
15	10.6	-13.7	3	8.3	6.8	12	57.9	51.4	-3	29.9	31.0	3	2.7	0.4
16	5.6	- 6.1	4	22.7	25.2	13	31.8	29.0	-4	7.7	- 5.4	4	20.5	-19.3
17	20.5	22.1	5	7.6	1.5	14	34.9	-30.2	-5	21.7	-18.8	5	8.4	7.6
1 0 5	6.5	- 2.1	6	5.5	2.6	16	2.7	- 0.2	-6	32.3	36.9	6	2.7	4.2
1	2.8	- 3.0	-1	22.5	23.2	17	14.4	-10.1	-7	23.5	23.7	7	23.4	23.3
2	2.8	- 4.9	-2	1.5	- 3.1	18	10.3	10.6	-8	51.4	-53.1	-1	14.2	-12.8
3	24.3	27.9	-3	18.4	16.9	-1	30.9	-30.2	-9	22.0	18.4	-2	29.6	28.1
4	17.6	-19.3	-4	13.8	-16.7	-2	32.2	30.5	-10	16.9	13.3	-3	1.4	- 6.0
5	2.8	- 1.7	-5	17.6	-17.1	-3	44.6	43.2	-11	7.0	-10.0	-4	5.7	4.7
6	25.7	35.0	-6	50.8	48.5	-4	50.3	-49.5	-12	17.9	19.3	-5	42.3	39.1
7		- 6.6	-7	5.0	0.2	-5	6.4	1.3	-13	13.4	-15.8	-6	6.1	- 5.4
8	12.8	-16.0	-8	29.2	-28.1	-6	62.6	61.3	-14	2.7	1.3	-7	21.2	-22.6
9	19.9	27.7	-9	24.3	24.8	-7	24.0	22.8	-15	30.4	32.9	-8	23.4	23.4
10	10.0	-11.9	-10	26.1	28.1	-8	51.3	-50.5	6 0 -5	1.4	0.5	-9	28.0	29.1
11		- 8.6	-11	6.4	- 5.3	-9	23.2	19.6	1	29.9	29.4	-10	16.7	-21.2
12		- 5.3	5 0 5	32.5	32.1	-10	6.4	3.8	2	7.1	7.1	-11	8.8	- 9.4
13	9.0	9.5	1	9.0	8.6	-11	9.9	10.9	3		-26.8	-12	24.6	27.2
14		9.8	2	2.7	- 2.5	-12	2.8	- 0.6	4	13.1	10.7	0 1 -6	26.6	-25.9
15	19.5	-20.5	3	18.2	23.9	-13	17.2	-14.6	5	27.4	30.9	2	6.2	7.3
-1	2.8	1.8	4	5.4	-14.2	-14	7.2	10.2	6	21.9	-26.5	3	20.2	-20.5
-2	15.8	-15.4	-1	18.1	-17.4	-15	12.9	13.7	7	8.0	10.0	4	16.9	18.5
-3	48.8	55.4	-2	25.1	-24.8	-16	6.3	11.1	8	16.4	18.3	5	23.8	25.9
-4	2.8	- 0.3	-3	52.1	52.4	-17		1.6	9	20.6	-23.0	6	0.6	- 1.5
-5	47.7	-49.5	-4	9.1	- 9.3	-18	14.1	15.6	10	6.8	4.8	7	34.2	-33.9
-6	31.4	30.2	-5	18.8	-17.3	3 0 -5	43.2	-43.3	11	13.8	11.2	8	5.8	4.8
-7	5.7	-10.4	-6	31.2	29.1	1	86.2	86.8	-1	16.3	-17.8	9	41.9	44.6
-8	33.0	-34.9	-7	16.9	-16.6	2	31.6	30.8	0 0 6	55.3	54.3	10	45.4	-48.1
-9	28.0	27.1	-8	2.7	3.3	3	82.6	-82.6	1	26.5	-28.8	11	11.3	10.5
-10	11.3	-15.6	-9	19.9	18.3	4	35.1	35.2	2	49.8	-47.7	12	28.5	32.5
-11	24.0	-17.9	-10	6.3	7.0	5	39.0	38.9	3	34.2	28.7	13	36.1	-38.6
-12	32.1	32.9	6 0 5	33.8	-34.3	6	12.9	-12.4	4	6.8	7.2	14	22.6	23.9
-13	31.5	29.9	1	12.4	13.7	7	29.2	-29.2	5	8.8	- 4.3	15	23.9	25.3
-14	42.3	-41.4	2	28.4	27.8	8	27.9	25.5	6	5.1	0.5	16	9.7	-10.2
-15		15.6	0 1 -5	29.8	27.2	9	12.7	-12.0	7	38.5	36.1	1 0 -6	2.8	- 4.3
-16	6.4	2.8	2	11.0	9.2	10	28.4	30.8	8	2.7	6.0	1	35.9	36.4
-17	17.1	-17.2	3	59.0	-58.4	11	21.1	21.0	9	26.4	-27.7	2	15.9	-15.3
-18	34.3	32.6	4	23.8	24.0	12	42.7	-43.9	10	29.3	27.1	3	15.6	14.0
2 0 5		58.4	5		10.3	13	17.1	15.3	11	2.4	4.3	4	13.0	14.7
1	4.7	-13.6	6	32.4	-33.5	14	6.2	8.0	12	9.6	- 9.0	5	7.6	4.8
2	6.0	- 7.1	7	5.7	- 4.3	15	6.4	- 1.9	13	13.9	-13.5	6	36.5	-38.0
3	2.8	3.5	8	46.1	46.8	-1	36.6	37.2	14	10.4	15.3	7	59.4	57.0
4	9.5	-19.0	9	6.6	- 7.3	-2	26.3	24.9	15	14.4	19.0	8	2.3	- 5.6
5	5.0	8.6	10	13.9	15.1	-3	52.7	-50.5	1 0 6	2.8	0.3	9	45.4	-45.7
6		20.7	11	21.6	19.3	-4	35.1	38.4	1		55.2	10	41.1	39.6
7	2.8	- 2.4	12	37.2	-36.0	-5	52.9	54.0	2	32.6	-38.2	11	12.8	-11.3
8		-38.3	13	13.2	8.9	-6	33.5	-34.1	3	31.2	39.2	12	8.6	5.9
9		44.0	14	45.7	48.6	-7	2.9	0.4	4	24.6	31.1	13	20.9	20.8
10		17.2	15	32.8	-35.7	-8	51.8	54.1	5		-61.0	14	25.3	-24.2
11		-54.6	16	6.7	4.2	-9	28.5	-25.8	6		21.6	15	4.2	- 6.1
12		34.2	17	17.0	21.5	-10	9.8	11.8	7	24.8	32.7	-1	68.0	-69.2
13	9.6	- 2.1	18	12.7	-14.6	-11	33.8	32.5	8		-17.3	-2	42.7	44.0
14	10.5	-17.1	1 0 -5	29.0	26.3	-12	48.1	-47.2	9	11.3	-11.9	-3	5.6	5.9
-1		-16.3	1	11.1	12.5	-13	12.5	4.5	10	4.3	34.6	-4	19.3	-18.6
-2	9.2	11.1	2	28.5	27.1	-14	37.4	36.7	-1	18.4	-19.9	-5	7.0	6.8
-3	19.2	23.5	3	3.1	6.5	-15	5.4	- 1.7	-2	15.0	17.8	-6	28.4	-23.8
-4	14.0	-20.0	4	2.1	- 5.4	-16	14.6	-14.4	-3	2.8	- 1.5	-7	17.3	13.8
-5	2.8	3.6	5	31.5	32.2	4 0 -5	13.2	-12.8	-4	5.2	9.3	-8	20.2	21.4
-6	21.6	25.3	6	10.2	8.9	1	36.3	38.0	-5	8.5	3.0	-9	3.4	0.7
-7	17.3	-21.0	7	29.7	26.5	2	2.1	- 5.4	-6	17.5	-18.6	-10	42.1	-47.0
-8	28.3	-33.4	8	40.3	-43.5	3	35.0	-38.4	-7	17.5	-17.3	-11	27.0	29.8
-9	29.8	35.6	9	7.1	2.1	4	33.4	33.6	-8	36.1	37.4	-12	30.7	32.8
-10	10.0	11.5	10	55.3	55.6	5	11.1	7.0	-9	10.2	13.6	-13	37.3	-42.4
-11	9.9	-13.4	11	14.9	-12.8	6	2.8	2.0	-10	39.6	-39.4	-14	19.3	25.2
-12	2.8	- 4.9	12	8.7	8.9	7	13.7	-15.7	-12	15.2	19.4	-15	2.7	3.9
-13	2.8	1.3	13	7.8	5.1	8	23.9	27.5	-13	18.8	17.6	2 0 -6	35.4	33.5
-14	11.5	8.3	14	11.1	13.8	9	2.8	- 1.3	-14	10.0	- 3.7	1	2.8	- 1.3
-15	2.7	- 3.6	15	8.7	- 8.6	10	23.9	-24.7	-15	10.9	-13.2	2	62.0	-63.5
-16	5.2	- 1.0	16	9.6	3.9	11	26.5	27.8	-16	5.2	5.5	3	65.2	63.1
-17	2.7	2.5	17	20.1	20.9	12	3.3	- 7.7	2 0 6	16.6	-17.4	4	22.9	22.3
-18	14.7	-13.6	18	25.2	-27.8	13	17.8	18.6	1		-52.9	5	13.7	-12.2
3 0 5	31.6	-29.0	-1	47.6	-47.2	-1	24.1	-24.7	2		69.6	6	22.7	-21.6
1	35.6	36.5	-2	17.1	-18.7	-2	6.5	- 3.8	3	10.0	10.5	7	22.4	-19.5
2	50.5	49.4	-3	22.1	20.5	-3	60.1	65.6	4		-25.2	8	62.6	61.2
3	17.9	-22.2	-4	16.4	15.3	-4	1.8	- 1.5	5	5.0	9.8	9	18.7	-17.5
4	15.5	-16.6	-5	20.7	-21.9	-5	14.9	-16.7	6	13.8	14.6	10	3.2	- 8.3
5	35.9	35.2	-6	29.1	23.9	-6	23.1	23.3	7	7.7	- 8.1	11	6.6	- 7.0
6	23.4	-24.5	-7	10.6	6.8	-7	3.0	- 3.0	8	6.6	7.0	12	2.7	3.9
7	5.0	- 3.5	-8	15.6	-13.5	-8	26.7	28.9	9	10.8	11.4	13	13.6	14.4
8	25.0	22.6	-9	32.8	29.5	-9	10.8	- 9.3	10	14.7	-15.5	14	13.3	-12.7
9	31.1	-30.3	-10	9.9	8.2	-10	6.5	11.6	11	22.9	24.1	15	19.5	17.5
10	16.0	14.4	-11	31.0	-27.8	-11	12.8	- 9.8	12	3.1	- 6.6	-1	53.5	53.2
11	26.9	30.8	-12	20.4	20.6	-12	23.6	24.8	-1		99.2	-2	27.4	-22.4
-1	24.6	-27.6	-13	8.6	9.0	-13	10.8	12.6	-2		-16.7	-3	40.4	-40.1
-2	40.6	38.2	-14	6.9	5.9	-14	14.3	-16.3	-3	12.6	-16.4	-4	34.2	31.9
-3	24.2	-24.5	-15	9.6	9.4	-15	6.7	9.3	-4	14.0	16.9	-5	24.0	-20.9

Table 5. *(Continued)*

h k l	F_o	F_c	h k l	F_o	F_c	h k l	F_o	F_c	h k l	F_o	F_c	h k l	F_o	F_c
2 -6 -6	2.8	2.8	5 -5 -6	12.7	17.1	2 -11 7	32.5	43.9	3 1 -7	2.8	- 2.9	1 -2 8	18.4	21.9
-7	23.6	21.2	-6	7.4	6.2	3 0 7	5.0	8.7	2	48.4	46.5	-3	19.8	-24.6
-8	21.9	-20.3	-7	7.3	6.4	-1	7.2	- 2.5	3	20.9	-19.7	-4	2.7	2.5
-9	11.5	- 6.3	-8	19.6	-20.9	-2	19.8	20.7	4	2.8	3.5	-5	6.2	6.5
-10	24.8	27.1	-9	21.3	25.0	-3	28.3	-28.7	5	21.8	-22.0	-6	2.5	5.2
-11	15.5	10.7	-10	14.2	14.1	-4	0.8	- 8.0	6	9.0	9.4	-7	2.7	1.0
-12	33.5	-33.0	-11	6.3	1.0	-5	44.0	43.9	7	23.2	20.6	-8	26.9	-30.3
-13	14.9	10.8	-12	9.9	-11.2	0 1 -7	1.9	3.1	8	21.4	-19.6	2 0 8	43.8	-46.1
-14	13.1	-17.5	-13	2.3	5.5	2	42.2	41.3	9	13.5	-12.3	1	13.9	14.7
-15	3.0	5.4	6 0 -6	4.7	3.3	3	7.9	- 4.9	10	5.7	4.6	2	36.4	38.3
-16	26.2	25.3	1	35.9	-37.9	4	11.1	-13.7	11	16.9	18.0	-1	22.5	23.7
3 0 -6	14.6	13.1	2	27.8	30.5	5	10.4	8.0	-1	14.0	14.5	-2	8.4	8.8
1	23.3	-23.1	3	23.5	24.1	6	2.8	- 3.4	-2	6.3	- 1.0	-3	2.7	- 2.1
2	21.1	19.5	4	33.3	-37.5	7	17.2	18.7	-3	13.6	13.4	-4	7.6	8.0
3	8.2	- 1.2	5	9.8	11.3	8	4.2	1.6	-4	4.1	4.4	-5	14.1	-20.9
4	2.8	5.1	6	31.3	36.6	9	17.2	-18.5	-5	2.8	- 0.1	-6	2.7	0.2
5	11.1	5.2	7	24.5	-28.2	10	16.2	18.8	-6	14.6	-13.9	0 1 -8	24.2	-26.2
6	39.4	36.2	8	18.5	20.7	11	36.3	41.7	-7	12.8	16.4	2	27.6	25.7
7	31.6	-34.2	9	2.7	- 1.6	12	7.1	- 3.7	-8	31.2	32.6	3	27.6	29.6
8	9.2	14.8	10	15.4	-16.7	1 0 -7	37.6	-34.9	-9	36.0	-39.7	4	52.8	-51.1
9	16.0	17.4	0 0 7	14.1	- 8.7	1	6.0	- 7.3	-10	13.5	14.5	5	25.6	26.6
10	47.0	-49.2	1	27.4	25.0	2	23.3	21.8	-11	2.7	1.3	6	48.6	46.1
11	35.9	36.9	2	2.8	- 1.8	3	35.2	33.8	4 0 -7	13.0	-18.0	7	16.7	-18.4
12	21.2	22.2	3	43.9	-42.3	4	19.8	-20.9	1	28.9	-30.7	8	22.6	-25.9
13	37.5	-38.6	4	40.3	36.8	5	20.6	20.4	2	31.1	34.1	9	44.2	47.1
-1	32.8	32.3	5	27.1	24.4	6	19.5	-17.4	3	8.3	- 8.8	1 0 -8	40.4	-39.9
-2	68.9	-67.0	6	52.7	-49.4	7	23.0	23.9	4	17.9	-18.8	1	50.0	48.7
-3	31.4	31.9	7	28.4	28.0	8	34.1	32.4	5	33.5	35.6	2	2.7	- 2.0
-4	67.7	65.8	8	35.4	34.3	9	41.7	-44.8	-1	38.5	40.1	3	5.7	-13.1
-5	23.7	-21.5	9	27.3	-25.7	10	9.0	-13.1	-2	5.2	0.4	4	22.8	21.4
-6	10.6	10.3	10	33.0	33.8	11	28.1	28.7	-3	21.9	-19.9	5	10.9	18.2
-7	6.0	1.5	11	4.5	1.2	12	2.7	3.7	-4	7.7	- 9.3	6	15.1	- 9.6
-8	15.0	14.2	1 0 7		53.4	13	14.9	-18.7	-5	22.4	25.2	7	3.5	- 0.4
-9	5.3	- 5.5	1	10.3	-10.8	14	18.1	20.1	-6	13.6	-12.5	8	19.2	20.2
-10	5.6	0.6	2	11.4	-19.7	-1	13.5	17.1	-7	13.4	13.8	-1	6.1	6.5
-11	24.9	-24.3	3		45.9	-2	39.8	38.7	-8	2.2	5.4	-2	48.3	43.2
-12	11.4	13.7	4	19.2	-26.4	-3	22.5	-25.2	5 0 -7	18.7	20.4	-3	19.0	-17.3
-13	15.7	19.1	5	9.8	10.3	-4	10.2	8.3	1	6.7	7.3	-4	15.6	-13.8
-14	15.8	-16.2	6	21.5	35.8	-5	6.2	- 6.5	2	27.7	-27.8	-5	14.7	11.7
4 0 -6	9.1	11.0	7	24.2	-25.5	-6	12.4	- 2.3	3	28.6	32.2	-6	13.9	16.1
1	3.5	- 7.1	8	10.5	18.4	-7	18.9	17.8	4	7.3	- 2.7	-7	10.6	-11.0
2	24.0	-23.9	9	18.0	18.9	-8	6.5	- 6.8	5	16.4	-18.5	-8	11.4	15.6
3	3.2	5.0	10	16.8	-14.5	-9	15.3	16.9	6	31.2	37.0	2 0 -8	2.0	- 5.3
4	54.7	57.4	-1	6.9	-13.7	-10	20.1	-23.9	7	8.8	10.3	1	52.6	46.9
5	32.6	-35.6	-2	32.3	-36.6	-11	8.1	17.9	-1		-20.4	2	6.0	6.3
7	68.1	75.0	-3	22.2	28.2	-12	15.4	19.4	-2	7.5	7.9	3	29.0	-27.7
8	20.5	-23.9	-4	34.4	39.4	-13	2.4	- 5.6	-3	4.9	12.8	4	24.7	20.5
9	3.2	- 4.2	-5	33.9	-39.5	2 0 -7	39.3	32.7	-4	2.7	4.0	5	14.3	7.9
10	16.8	19.0	-6	15.9	20.2	1	1.4	2.2	-5	2.7	- 0.9	6	5.2	6.9
-1	12.6	-13.6	-7	10.6	13.9	2	51.8	-46.5	-6	18.1	21.5	7	16.4	-15.4
-2	34.7	32.7	-8	18.7	-20.5	3	43.2	38.0	-7	23.7	-25.2	8	2.7	0.6
-3	16.1	15.3	-9	22.9	25.4	4	15.2	14.4	-8	8.4	-16.8	9	7.4	- 7.8
-4	33.9	-32.1	-10	9.0	11.5	5	37.3	-33.9	-9	35.7	38.5	10	17.6	16.6
-5	47.2	47.4	-11	28.0	-27.5	6	44.8	38.7	6 0 -7	12.9	-12.6	-1	12.6	-13.8
-6	2.8	- 2.5	-12	10.8	10.2	7	3.5	- 0.7	1	4.0	- 3.1	-2	2.7	1.3
-7	13.1	- 9.5	-13	26.6	30.2	8	29.0	-26.9	2	11.4	16.6	-3	13.9	13.7
-8	38.6	40.2	2 0 7	2.7	- 2.5	9	9.3	8.2	3	7.0	7.3	-4	7.4	- 6.0
-9	8.3	-11.2	1	2.7	- 2.6	10	23.9	22.2	4	2.7	- 3.6	-5	10.5	13.8
-10	30.0	-30.2	2	5.2	0.8	11	26.8	-27.2	5	2.7	0.2	-6	24.3	22.2
-11	36.4	38.2	3	9.6	10.1	12	14.1	-14.2	6	11.2	13.9	-7	23.3	-23.0
-12	24.2	28.7	4	15.2	16.0	13	12.6	13.3	7	9.0	-12.7	-8	15.8	14.7
5 0 -6	21.7	22.4	5	2.7	3.8	14	2.7	- 3.1	0 0 8	17.5	14.8	-9	6.6	9.5
1	7.5	- 9.1	6	11.2	-11.8	-1	14.0	-10.9	1	18.4	-16.0	3 0 -8	21.9	21.5
2	10.0	- 9.5	7	2.7	3.9	-2	6.3	- 5.0	2		- 6.6	1	42.1	-46.1
3	28.4	29.3	8	8.6	9.1	-3	2.0	6.0	3	19.3	17.7	2	14.6	14.3
4	3.8	4.5	9	10.5	11.1	-4	2.8	- 1.4	4	7.8	14.6	3	19.0	22.6
5	8.4	- 8.9	-1	4.0	12.8	-5	8.8	9.7	5	6.9	-11.0	4	24.3	-28.3
6	2.7	3.8	-2	2.7	4.3	-6	45.4	42.6	6	6.8	4.9	5	11.0	8.6
7	18.7	21.4	-3	13.0	13.7	-7	43.3	-39.0	7	14.3	12.5	6	7.1	9.7
8	6.9	- 7.3	-4	12.8	13.5	-8	3.0	-13.9	1 0 8	15.2	15.7	-1	2.7	2.5
9	7.4	- 7.8	-5	8.7	- 9.2	-9	47.2	43.3	1	2.7	3.8	-2	14.0	-13.0
10	29.4	34.6	-6	15.8	-16.6	-10	30.2	-29.0	2	2.7	- 3.7	-3	37.8	39.9
-1	18.5	22.1	-7		31.0	-11	4.1	-10.8	3	2.7	- 3.4	-4	2.7	3.4
-2	10.4	-11.4	-8		14.3	-12	10.1	12.9	4	11.0	-14.7	-5	27.4	-27.3
-3	23.7	-26.0	-9	23.3	-37.5	-13	5.2	- 1.5	5	13.2	13.9	-6	8.4	15.1
-4	9.2	12.5	-10	19.5	-12.4	3 0 -7	36.6	-39.3	-1	9.1	- 7.8			

Description of the structure

The Mg and Fe atoms are surrounded octahedrally by six oxygen atoms; the sulfur atoms are surrounded tetrahedrally by four oxygen atoms. The average interatomic distances are quite normal: 2.07 A for Mg—O, 2.01 Å for Fe^{3+}—O, and 1.47 A for S—O. The interatomic distances and angles are compiled in Table 6.

The sulfate tetrahedra and the coordination octahedra of Fe are connected to form one-dimensional, infinite complexes along [101]. Within a complex, two Fe octahedra are directly connected by a com-

Table 6. *Interatomic distances and angles in copiapite*

Atoms			Distances			Angles
A	*B*	*C*	*B—A*	*B—C*	*A—C*	*A—B—C*
O(16)*w*	Mg	O(18)*w*	2.08 ± .01 Å	2.06 ± .01 Å	2.91 ± .02 Å	89.3 ± .4°
O($\overline{16}$)*w*		O(18)*w*	2.08	2.06	2.94	90.7
O(16)*w*		O(20)*w*	2.08	2.06	2.90	88.8
O($\overline{16}$)*w*		O(20)*w*	2.08	2.06	2.96	91.2
O(18)*w*		O(20)*w*	2.06	2.06	2.89	89.0
O($\overline{18}$)*w*		O(20)*w*	2.06	2.06	2.94	91.0
O(3)	Fe(1)	O(7)	1.98 ± .01 Å	2.04 ± .01 Å	2.78 ± .02 Å	87.6 ± .4°
O(3)		O(12)	1.98	1.98	2.75	88.1
O(3)		O(14)*w*	1.98	2.06	2.87	90.8
O(3)		O(15)*w*	1.98	2.04	2.80	88.3
O(13)*h*		O(7)	1.95	2.04	2.87	92.2
O(13)*h*		O(12)	1.95	1.98	2.87	94.0
O(13)*h*		O(14)*w*	1.95	2.06	2.82	89.3
O(13)*h*		O(15)*w*	1.95	2.04	2.81	89.6
O(7)		O(15)*w*	2.04	2.04	2.83	87.9
O(7)		O(12)	2.04	1.98	2.90	92.7
O(14)*w*		O(12)	2.06	1.98	2.88	91.0
O(14)*w*		O(15)*w*	2.06	2.04	2.85	88.3
O(1)	Fe(2)	O(5)	2.00 ± .01 Å	1.99 ± .01 Å	2.68 ± .02 Å	84.4 ± .4°
O(1)		O(10)	2.00	2.00	2.76	87.3
O(1)		O(17)*w*	2.00	2.04	2.84	89.5
O(1)		O(19)*w*	2.00	1.99	3.04	99.1
O(13)*h*		O(5)	1.96	1.99	2.77	89.1
O(13)*h*		O(10)	1.96	2.00	2.86	92.6
O(13)*h*		O(17)*w*	1.96	2.04	2.85	90.7
O(13)*h*		O(19)*w*	1.96	1.99	2.73	87.4
O(10)		O(5)	2.00	1.99	2.89	93.1
O(10)		O(19)*w*	2.00	1.99	2.87	92.1
O(17)*w*		O(5)	2.04	1.99	2.77	86.8
O(17)*w*		O(19)*w*	2.04	1.99	2.81	88.2
O(1)	S(1)	O(2)	1.50 ± .01 Å	1.45 ± .01 Å	2.37 ± .02 Å	107.0 ± .5°
O(1)		O(3)	1.50	1.49	2.38	105.9
O(1)		O(4)	1.50	1.45	2.43	110.7
O(2)		O(3)	1.45	1.49	2.40	109.4
O(2)		O(4)	1.45	1.45	2.43	113.1
O(3)		O(4)	1.49	1.45	2.41	110.4
O(5)	S(2)	O(6)	1.48 ± .01 Å	1.46 ± .01 Å	2.40 ± .02 Å	109.1 ± .5°
O 5)		O(7)	1.48	1.49	2.44	110.3
O 5)		O(8)	1.48	1.46	2.37	107.8
O(6)		O(7)	1.46	1.49	2.41	109.6
O(6)		O(8)	1.46	1.46	2.40	110.7
O(7)		O(8)	1.49	1.46	2.40	109.3

Table 6. *(Continued)*

Atoms			Distances			Angles
A	*B*	*C*	*B—A*	*B—C*	*A—C*	*A—B—C*
O(9)	S(3)	O(10)	1.47 ± .01 Å	1.48 ± .01 Å	2.41 ± .02 Å	109.4 ± .5°
O(9)		O(11)	1.47	1.46	2.41	110.5
O(9)		O(12)	1.47	1.50	2.41	108.6
O(10)		O(11)	1.48	1.46	2.41	110.0
O(10)		O(12)	1.48	1.50	2.42	108.9
O(11)		O(12)	1.46	1.50	2.42	109.4

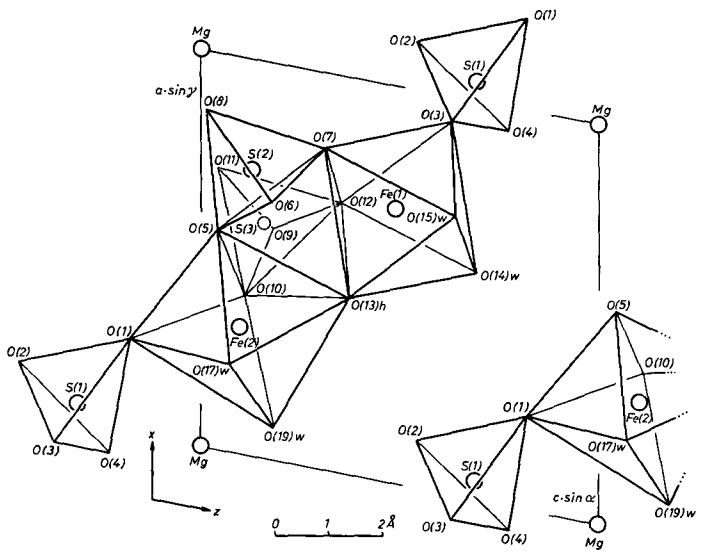

Fig. 1. The one-dimensional infinite octahedra-tetrahedra complexes in copiapite

mon oxygen atom and are also linked by two sulfate tetrahedra, as shown in Fig. 1. These groups of two tetrahedra and two octahedra are connected through a third tetrahedron to form the infinite complexes. The coordination octahedra of Mg lie between the complexes.

Oxygen chemistry and hydrogen bonding

A differential Fourier synthesis was used to locate the hydrogen atoms, but the results were highly inaccurate. It was, however, possible to determine probable hydrogen positions indirectly by finding the system of hydrogen bonds.

Of the twenty-three oxygen atoms in the structure, twelve belong to sulfate groups. They are potential acceptors of hydrogen bonds,

Table 7. *Distances and angles of hydrogen bonds in copiapite*

Acceptor *A*	Donor *B*	Acceptor *C*	Distances		Angles
			B—*A*	*B*—*C*	*A*—*B*—*C*
O(22)*w*	O(13)*h*		2.77 ± .02 Å		
O(1)	O(14)*w*	O(11)	2.99	2.75 ± .02 Å	80.2 ± .4°
O(8)	O(15)*w*	O(22)*w*	2.69	2.75	113.1
O(9)	O(16)*w*	O(21)*w*	2.92	2.81	102.9
O(6)	O(17)*w*	O(8)	2.71	2.66	98.7
O(21)*w*	O(18)*w*	O(23)*w*	2.82	2.82	95.3
O(2)	O(19)*w*	O(11)	2.68	2.69	102.2
O(4)	O(20)*w*	O(9)	2.93	2.97	101.4
O(2)	O(21)*w*	O(23)*w*	2.90	2.84	121.9
O(6)	O(22)*w*	O(7)	2.72	3.10	119.0
O(6)	O(22)*w*	O(17)*w*	2.72	3.04	157.0
O(4)	O(23)*w*	O(9)	2.84	2.90	110.2

especially those which are bound only to sulfur. Of the remaining eleven oxygen atoms, ten are oxygen atoms of water molecules and one is an hydroxyl oxygen. O(13), the only oxygen atom bound to two Fe atoms, is most likely the hydroxyl oxygen. The oxygen chemistry is assumed to be as follows: O(1) to O(12) are oxygen atoms of sulfate groups. O(2), O(4), O(6), O(8), O(9), and O(11) are bound only to sulfur; O(1), O(3), O(5), O(7), O(10), and O(12) are bound to sulfur and iron. O(13) is the hydroxyl oxygen. O(14) to O(23) are oxygen atoms of water

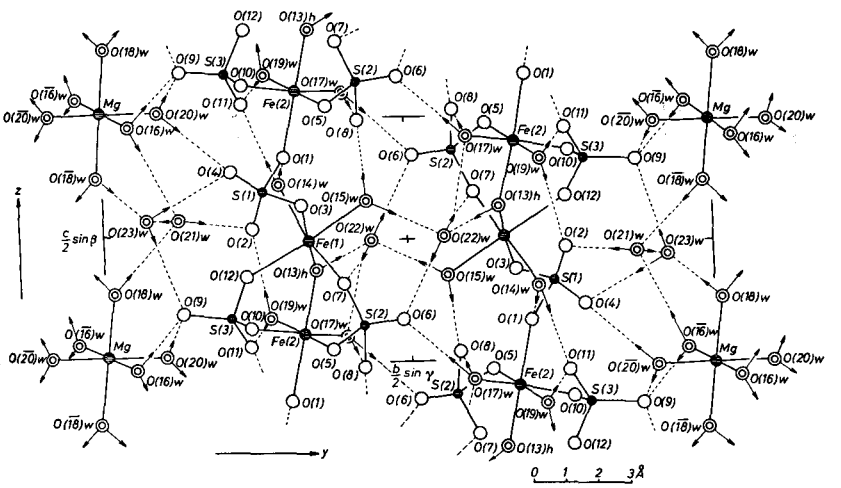

Fig. 2. The structure of copiapite projected along the *a* axis

Table 8. *Distances and angles about* O(21)w, O(22)w, and O(23)w

Atoms			Distances		Angles
A	*B*	*C*	*B—A*	*B—C*	*A—B—C*
O(2)	O(21)w	O(16)w	2.90 ± .02 Å	2.81 ± .02 Å	111.3 ± .04°
O(2)		O(18)w	2.90	2.82	112.9
O(2)		O(23)w	2.90	2.84	121.9
O(16)w		O(18)w	2.81	2.82	115.4
O(16)w		O(23)w	2.81	2.84	103.2
O(18)w		O(23)w	2.82	2.84	90.9
O(6)	O(22)w	O(7)	2.72	3.10	119.0
O(6)		O(13)h	2.72	2.77	124.6
O(6)		O(15)w	2.72	2.75	86.5
O(7)		O(13)h	3.10	2.77	108.1
O(7)		O(15)w	3.10	2.75	100.6
O(13)h		O(15)w	2.77	2.75	112.8
O(17)w		O(6)	3.04	2.72	157.0
O(17)w		O(13)h	3.04	2.77	58.6
O(17)w		O(15)w	3.04	2.75	72.7
O(4)	O(23)w	O(9)	2.84	2.90	110.2
O(4)		O(18)w	2.84	2.82	91.3
O(4)		O(21)w	2.84	2.84	118.5
O(9)		O(18)w	2.90	2.82	124.6
O(9)		O(21)w	2.90	2.84	90.7
O(18)w		O(21)w	2.82	2.84	123.5

molecules. O(14), O(15), O(17), and O(19) are bound to iron; O(16), O(18), and O(20) are bound to magnesium; and O(21), O(22), and O(23) are not bound to cations. The hydroxyl oxygen will be referred to as O(13)h and the oxygen atoms of water molecules as O(14)w, O(15)w, etc.

The temperature coefficients and corresponding root-mean-square amplitudes of the oxygen atoms show a correlation to their bonding. They tend to be smaller for those sulfate oxygen atoms which are bound to iron than for those bound to sulfur only. A similar observation can be made for the hydroxyl and water oxygen atoms. Their temperature coefficients and root-mean-square amplitudes are smaller for the oxygen atoms which are bound to iron than for those bound to magnesium or to no cations.

The pairs of oxygen atoms between which hydrogen bonding is likely to take place were found by looking for proper bond angles and

oxygen-oxygen distances outside the cation polyhedra. The angles and distances between presumably hydrogen-bonded oxygen atoms are compiled in Table 7. The water oxygen atoms O(21)*w*, O(22)*w*, and O(23)*w* each receive and donate two hydrogen bonds. The coordination angles and distances about these three oxygen atoms are given in Table 8. There are three oxygen atoms that are possible acceptors of the two hydrogen bonds of O(22)*w*: O(6), O(7), and O(17)*w*. Bond-angle considerations suggest that O(6) receives one hydrogen bond, and O(7) and O(17)*w* receive the other.

A view of the whole structure is shown in Fig. 2. Hydrogen bonds are indicated by dashes. The arrows point to the acceptor oxygen atoms. The hydrogen atoms may be assumed to be located at or near the vertices of the arrows.

Bond lengths and valence balance

Some of the cation-anion distances deviate considerably from the mean values. These deviations may be explained electrostatically if a correlation is assumed between valence-bond strengths of all bonds between nearest neighbors. For the Fe—O, Mg—O, and S—O bonds, valence strengths were computed according to DONNAY and ALLMANN (1970). The correlation between hydrogen bond strength and O—H···O bond length was taken from ZACHARIASEN (1963). The total sum of bond strengths for each atom is given under the heading ΣQ. The sums are close to the ideal values of 2 for O^{2-}, 1 for OH^-, and 0 for H_2O, as required by PAULING's second rule (PAULING, 1929).

Although second-nearest neighbor interactions are ignored, these considerations explain most of the deviations from the mean bond lengths. For instance, the bond Fe(1)—O(14)*w* is relatively long because the sum of the bond strengths of the two hydrogen bonds of O(14)*w* is well below −0.50. In order to make the total sum of bond valences for O(14)*w* about equal to zero, the bond strength of Fe(1)—O(14)*w* must be less than 0.50, and consequently the bond length has to be longer than average. The short bond lengths of Fe(1) and Fe(2) to O(13)*h* and the tendency of S—O bonds to be shorter than average when the oxygen is bound to sulfur only can be similarly explained.

Conclusions

There are about thirty ferric sulfate minerals known in nature. The crystal structures of nine of them have been determined: jarosite (HENDRICKS, 1937), krausite (GRAEBER *et al.*, 1965), amarantite

(SÜSSE, 1968a), botryogen (SÜSSE, 1968b), roemerite (FANFANI *et al.*, 1970), ransomite (WOOD, 1970), parabutlerite (BORÈNE, 1970), coquimbite (FANG and ROBINSON, 1970), and copiapite. A common feature of all these structures is the connection of sulfate tetrahedra and coordination octahedra of ferric iron to complexes. There are isolated tetrahedra-octahedra complexes in roemerite and coquimbite; one-dimensional infinite complexes in parabutlerite, amarantite, botryogen, ranso-

Table 9. *The elect*

	Mg/2	Fe(1)	Fe(2)	S(1)	S(2)	S(3)	O(1)	O(2)	O(3)	O(4)	O(5)	O(6)	O(7)	O(8)	O(9)
Mg/2															
Fe(1)									− 0.54				− 0.45		
Fe(2)							− 0.50				− 0.51				
S(1)							− 1.40	− 1.57	− 1.43	− 1.57					
S(2)											− 1.47	− 1.54	− 1.43	− 1.54	
S(3)															− 1.54
O(1)			0.50	1.40											
O(2)				1.57											
O(3)		0.54		1.43											
O(4)				1.57											
O(5)			0.51		1.47										
O(6)					1.54										
O(7)		0.45			1.43										
O(8)					1.54										
O(9)						1.54									
O(10)			0.50			1.50									
O(11)						1.57									
O(12)		0.54				1.42									
O(13)*h*		0.59	0.55												
O(14)*w*		0.44					− 0.14								
O(15)*w*		0.46												− 0.26	
O(16)*w*	0.33														− 0.16
O(17)*w*			0.45									− 0.25		− 0.27	
O(18)*w*	0.34														
O(19)*w*			0.51					− 0.26							
O(20)*w*	0.34									− 0.16					− 0.15
O(21)*w*								− 0.17							
O(22)*w*												− 0.24	− 0.10		
O(23)*w*										− 0.19					− 0.17
ΣQ	1.01	3.02	3.02	5.97	5.98	6.03	− 2.04	− 2.00	− 1.97	− 1.92	− 1.98	− 2.03	− 1.98	− 2.07	− 2.02

mite, krausite, and copiapite; and two-dimensional infinite complexes in jarosite. The complexes are connected to each other only by hydrogen bonds or by large cations such as K^+. The physical properties of the crystal (habit, cleavage, etc.) correspond to the kind of octahedra-tetrahedra complex in the structures. Copiapite seems to make an exception. The crystals are tabular parallel to (010) rather than elongated along [101], the direction in which the one-dimensional infinite

balance in copiapite

O(12)	O(13)h	O(14)w	O(15)w	O(16)w	O(17)w	O(18)w	O(19)w	O(20)w	O(21)w	O(22)w	O(23)w	ΣQ
				− 0.33		− 0.34		− 0.34				− 1.01
− 0.54	− 0.59	− 0.44	− 0.46									− 3.02
	− 0.55				− 0.45		− 0.51					− 3.02
												− 5.97
												− 5.98
− 1.42												− 6.03
		0.14										2.04
							0.26		0.17			2.00
												1.97
								0.16			0.19	1.92
												1.98
					0.25					0.24		2.03
										0.10		1.98
			0.26		0.27							2.07
				0.16				0.15			0.17	2.02
												2.00
		0.23					0.26					2.06
												1.96
										− 0.22		0.92
												0.07
										− 0.23		− 0.03
									− 0.20			− 0.03
										0.12		0.05
									− 0.20		− 0.20	− 0.06
												− 0.01
												0.03
				0.20		0.20					− 0.19	0.04
	0.22		0.23		− 0.12							− 0.01
						0.20			0.19			0.03
− 1.96	− 0.92	− 0.07	0.03	0.03	− 0.05	0.06	0.01	− 0.03	− 0.04	0.01	− 0.03	0.00

complexes run. The cleavage is perfect parallel to (010) and imperfect parallel to ($\bar{1}01$). The reason for this must lie in the way the one-dimensional complexes are packed. In the [$\bar{1}01$] direction they are about 5.5 Å apart (center to center), while in the [010] direction the distance is about 9 Å, the wide gap being filled by the $Mg(H_2O)_6$ octahedra and the three water molecules not bound to cations. Hydrogen bonding in this direction takes place only via these intermediate groups, while in the direction [$\bar{1}01$] relatively strong hydrogen bonds directly connect the one-dimensional complexes. This accounts for the less perfect cleavage parallel to ($\bar{1}01$) compared with the perfect cleavage parallel to (010) as well as for the tabular habit of the crystals parallel to (010).

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References

L. G. BERRY (1947), Composition and optics of copiapite. Univ. Toronto Studies, Geol. Ser. **51**, 21—34.

JACQUES BORÈNE (1970), Structure cristalline de la parabutlérite. Bull. Soc. franç. Minéral. Cristallogr. **93**, 185—189.

GABRIELLE DONNAY and RUDOLF ALLMANN (1970), How to recognize O^{2-}, OH^-, and H_2O in crystal structures determined by X-rays. Amer. Mineral. **55**, 1003—1015.

L. FANFANI, A. NUNZI and P. F. ZANAZZI (1970), The crystal structure of roemerite. Amer. Mineral. **55**, 78—89.

J. H. FANG and PAUL D. ROBINSON (1970), Crystal structures and mineral chemistry of hydrated ferric sulfates. I. The crystal structure of coquimbite. Amer. Mineral. **55**, 1534—1540.

EDWARD J. GRAEBER, BRUNO MOROSIN and ABRAHAM ROSENZWEIG (1965), The crystal structure of krausite, $KFe(SO_4)_2 \cdot H_2O$. Amer. Mineral. **50**, 1929—1936.

STERLING B. HENDRICKS (1937), The crystal structure of alunite and the jarosites. Amer. Mineral. **22**, 773—784.

JAMES H. JOLLY and HELEN L. FOSTER (1967), X-ray diffraction data of alumino-copiapite. Amer. Mineral. **52**, 1220—1223.

G. LINCK (1889), Beitrag zur Kenntnis der Sulfate von Tierra amarilla bei Copiapó in Chile. Z. Kristallogr. **15**, 1—28.

CHARLES PALACHE, M. A. PEACOCK and L. G. BERRY (1946), Crystallography of copiapite. Univ. Toronto Studies, Geol. Ser. **50**, 9—26.

LINUS PAULING (1929), The principles determining the structure of complex ionic crystals. J. Amer. Chem. Soc. **51**, 1010—1026.

HEINRICH ROSE (1833), Über einige in Südamerika vorkommende Eisenoxydsalze. Ann. Physik **103**, 309—319.

P. SÜSSE (1968a), The crystal structure of amarantite, $Fe_2(SO_4)_2O \cdot 7H_2O$. Z. Kristallogr. **127**, 261—275.

P. SÜSSE (1968b), Die Kristallstruktur des Botryogens. Acta Crystallogr. B**24**, 760—767.

MICHAEL M. WOOD (1970), The crystal structure of ransomite. Amer. Mineral. **55**, 729—734.

W. H. ZACHARIASEN (1963), The crystal structure of monoclinic metaboric acid. Acta Crystallogr. **16**, 385—389.