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Crystal structure of babingtonite

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Auszug

Babingtonit, $Ca_2(Fe,Mn,Mg)FeHSi_5O_{15}$ hat die Raumgruppe $P\bar{1}$ und die Gitterkonstanten $a = 7{,}509 \pm 0{,}019$ Å, $b = 11{,}697 \pm 0{,}028$ Å, $c = 6{,}719 \pm 0{,}017$ Å, $\alpha = 91{,}433 \pm 0{,}041°$, $\beta = 93{,}886 \pm 0{,}030°$, $\gamma = 104{,}255 \pm 0{,}029°$, $Z = 2$. Die Struktur wurde aus dreidimensionalen Pattersondiagrammen mittels der Minimumfunktions-Methode bestimmt. Die Verfeinerung mit isotropen Temperaturfaktoren ergab $R = 0{,}0612$.

Das Strukturgerüst wird von zwei Einzelketten aus SiO_4-Tetraedern parallel [110] und mit je fünf Oktaedern je Elementarzelle gebildet. Die Ketten sind durch Oktaeder um Fe,Mn,Mg zusammengehalten. In den großen leeren Räumen zwischen den Ketten und Oktaedern liegen die Ca-Atome inmitten von Polyedern aus acht O-Atomen. Der Abstand vom Si zu den brückenbildenden O-Atomen ist 1,652 Å, für die übrigen O-Atome ist Si—O = 1,614 Å. Fe^{2+}—O ist 2,066 bis 2,239 Å, Fe^{3+}—O 1,934 bis 2,206 Å und Ca—O 2,287 bis 3,084 Å. Die Struktur von Babingtonit ist der von Rhodonit deutlich ähnlich.

Abstract

Babingtonite, $Ca_2(Fe,Mn,Mg)FeHSi_5O_{15}$, from the Yakuki mine, Japan, has triclinic space group $P\bar{1}$ and unit-cell constants $a = 7.509 \pm 0.019$ Å, $b = 11.697 \pm 0,028$ Å, $c = 6.719 \pm 0.017$ Å, $\alpha = 91.433 \pm 0.041°$, $\beta = 93.886 \pm 0.030°$, $\gamma = 104.255 \pm 0.029°$, and $Z = 2$. Three-dimensional intensities were collected with the 2θ scan method and by using Zr-filtered Mo$K\alpha$ radiation. The structure was determined by solving three-dimensional Patterson maps with the minimum-function method. The final least-squares refinement for isotropic temperature factors, using 3265 reflections, gave $R = 0.0612$.

The structure consists of two single chains of silica tetrahedra, containing five tetrahedra per repeat unit, running parallel to the [110] zone and connected by Fe,Mn,Mg octahedra. Ca atoms occupy the large openings existing between the tetrahedral chains and the octahedra, and form irregular polyhedra each with eight oxygen atoms. The average distance from Si to the nonbridging

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oxygen atoms is 1.614 Å and from Si to bridging oxygen atoms is 1.652 Å. The range of Fe^{2+}—O distances is between 2.066 and 2.239 Å; of Fe^{3+}—O, between 1.934 and 2.206 Å; and of Ca—O between 2.287 and 3.084 Å. The structure of babingtonite distinctly resembles that of rhodonite.

Introduction

Although the crystal structure of babingtonite had not been determined prior to this study the mineral was usually classified, together with rhodonite, as a single-chain silicate, containing five tetrahedra per repeat unit (PEACOR and NIIZEKI, 1963; STRUNZ, 1970) on the basis of morphological and cell data. PREWITT and PEACOR (1964) have suggested for babingtonite a possible five-membered single-chain structure on the basis of the resemblance between the b-axis diffraction patterns of babingtonite and rhodonite. However, a double-chain structure was inferable from the chemical composition of the mineral, provided that OH is not in tetrahedral-corner position.

A comprehensive description of babingtonite from the contact-metamorphic iron deposits of the Yakuki mine, Japan, was published recently by NAMBU, TANIDA and KITAMURA (1969). The specific gravity of these specimens was determined by the authors of that paper as 3.37 g/cm³, and the chemical formula was given as:

$$(Ca_{3.85}Mn_{0.11}Na_{0.03}K_{0.03})_{4.02}(Fe_{1.26}Mn_{0.49}Mg_{0.26})_{2.01}$$
$$(Fe^{3+}_{1.97}Al_{0.01})_{1.98}(Si_{9.83}Al_{0.17})_{10.0}O_{27.73}(OH)_{2.27}\,.$$

One of us collected from the same locality the specimens which were used in the following study.

Experimental

A small prismatic fragment cut from a larger babingtonite crystal, measuring about 0.45, 0.42 and 0.27 mm along the a, b and c axes, was mounted on an automated Hilger-Watts four-circle diffractometer with the b axis in approximate coincidence with the instrument's φ axis. Intensities of 3275 upper-hemisphere reflections, within the limit of $\sin\theta \leq 0.5$ were measured, using Zr-filtered Mo$K\alpha$ radiation. Scanning across the diffraction peaks was done with a stepwise, stationary-counter, stationary-crystal, 2θ scan technique by applying a symmetrical scan range of 1° and a rate of 1°/100 seconds. Background measurements were made every 50 seconds on both sides of the peaks. The scintillation counter was set at the crystal-to-counter distance of 20 cm, and an aperture 6 mm in diameter was used.

Absorption corrections were calculated for the polyhedral-shaped crystal by using a Gaussian integral method with divisions of 7 (BURNHAM, 1966), and all reflections were corrected. Weights for all reflections were assigned by considering counting statistics, long-period source fluctuation which was deduced from repeated measurements on selected standard reflections, and from errors in crystal-size measurements. 313 reflections had intensities lower than $2\sigma(I)$ and these were set to be equal to $\sigma(I)$.

The unit-cell constants of babingtonite were refined by a least-squares method by using the initial data obtained from precession photographs and from a Cu$K\alpha$ powder diffractometer chart. The refined parameters with corresponding standard deviations are:

$$\begin{aligned} a &= 7.509 \pm 0.019 \text{ Å} & \alpha &= 91.433 \pm 0.041^\circ \\ b &= 11.697 \pm 0.028 \text{ Å} & \beta &= 93.886 \pm 0.030^\circ \\ c &= 6.719 \pm 0.017 \text{ Å} & \gamma &= 104.255 \pm 0.029^\circ. \end{aligned}$$

These lattice parameters agree closely with those previously reported by RICHMOND (1937).

Structure determination

An $N(z)$ test for the detection of the presence of a center of inversion was carried out. The results indicated strongly that the structure of babingtonite is centric, so space group $P\bar{1}$ was accepted in consequent calculations.

A three-dimensional Patterson synthesis was calculated from the 3275 observed intensities and a search was initiated for locating potential inversion peaks. Since there were possible overlapping of peaks in the Patterson maps, those peaks with heights larger than that of Fe—Fe single-vector peaks were ignored. Seven peaks showing possible inversion and conjugate relationships and having no prominent peaks in forbidden zones were selected as probable inversion peaks.

By using the inversion-peak candidate located at 0.08, 0.475, 0.35 in x, y, and z coordinates of the Patterson synthesis, M_2 maps were prepared. These maps contained a number of relatively large symmetrical peaks equal to the number of atoms anticipated in a unit cell. In addition to these peaks, however, there were many others of relatively low height and more irregular peaks as well. With the aid of standard interatomic distances and coordination

polyhedra the major features of the babingtonite structure were easily deduced. A typical section of the M_2 maps is shown in Fig. 1. Structure factors were calculated from the approximate atomic coordinates of the M_2 maps by using arbitrary temperature factors. An R value of 33.9% was obtained. A subsequent Fourier synthesis disclosed better-defined atomic positions and the input of these coordinates decreased the R value to 25.7%. The shifts in the atomic positions in a second Fourier synthesis were negligible and further syntheses were judged to be unnecessary.

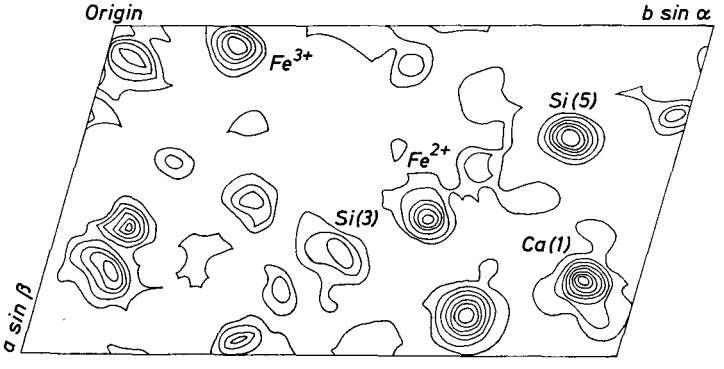

Fig. 1. M_2 section at $z = 0.125$ showing parts of Fe^{2+}, Fe^{3+}, Ca(1), Si(3), Si(5) and oxygen atoms

Four cycles of least-squares refinement of the atomic positions and isotropic temperature factors were calculated. The percentage of Mg occupancy in the Fe^{2+} position was also computed. Because of the small difference in f curves between Mn^{2+} and Fe^{2+} (although the Fe^{2+} site was presumed to be partly replaced by Mn^{2+} and Mg^{2+}) the calculations of these occupancy ratios were omitted. In these calculations, fully ionized states were assumed for all atoms except oxygen, which was assumed to be half ionized (CROMER and MANN, 1968). Ten reflections out of the 3275 were excluded from the calculations because their intensity measurements appeared to be less reliable due to possible machine failure. No corrections for secondary-extinction effects were made. The final conventional R value and weighted R for 3265 reflections were 6.12 and 6.92%, respectively.

The final atomic coordinates and temperature factors with corresponding standard deviations are listed in Table 1. All observed and calculated structure factors are tabulated in Table 2.

Table 1. *Final atomic parameters and their standard deviations* (lower rows)

Atom	x	y	z	B	Occupancy
Ca(1)	0.78195	0.94185	0.14246	0.8282	
	0.00011	0.00007	0.00012	0.0140	
Ca(2)	0.23789	0.52034	0.30414	0.6958	
	0.00010	0.00007	0.00012	0.0136	
Fe^{2+}	0.59363	0.64411	0.06137	0.4954	0.8561
	0.00008	0.00005	0.00009	0.0165	0.0058
Fe^{3+}	0.04655	0.23532	0.18443	0.5599	
	0.00007	0.00005	0.00008	0.0116	
Si(1)	0.28767	0.05351	0.34126	0.5788	
	0.00014	0.00009	0.00015	0.0166	
Si(2)	0.46011	0.31355	0.42474	0.5224	
	0.00014	0.00009	0.00015	0.0162	
Si(3)	0.80613	0.44506	0.20977	0.4960	
	0.00014	0.00009	0.00015	0.0161	
Si(4)	0.98773	0.71336	0.30999	0.5226	
	0.00014	0.00009	0.00015	0.0163	
Si(5)	0.32721	0.83592	0.10650	0.5822	
	0.00014	0.00009	0.00016	0.0165	
O(1)	0.19767	0.98774	0.53409	1.0594	
	0.00039	0.00026	0.00044	0.0437	
O(2)	0.13003	0.08047	0.18484	0.7000	
	0.00036	0.00024	0.00041	0.0390	
O(3)	0.43302	0.17111	0.43607	0.8866	
	0.00038	0.00025	0.00042	0.0414	
O(4)	0.31691	0.33841	0.24601	0.7178	
	0.00036	0.00024	0.00041	0.0394	
O(5)	0.55045	0.62029	0.36622	0.7403	
	0.00037	0.00024	0.00041	0.0394	

Table 1. *(Continued)*

Atom	x	y	z	B	Occupancy
O(6)	0.67737	0.37087	0.37284	0.7535	
	0.00036	0.00024	0.00041	0.0398	
O(7)	0.96850	0.38455	0.15858	0.7506	
	0.00037	0.00024	0.00041	0.0399	
O(8)	0.67837	0.47453	0.02701	0.6870	
	0.00036	0.00024	0.00041	0.0391	
O(9)	0.92555	0.56897	0.33717	0.6869	
	0.00035	0.00023	0.00040	0.0389	
O(10)	0.87215	0.75533	0.12528	0.7549	
	0.00037	0.00024	0.00041	0.0399	
O(11)	0.02110	0.22100	0.47837	0.8925	
	0.00038	0.00025	0.00042	0.0414	
O(12)	0.20394	0.73700	0.24969	0.7727	
	0.00037	0.00024	0.00041	0.0401	
O(13)	0.50958	0.79949	0.05626	0.8886	
	0.00038	0.00025	0.00043	0.0415	
O(14)	0.80576	0.14201	0.08167	0.8142	
	0.00037	0.00024	0.00042	0.0405	
O(15)	0.39447	0.96755	0.22562	0.9076	
	0.00038	0.00025	0.00043	0.0416	

Description of the structure

The c-axis projection of the babingtonite structure is illustrated in Fig. 2. The major bond distances and angles, with their standard deviations, are listed in Tables 3 and 4, respectively.

The dominant feature in the babingtonite structure is the single chain of silica tetrahedra containing five tetrahedra per repeat unit. There are two chains per unit cell, both extending parallel in the direction of [110]. These chains are connected by bands of Fe octahedra and Ca polyhedra.

There are two kinds of iron octahedra (which contain Mn and Mg) in the structure. In one octahedron the Fe—O distances range from

Table 2. *List of observed and calculated structure factors*

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
-10	1	-2	19.4	-18.4	-9	7	1	2.6	- 3.9	-8	7	-5	54.4	-50.9	-7	4	-4	5.0	4.6	-7	12	-1	29.2	-27.6
		0	12.1	14.5			2	6.7	6.9			-4	28.0	-27.6			-3	4.5	4.1			0	44.1	-46.3
		1	4.2	- 3.1			3	4.6	- 3.5			-3	36.1	34.8			-2	11.0	10.7			1	56.6	60.4
		2	9.8	9.0			4	8.5	11.2			-2	12.5	12.8			-1	2.4	2.0			2	22.2	21.6
-10	2	-1	12.1	-11.0	-9	8	-3	26.0	25.4			-1	2.6	- 0.2			0	9.3	- 8.4			3	5.3	- 4.9
		0	16.7	18.5			-2	7.1	- 5.4			0	16.0	-16.9			1	28.9	-30.3			4	6.0	5.3
		1	2.7	- 3.8			-1	13.3	-14.2			1	8.4	- 8.9			2	10.2	-11.7	-7	13	-3	6.9	- 5.1
		2	20.8	-19.9			0	2.8	- 4.4			2	22.3	-23.6			3	2.4	4.8			-2	20.3	-19.9
		3	61.3	-64.3			1	6.7	- 7.0			3	24.3	26.8			4	23.5	-25.1			-1	9.8	- 8.1
-10	3	-2	9.4	- 9.9			2	2.6	1.0			4	17.8	18.3			5	9.9	-10.2			0	14.1	14.2
		-1	70.6	70.3			3	70.0	72.6			5	28.7	31.5			6	10.7	-10.8			1	2.7	- 4.4
		0	12.8	14.8			4	49.8	50.7	-8	8	-4	15.0	14.8			7	12.8	11.9			2	2.7	- 1.4
		1	36.7	-34.7	-9	9	-3	3.0	0.1			-3	8.8	7.2	-7	5	-6	4.3	3.7			3	9.8	10.1
		2	2.7	3.7			-2	4.5	7.2			-2	20.3	19.9			-5	23.8	-23.2	-7	14	-1	21.8	-21.1
		3	8.8	-10.7			-1	50.3	-49.5			-1	8.7	9.1			-4	5.9	- 5.8			0	2.8	- 1.0
-10	4	-2	2.9	- 5.6			0	43.2	-43.6			0	15.1	-15.5			-3	25.8	25.4			1	24.3	26.4
		-1	15.6	-14.8			1	18.0	17.4			1	47.0	-49.2			-2	9.9	- 8.5			2	16.6	16.7
		0	7.4	2.7			2	2.7	1.5			2	30.3	-31.8			-1	24.1	25.3	-6	1	-7	5.2	- 3.1
		1	20.7	19.9			3	3.9	- 1.9			3	12.5	14.6			0	26.5	25.4			-6	20.3	18.5
		2	8.7	- 7.5	-9	10	-2	4.2	6.3			4	29.2	-29.8			1	21.2	21.5			-5	43.5	-42.6
		3	5.2	2.7			-1	9.9	8.8			5	8.4	- 5.3			2	21.5	23.5			-4	13.1	12.5
-10	5	-2	4.5	- 2.9			0	30.7	31.5	-8	9	-4	12.9	-12.2			3	26.0	-27.4			-3	24.3	24.8
		-1	2.8	- 1.4			1	32.3	-34.2			-3	30.9	29.6			4	19.8	-21.0			-2	5.5	- 4.2
		0	12.7	12.1			2	11.3	-11.2			-2	18.2	18.2			5	18.5	-17.5			-1	36.7	36.9
		1	9.8	9.2			3	2.7	0.9			-1	11.7	-10.4			6	6.2	- 7.3			0	12.5	12.3
		2	15.4	15.9	-9	11	-1	5.6	- 4.4			0	24.9	25.3			7	5.4	5.0			1	14.4	15.2
		3	25.4	-27.6			0	9.0	9.9			1	36.9	36.4	-7	6	-6	7.9	- 8.8			2	8.9	9.9
-10	6	-1	2.8	1.4			1	18.9	-19.4			2	49.4	50.3			-5	2.9	4.9			3	14.7	-16.0
		0	13.0	14.8			2	16.5	-16.9			3	12.8	-12.4			-4	10.8	8.2			4	21.8	-22.9
		1	46.9	47.3	-8	1	-5	19.4	18.8			4	23.6	-24.8			-3	60.5	-57.5			5	16.7	-17.9
		2	48.7	51.5			-4	8.8	9.2			5	14.3	-13.3			-2	18.8	-16.9			6	18.4	19.3
		3	16.5	-17.7			-3	13.9	-14.0	-8	10	-4	5.4	5.2			-1	37.4	38.5			7	18.1	-17.9
-10	7	-1	2.8	2.3			-2	14.2	-14.3			-3	40.4	-38.5			0	5.9	4.3			8	31.1	-30.5
		0	8.0	- 6.6			-1	29.1	-29.8			-2	60.9	-56.6			1	2.4	- 1.5	-6	2	-7	22.4	20.5
		1	22.6	-21.3			0	33.5	33.9			-1	29.3	30.8			2	8.7	-10.4			-6	8.1	- 7.8
		2	24.0	-22.7			1	76.1	80.5			0	18.4	18.2			3	10.7	-10.9			-5	5.8	5.6
-10	8	0	21.1	-19.9			2	6.6	- 5.0			1	2.6	- 1.1			4	18.9	18.6			-4	46.0	-46.8
		1	7.5	- 5.8			3	2.5	0.1			2	16.6	15.6			5	65.5	68.6			-3	85.1	-83.6
-9	1	-3	23.3	-23.2			4	12.8	11.3			3	13.3	-14.5			6	10.4	10.3			-2	33.0	33.3
		-2	18.8	-19.1			5	15.4	15.8			4	5.8	- 5.3			7	41.2	-40.5			-1	20.2	17.2
		-1	8.6	7.9			6	2.7	- 1.7	-8	11	-3	8.4	7.5	-7	7	-6	3.1	4.1			0	19.2	-18.9
		0	12.8	14.2	-8	2	-5	12.1	12.7			-2	23.0	22.5			-5	15.4	-14.9			1	2.2	- 2.1
		1	14.4	16.0			-4	22.1	-20.3			-1	6.3	6.6			-4	2.8	0.1			2	15.9	-17.1
		2	24.7	25.6			-3	37.7	-35.7			0	10.2	- 8.7			-3	23.4	22.9			3	13.0	-13.5
		3	47.9	-50.7			-2	7.5	- 8.4			1	22.1	-21.5			-2	7.2	7.1			4	50.8	55.0
		4	29.4	-30.8			-1	21.6	-23.8			2	38.0	-40.4			-1	10.0	11.7			5	84.6	91.4
		5	28.6	-30.0			0	2.5	2.6			3	6.2	6.3			0	7.7	- 7.7			6	3.7	- 5.3
-9	2	-4	15.4	-14.5			1	22.1	-21.2			4	9.8	8.5			1	56.2	-59.6			7	9.6	- 9.8
		-3	19.9	-20.9			2	26.2	-27.3	-8	12	-2	16.9	15.8			2	33.0	-36.0			8	15.0	14.5
		-2	10.3	- 9.7			3	4.7	6.1			-1	25.0	26.8			3	12.4	- 0.6	-6	3	-7	80.1	76.1
		-1	13.2	12.6			4	2.5	1.7			0	4.3	- 1.4			4	3.7	- 3.4			-6	14.4	-13.0
		0	17.3	17.3			5	10.6	10.6			1	4.6	- 4.3			5	10.1	- 8.3			-5	23.2	-22.0
		1	71.3	73.7			6	2.7	- 0.9			2	22.6	20.7			6	7.9	- 8.1			-4	16.6	15.5
		2	16.2	17.2	-8	3	-5	11.1	11.2			3	12.8	-13.4	-7	8	-5	2.9	3.0			-3	36.6	35.7
		3	9.5	-10.6			-4	7.7	- 6.0	-8	13	-1	2.8	- 1.1			-4	7.3	- 7.8			-2	2.4	- 0.3
		4	18.1	18.1			-3	35.9	35.6			0	16.7	-16.5			-3	36.1	33.8			-1	22.0	23.8
		5	6.9	- 6.2			-2	35.8	31.7			1	5.4	6.6			-2	7.5	6.8			0	48.8	-51.3
-9	3	-4	2.9	2.7			-1	20.9	19.8	-7	1	-6	24.2	22.4			-1	29.3	30.8			1	105.5	-115.1
		-3	56.5	-55.1			0	9.0	-10.7			-5	47.1	45.6			0	10.2	-10.3			2	2.2	- 2.3
		-2	2.7	- 1.5			1	7.1	4.7			-4	7.0	7.0			1	26.9	29.1			3	7.7	7.9
		-1	12.5	10.6			2	5.3	5.1			-3	24.9	25.8			2	33.8	34.9			4	15.5	-16.0
		0	33.6	-33.0			3	6.1	- 3.7			-2	43.4	-43.3			3	22.8	-24.4			5	18.6	-19.0
		1	34.1	-32.8			4	7.9	8.2			-1	79.3	-81.5			4	2.5	0.5			6	4.5	- 2.4
		2	5.7	- 6.0			5	12.9	-13.1			0	9.5	9.2			5	14.3	13.0			7	15.8	16.4
		3	28.2	28.3			6	30.4	-31.9			1	26.0	-28.1			6	4.4	- 2.0			8	5.9	5.5
		4	7.1	7.1	-8	4	-5	38.6	-35.0			2	33.9	-35.5	-7	9	-5	6.8	- 8.0	-6	4	-7	31.8	-30.7
		5	36.0	35.2			-4	11.3	- 9.6			3	5.5	- 4.7			-4	13.5	11.2			-6	6.1	- 6.6
-9	4	-4	15.8	16.3			-3	29.3	30.0			4	30.5	32.9			-3	44.7	-43.1			-5	4.8	- 5.2
		-3	45.4	40.3			-2	17.0	-16.1			5	2.5	4.0			-2	35.5	-33.2			-4	13.8	11.9
		-2	22.0	20.0			-1	18.8	-19.8			6	25.4	26.0			-1	15.8	-14.0			-3	35.7	33.0
		-1	26.7	-27.7			0	2.7	- 2.2			7	15.3	16.1			0	27.0	-27.6			-2	19.2	18.4
		0	13.4	-12.8			1	2.4	- 2.2	-7	2	-6	14.8	12.0			1	31.4	34.9			-1	4.8	- 2.6
		1	17.2	-14.8			2	18.2	17.4			-5	37.4	35.3			2	13.0	-14.2			0	5.1	- 4.8
		2	5.4	- 4.7			3	79.6	85.3			-4	2.7	- 3.4			3	9.0	- 9.2			1	73.5	79.6
		3	13.5	14.6			4	2.6	- 0.8			-3	12.5	13.5			4	4.7	- 5.7			2	31.7	33.3
		4	3.8	- 1.9			5	31.9	-34.1			-2	29.8	29.6			5	5.5	- 3.8			3	29.6	-32.4
		5	48.2	-49.8			6	3.9	- 0.9			-1	90.2	94.0			6	27.1	27.8			4	5.8	6.5
-9	5	-4	12.5	12.7	-8	5	-5	30.7	27.7			0	16.3	-18.1	-7	10	-5	31.0	29.3			5	17.9	-18.9
		-3	15.5	-15.5			-4	23.6	23.3			1	44.7	-49.0			-4	28.9	25.8			6	2.6	- 1.7
		-2	2.8	4.8			-3	11.5	11.2			2	20.9	-23.2			-3	37.9	-36.4			7	21.9	23.0
		-1	11.7	-14.0			-2	11.2	1.6			3	10.8	-11.2			-2	6.8	- 5.6	-6	5	-7	16.8	17.0
		0	5.1	- 4.3			-1	66.5	-66.0			4	25.4	28.0			-1	24.3	24.5			-6	16.5	-15.6
		1	43.2	44.7			0	18.6	-20.8			5	24.3	24.5			0	35.4	36.4			-5	2.8	- 4.1
		2	11.5	12.8			1	20.4	19.8			6	6.6	- 6.0			1	15.4	16.6			-4	15.2	-15.1
		3	27.8	-27.7			2	12.8	-14.1			7	55.8	-57.6			2	15.3	-14.9			-3	57.5	-55.1
		4	9.8	11.1			3	13.7	-13.6	-7	3	-6	31.5	-30.8			3	59.9	-60.8			-2	9.7	10.0
		5	5.9	4.8			4	12.7	12.4			-5	94.3	-89.2			4	39.6	-40.5			-1	7.0	- 6.8
-9	6	-4	4.5	0.1			5	20.5	20.4			-4	15.5	-15.1			5	26.2	27.3			0	6.7	6.9
		-3	23.4	-22.2			6	2.8	3.9			-3	41.3	41.4	-7	11	-4	47.8	-45.0			1	16.8	18.3
		-2	4.6	- 4.4	-8	6	-5	16.0	13.6			-2	2.5	0.0			-3	5.3	- 4.2			2	7.1	7.5
		-1	21.5	-23.5			-4	15.9	16.2			-1	17.3	17.9			-2	2.8	- 0.6			3	18.0	-21.0
		0	2.7	- 1.4			-3	22.2	23.3			0	9.7	-11.3			-1	30.1	29.6			4	17.6	-18.3
		1	17.2	-17.0			-2	2.7	5.0			1	24.0	-26.0			0	38.3	39.3			5	10.4	10.6
		2	15.1	-14.0			-1	32.8	33.1			2	13.1	-14.5			1	8.9	10.2			6	39.3	39.3
		3	16.2	17.5			0	5.1	2.2			3	53.9	58.4			2	4.3	- 3.3			7	32.1	31.2
		4	2.7	- 1.1			1	50.7	-53.1			4	14.3	14.7			3	13.5	14.0	-6	6	-7	3.0	1.5
		5	9.9	- 8.7			2	8.7	- 9.4			5	35.8	37.8			4	19.0	20.0			-6	8.9	- 6.8
-9	7	-3	4.2	0.5			3	3.7	2.1			6	12.9	12.7			5	27.4	-27.1			-5	36.6	34.1
		-2	28.5	26.3			4	2.6	- 4.1			7	10.6	-13.3	-7	12	-4	10.1	-10.3			-4	23.6	-23.7
		-1	22.2	19.7			5	18.5	17.9	-7	4	-6	17.0	-16.2			-3	21.0	-20.8			-3	17.3	-16.9
		0	7.7	6.7			6	14.9	15.3			-5	2.8	1.9			-2	4.4	1.9			-2	14.2	13.3

Table 2. *(Continued)*

h	k	l	$\|F_o\|$	F_c
-6	6	-1	38.7	39.0
		0	22.8	24.2
		1	6.5	8.0
		2	15.0	-13.8
		3	72.3	-78.7
		4	2.4	0.0
		5	6.2	- 7.5
		6	12.1	- 9.9
		7	13.0	12.6
-6	7	-6	2.9	- 0.8
		-5	30.6	-28.1
		-4	30.1	-28.7
		-3	18.9	-18.0
		-2	5.3	- 6.3
		-1	71.3	71.7
		0	10.5	10.5
		1	19.5	21.5
		2	18.4	18.3
		3	36.7	38.2
		4	5.4	- 4.5
		5	54.1	-56.8
		6	9.3	-10.0
		7	12.1	-12.1
-6	8	-6	13.3	13.3
		-5	4.9	4.0
		-4	16.7	-16.6
		-3	4.8	- 4.7
		-2	6.1	- 4.1
		-1	108.3	-110.3
		0	31.8	-33.3
		1	66.8	71.7
		2	6.8	- 7.5
		3	14.2	15.0
		4	6.5	- 6.2
		5	17.3	-17.1
		6	2.7	- 1.5
		7	39.5	38.3
-6	9	-6	17.5	16.2
		-5	91.3	85.7
		-4	46.9	44.9
		-3	22.5	-21.4
		-2	10.3	-11.0
		-1	3.6	- 4.1
		0	5.9	4.8
		1	12.0	-11.7
		2	25.4	27.3
		3	22.3	-25.5
		4	22.5	-23.1
		5	13.1	+13.6
		6	18.1	-18.1
-6	10	-6	9.6	9.9
		-5	10.7	10.8
		-4	29.0	-28.1
		-3	2.8	- 2.2
		-2	12.2	-12.2
		-1	2.5	- 1.9
		0	21.6	21.9
		1	14.5	15.2
		2	2.4	0.7
		3	11.1	10.4
		4	29.9	30.8
		5	6.7	- 6.2
		6	34.8	35.7
-6	11	-5	3.0	3.4
		-4	12.5	- 9.6
		-3	6.8	- 5.9
		-2	5.0	- 5.4
		-1	2.6	- 2.7
		0	6.7	- 7.4
		1	26.1	-25.2
		2	43.7	-45.5
		3	23.9	25.8
		4	24.1	25.1
		5	2.7	2.4
-6	12	-5	3.0	0.5
		-4	20.3	-18.2
		-3	44.4	43.4
		-2	26.3	23.7
		-1	21.4	-21.8
		0	10.0	-10.0
		1	9.8	10.3
		2	15.1	16.2
		3	12.7	13.2
		4	12.1	-12.2
		5	43.0	-43.0
-6	13	-4	3.1	4.4
		-3	13.8	-13.4
		-2	26.0	-24.4
		-1	7.0	7.2
		0	4.4	3.8
		1	19.1	20.1
		2	31.1	33.0
		3	21.4	23.4
		4	8.4	- 8.6
-6	14	-3	8.3	7.6
		-2	20.0	-19.4
		-1	15.9	-16.0
		0	2.7	- 0.1
		1	24.8	-25.8
		2	32.9	-34.5
-6	14	3	17.8	18.0
-6	15	-1	10.9	11.7
		0	20.0	19.6
		1	20.0	-19.7
-5	1	-7	11.6	10.9
		-6	18.0	-16.4
		-5	14.5	-13.6
		-4	39.4	-38.2
		-3	32.4	-30.6
		-2	45.9	45.9
		-1	21.9	-21.6
		0	54.9	57.9
		1	14.5	-14.0
		2	10.4	-11.1
		3	38.8	-44.2
		4	5.1	5.5
		5	27.0	28.0
		6	24.0	24.4
		7	26.2	26.5
		8	2.9	1.4
-5	2	-7	16.1	15.6
		-6	10.8	7.0
		-5	22.1	20.7
		-4	30.2	-28.9
		-3	9.6	- 9.7
		-2	24.0	23.8
		-1	54.9	55.9
		0	13.7	14.0
		1	15.2	16.1
		2	49.9	-52.7
		3	102.8	-116.4
		4	13.2	15.3
		5	37.7	-39.6
		6	20.2	-20.8
		7	16.4	15.9
		8	7.9	7.5
-5	3	-7	10.1	8.8
		-6	18.5	-17.3
		-5	25.2	-24.5
		-4	17.3	-16.3
		-3	28.0	-27.0
		-2	30.7	30.3
		-1	65.7	65.2
		0	9.7	9.7
		1	26.4	27.6
		2	55.8	59.3
		3	76.1	84.3
		4	20.6	-21.7
		5	41.1	-45.0
		6	14.2	-14.0
		7	24.0	-24.2
		8	21.9	20.8
-5	4	-7	2.9	2.2
		-6	2.8	3.5
		-5	8.0	7.1
		-4	2.6	3.1
		-3	4.9	- 2.8
		-2	87.2	-84.7
		-1	179.2	-193.0
		0	11.7	12.6
		1	67.4	72.6
		2	5.8	6.6
		3	16.8	17.9
		4	2.3	3.3
		5	26.1	-27.4
		6	15.9	17.5
		7	57.9	58.4
		8	2.9	- 3.4
-5	5	-7	15.2	-13.3
		-6	47.4	44.6
		-5	87.3	82.4
		-4	32.0	31.0
		-3	31.3	-29.9
		-2	22.4	-21.0
		-1	2.2	- 1.7
		0	4.6	6.5
		1	12.7	13.2
		2	4.6	4.7
		3	65.9	-71.4
		4	7.3	8.7
		5	5.4	6.2
		6	2.6	4.2
		7	12.7	-11.7
		8	2.9	- 3.1
-5	6	-7	19.2	-16.6
		-6	7.0	7.3
		-5	13.3	-12.6
		-4	18.0	-16.2
		-3	4.0	3.1
		-2	20.5	18.9
		-1	20.6	-21.4
		0	26.8	27.4
		1	13.0	14.4
		2	12.1	-12.6
		3	38.3	41.6
		4	4.0	- 0.9
		5	14.3	-14.2
		6	28.8	30.1
		7	25.0	-23.8
		8	21.1	-21.6
-5	7	-7	10.7	9.9
		-6	10.9	-10.5
		-5	7.4	8.7
		-4	6.4	7.2
		-3	8.6	- 8.5
		-2	5.3	- 5.8
		-1	18.5	-18.2
		0	12.6	13.6
		1	27.5	-29.0
		2	5.9	6.5
		3	16.9	18.3
		4	7.0	- 6.4
		5	8.6	8.5
		6	13.1	-13.4
		7	2.8	1.2
-5	8	-7	18.0	-17.0
		-6	3.0	- 3.9
		-5	5.4	- 5.9
		-4	5.6	5.6
		-3	93.1	90.7
		-2	4.3	- 5.3
		-1	45.5	-42.4
		0	32.0	33.6
		1	15.3	15.6
		2	13.2	15.0
		3	2.3	0.5
		4	17.9	-18.0
		5	74.9	-79.8
		6	22.0	-22.4
		7	12.6	11.3
-5	9	-6	9.7	-11.3
		-5	23.8	23.2
		-4	2.7	2.9
		-3	34.5	-34.4
		-2	27.5	-24.7
		-1	10.8	-11.5
		0	3.6	1.1
		1	54.2	57.7
		2	45.2	48.2
		3	3.7	- 4.7
		4	2.5	2.3
		5	35.6	35.7
		6	24.6	25.5
		7	46.0	-43.7
-5	10	-6	49.5	46.4
		-5	21.3	-20.6
		-4	10.3	10.9
		-3	7.9	- 6.6
		-2	32.0	-30.9
		-1	11.9	-12.3
		0	2.6	0.1
		1	70.8	-77.4
		2	29.4	-30.9
		3	19.7	20.5
		4	4.7	- 5.6
		5	8.9	9.6
		6	17.9	17.8
-5	11	-6	8.1	- 8.1
		-5	11.8	12.7
		-4	7.0	5.5
		-3	44.9	43.0
		-2	29.2	28.2
		-1	2.6	2.4
		0	3.8	- 2.6
		1	28.7	-30.4
		2	2.4	- 0.6
		3	9.6	9.8
		4	29.4	30.9
		5	9.3	8.3
		6	27.8	-27.1
-5	12	-5	33.6	-32.4
		-4	2.9	2.0
		-3	33.8	31.8
		-2	4.8	- 5.9
		-1	13.1	-12.4
		0	35.7	-37.0
		1	17.2	-18.8
		2	21.6	22.6
		3	43.7	44.7
		4	17.5	17.6
		5	4.1	2.5
-5	13	-4	36.9	33.6
		-3	5.7	4.2
		-2	12.2	12.6
		-1	12.3	-11.7
		0	24.7	-26.3
		1	4.3	- 4.8
		2	6.1	7.0
		3	42.4	-43.7
		4	26.3	-26.3
-5	14	-4	5.9	- 5.5
		-3	3.0	5.0
		-2	9.1	9.3
		-1	53.3	51.2
		0	53.6	56.9
		1	39.2	-40.6
		2	7.0	- 6.8
		3	2.7	- 0.2
		4	2.8	0.8
-5	15	-2	9.9	9.9
-5	15	-1	9.4	9.3
		0	22.5	-23.4
		1	9.9	10.5
		2	7.8	9.0
-4	1	-8	7.8	- 7.9
		-7	35.6	-32.9
		-6	69.0	65.5
		-5	56.9	54.0
		-4	15.7	-14.8
		-3	19.1	-18.8
		-2	12.7	12.1
		-1	2.0	0.7
		0	6.4	- 4.6
		1	36.4	38.1
		2	61.4	-65.5
		3	21.7	-22.3
		4	46.0	50.7
		5	24.4	-26.5
		6	9.2	- 8.7
		7	15.0	-15.8
		8	15.4	14.8
-4	2	-8	11.9	-12.2
		-7	2.8	0.8
		-6	2.7	3.4
		-5	32.9	-29.9
		-4	12.3	-11.6
		-3	7.9	6.6
		-2	32.3	30.3
		-1	9.7	8.4
		0	18.2	18.8
		1	5.7	5.0
		2	31.1	31.9
		3	68.3	73.6
		4	48.5	-52.6
		5	3.9	2.8
		6	2.4	0.3
		7	12.4	-12.6
		8	2.8	3.3
-4	3	-8	2.9	- 1.8
		-7	9.9	- 8.4
		-6	2.7	2.0
		-5	6.1	5.1
		-4	6.8	- 5.5
		-3	11.0	11.0
		-2	2.1	- 2.5
		-1	57.7	-57.5
		0	55.0	-56.4
		1	48.3	-50.7
		2	10.5	11.6
		3	24.1	27.0
		4	20.3	-22.1
		5	9.1	- 9.7
		6	15.1	-14.6
		7	24.0	24.0
		8	33.3	33.1
-4	4	-8	14.3	-13.5
		-7	27.6	-25.5
		-6	16.5	15.6
		-5	12.5	10.9
		-4	93.0	89.3
		-3	80.8	77.0
		-2	25.3	-25.5
		-1	25.0	-24.9
		0	34.9	36.4
		1	3.4	5.1
		2	20.8	21.8
		3	21.7	22.3
		4	62.8	-68.8
-4	5	-8	36.5	-34.4
		-7	62.3	-58.5
		-6	23.4	21.6
		-5	13.3	12.8
		-4	27.2	-25.8
		-3	65.9	-63.6
		-2	21.0	-19.5
		-1	28.4	-28.4
		0	72.6	77.1
		1	42.5	45.2
		2	19.3	19.6
		3	3.5	- 4.5
		4	19.6	19.6
		5	60.1	64.0
		6	7.9	- 7.6
		7	35.3	-33.8
		8	4.3	- 0.2
-4	6	-8	3.0	3.0
		-7	68.8	65.2
		-6	13.7	11.9
		-5	7.4	- 7.5
		-4	5.3	- 1.1
		-3	24.8	-22.7
		-2	20.2	-20.1
		-1	4.3	4.1
		0	44.5	-45.7
		1	91.6	-100.0
		2	27.2	29.8
-4	6	3	31.2	33.3
		4	27.8	29.4
		5	23.5	24.3
		6	2.6	2.8
		7	24.5	-23.0
		8	12.7	-12.5
-4	7	-7	24.3	-24.9
		-6	12.2	11.3
		-5	2.7	1.5
		-4	20.5	19.3
		-3	59.0	55.8
		-2	31.5	-29.8
		-1	6.3	5.1
		0	25.3	-25.9
		1	27.7	-29.6
		2	7.9	8.2
		3	27.5	30.6
		4	19.0	19.7
		5	9.8	-10.2
		6	29.1	-27.8
		7	34.2	-33.1
		8	2.9	2.1
-4	8	-7	30.6	-28.6
		-6	7.4	- 7.5
		-5	31.3	-30.0
		-4	33.2	32.6
		-3	2.5	0.6
		-2	8.4	8.5
		-1	4.6	3.9
		0	27.8	-29.3
		1	18.5	-19.4
		2	2.2	2.1
		3	60.4	66.2
		4	12.6	12.8
		5	20.9	21.0
		6	11.5	10.6
		7	9.2	8.2
-4	9	-7	9.1	- 9.4
		-6	21.5	-17.5
		-5	9.0	9.6
		-4	49.7	47.3
		-3	8.3	- 8.1
		-2	27.7	26.8
		-1	20.9	-20.7
		0	6.5	- 7.6
		1	13.5	-14.5
		2	30.4	-31.0
		3	90.8	-98.7
		4	11.6	-12.1
		5	53.3	54.4
		6	11.7	-11.1
		7	13.4	12.8
-4	10	-7	9.1	- 9.1
		-6	9.4	- 9.4
		-5	17.8	-16.8
		-4	11.6	-10.3
		-3	6.2	- 5.6
		-2	34.4	32.6
		-1	120.4	120.5
		0	70.2	75.0
		1	54.5	-59.5
		2	2.3	- 1.6
		3	8.2	- 7.7
		4	2.5	- 0.1
		5	6.4	5.5
		6	4.2	- 2.8
		7	44.9	-42.0
-4	11	-6	13.6	-11.6
		-5	64.7	-60.2
		-4	42.8	-41.0
		-3	11.4	-11.0
		-2	21.3	21.7
		-1	7.5	- 8.3
		0	38.7	-41.1
		1	8.4	10.0
		2	5.0	- 4.0
		3	16.9	17.1
		4	47.4	46.9
		5	5.1	- 5.9
		6	11.3	-11.6
-4	12	-6	12.4	-13.2
		-5	29.7	26.5
		-4	35.6	34.4
		-3	13.7	-13.4
		-2	2.7	- 2.3
		-1	12.2	-11.1
		0	24.0	-24.4
		1	15.6	-17.3
		2	4.8	5.7
		3	13.7	-14.0
		4	9.2	- 8.4
		5	16.2	15.1
		6	18.9	-17.4
-4	13	-5	8.9	7.3
		-4	3.0	- 1.6
		-3	2.9	5.2
		-2	2.8	0.7
		-1	2.6	- 2.7
		0	10.7	11.1
		1	21.3	21.4

Table 2. *(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
-4 13 2	2.6	3.7	-3 5 -2	10.6	- 9.2	-3 11 2	27.1	-28.1	-2 3 4	2.2	0.6	-2 9 1	11.1	-12.0
3	31.5	-30.9	-1	11.2	- 9.5	3	2.6	1.7	5	2.5	2.6	2	16.4	17.4
4	6.7	6.4	0	5.6	5.0	4	26.2	-26.7	6	36.8	35.3	3	30.5	31.0
5	3.0	2.0	1	26.4	-27.4	5	56.0	-53.7	7	26.1	24.3	4	33.1	-32.5
-4 14 -4	7.6	8.6	2	105.5	-114.2	6	20.5	-21.3	8	44.7	-42.8	5	17.3	17.4
-3	49.8	-47.7	3	121.2	-135.8	-3 12 -6	26.8	-26.2	9	8.4	- 5.8	6	18.1	17.7
-2	12.1	-10.7	4	3.6	4.0	-5	16.5	16.0	-2 4 -8	8.8	8.7	7	7.2	7.5
-1	30.9	30.6	5	40.1	41.0	-4	4.5	- 5.1	-7	21.1	-21.0	-2 10 -7	22.7	20.7
0	6.3	- 0.6	6	25.7	26.3	-3	5.2	- 6.2	-6	37.2	37.3	-6	38.2	39.1
1	2.6	- 3.7	7	22.6	21.7	-2	12.2	12.2	-5	52.7	50.1	-5	15.2	16.1
2	19.1	-18.8	8	13.6	-11.2	-1	7.6	8.0	-4	11.3	- 9.9	-4	18.7	-18.8
3	14.4	-13.5	-3 6 -8	22.2	22.9	0	5.0	4.3	-3	15.2	-14.6	-3	25.7	26.2
4	14.7	15.4	-7	7.4	6.7	1	70.8	75.7	-2	7.4	- 6.7	-2	35.8	-34.3
-4 15 -3	9.4	10.2	-6	15.7	-16.6	2	21.8	21.8	-1	6.2	- 6.8	-1	22.4	-21.7
-2	53.4	49.1	-5	29.0	-26.8	3	15.3	-15.3	0	33.6	-34.6	0	42.5	46.2
-1	17.4	-17.8	-4	2.5	0.1	4	21.2	-19.1	1	24.0	25.6	1	12.1	11.7
0	16.4	16.4	-3	14.8	-13.8	5	23.4	-23.1	2	59.0	-60.0	2	7.9	- 7.3
1	2.6	1.7	-2	81.1	77.3	6	8.2	- 7.4	3	106.5	-111.2	3	15.6	-14.8
2	34.2	-35.0	-1	151.0	154.5	-3 13 -5	6.2	- 6.1	4	18.2	18.8	4	5.2	- 3.4
3	9.9	- 9.6	0	20.5	-22.1	-4	4.9	- 3.2	5	14.7	12.7	5	24.9	-22.7
-4 16 -1	13.6	14.3	1	32.0	-33.5	-3	57.8	-52.7	6	11.2	-10.9	6	25.9	-25.3
0	15.3	15.4	2	15.5	-17.1	-2	21.4	-20.7	7	15.7	13.8	7	27.3	-26.1
1	28.7	29.4	3	12.8	-12.7	-1	11.7	-10.7	8	11.7	-11.0	-2 11 -7	4.1	- 2.9
-3 1 -8	41.8	-39.5	4	5.9	4.8	0	20.6	21.8	9	19.4	-17.3	-6	9.3	-11.9
-7	34.4	-30.6	5	27.4	27.4	1	16.1	15.6	-2 5 -8	2.8	- 6.0	-5	24.4	-23.6
-6	20.9	19.5	6	40.7	-41.0	2	9.4	-10.3	-7	5.0	- 2.7	-4	4.0	- 2.8
-5	2.5	0.3	7	58.0	-55.5	3	17.6	18.4	-6	6.1	6.5	-3	17.7	16.4
-4	46.8	-44.5	8	15.4	15.4	4	26.9	-24.9	-5	6.2	5.1	-2	13.7	-12.7
-3	34.2	-32.4	-3 7 -8	4.7	2.3	5	9.9	- 7.7	-4	4.0	- 2.9	-1	2.7	- 2.0
-2	22.7	-21.4	-7	40.8	40.6	-3 14 -4	14.9	-14.8	-3	34.1	-31.6	0	9.0	-10.4
-1	54.6	-55.2	-6	23.4	-23.0	-3	3.0	- 3.0	-2	59.5	55.1	1	19.1	19.6
0	82.9	87.2	-5	78.8	-75.1	-2	10.1	- 8.4	-1	114.2	111.9	2	29.2	27.9
1	30.5	32.2	-4	11.3	- 9.9	-1	33.4	-31.5	0	115.4	128.5	3	87.6	85.7
2	11.8	-12.1	-3	2.5	1.5	0	32.9	33.6	1	37.7	38.5	4	20.0	20.4
3	28.8	29.7	-2	16.5	15.1	1	2.6	- 3.2	2	55.8	-58.5	5	22.6	-20.8
4	42.4	44.5	-1	50.8	-48.6	2	2.7	1.9	3	6.1	- 6.2	6	2.8	- 1.0
5	30.1	31.7	0	31.2	-33.1	3	17.2	-17.0	4	9.3	9.7	-2 12 -6	7.7	9.2
6	52.1	-53.6	1	26.8	28.9	4	15.9	-15.1	5	10.1	9.1	-5	22.4	21.6
7	22.5	-20.7	2	17.4	18.3	-3 15 -3	3.2	1.6	6	26.6	24.7	-4	16.1	15.4
8	28.2	-28.4	3	65.7	70.8	-2	11.4	-10.3	7	13.7	-13.0	-3	29.4	29.3
9	17.7	-17.6	4	2.4	- 2.9	-1	3.0	- 3.1	8	37.7	-37.5	-2	29.1	-27.4
-3 2 -8	29.1	28.8	5	6.1	- 6.5	0	2.7	1.0	-2 6 -8	13.7	14.3	-1	90.8	-85.6
-7	62.5	60.2	6	2.7	0.3	1	2.7	2.6	-7	16.6	14.7	0	30.7	-33.3
-6	20.1	-19.1	7	34.2	32.9	2	15.5	14.3	-6	36.9	-36.6	1	19.7	17.9
-5	4.6	2.6	8	28.3	-26.7	3	49.5	46.7	-5	19.8	21.2	2	11.4	10.9
-4	8.3	8.0	-3 8 -8	26.5	27.3	-3 16 -2	11.0	- 9.9	-4	82.6	-77.8	3	10.0	- 9.6
-3	7.6	- 6.8	-7	2.8	- 0.5	-1	35.9	-33.4	-3	73.0	-68.2	4	41.1	-40.3
-2	31.4	-29.6	-6	6.6	- 5.4	0	47.8	-49.7	-2	48.3	46.4	5	7.5	8.3
-1	5.8	5.0	-5	49.4	46.6	1	2.8	4.2	-1	15.7	14.5	6	8.5	9.0
0	100.7	-110.1	-4	18.7	-17.9	-2 1 -9	11.8	10.7	0	19.6	-20.4	-2 13 -5	36.7	36.8
1	11.6	-13.8	-3	21.9	-20.5	-8	12.4	11.0	1	41.6	-43.7	-4	35.0	35.6
2	90.3	98.9	-2	20.4	18.9	-7	6.7	4.6	2	64.5	-68.2	-3	2.9	0.6
3	20.6	21.2	-1	23.9	-22.6	-6	6.5	4.1	3	7.4	- 7.0	-2	24.3	-23.1
4	13.2	14.3	0	27.3	-28.7	-5	16.4	14.0	4	70.1	70.4	-1	49.5	48.2
5	28.2	29.4	1	2.1	- 3.3	-4	16.0	-13.5	5	50.8	49.8	0	35.1	33.9
6	22.1	-21.6	2	2.2	1.4	-3	33.3	30.8	6	4.8	- 4.2	1	20.3	-19.4
7	33.0	-31.9	3	43.9	-45.1	-2	18.1	-17.4	7	9.8	7.0	2	2.9	2.8
8	18.9	18.1	4	21.4	13.9	-1	40.9	39.5	8	13.7	13.2	3	37.0	-35.9
9	39.8	38.1	5	28.7	27.2	0	35.1	-34.0	-2 7 -8	25.2	24.4	4	43.3	-40.5
-3 3 -8	15.7	-15.2	6	10.4	-10.8	1	33.8	-39.3	-7	31.8	32.1	5	4.5	2.8
-7	29.7	-28.9	7	29.2	27.5	2	95.2	-102.9	-6	2.7	2.9	-2 14 -5	35.8	-35.4
-6	2.7	- 2.7	8	11.8	-10.7	3	64.5	-67.1	-5	21.7	-20.4	-4	8.4	- 8.4
-5	24.0	-23.0	-3 9 -7	9.7	- 7.5	4	69.6	72.3	-4	7.1	6.8	-3	21.2	21.0
-4	79.7	76.4	-6	3.0	- 2.8	5	11.6	10.5	-3	122.9	117.7	-2	19.3	-17.5
-3	126.0	122.3	-5	10.1	-10.6	6	41.5	41.0	-2	33.6	-31.0	-1	2.8	1.9
-2	41.3	-37.6	-4	2.7	2.6	7	8.2	9.5	-1	15.0	13.8	0	16.6	16.9
-1	18.7	-19.7	-3	2.7	- 1.5	8	10.9	- 9.8	0	22.1	-22.8	1	18.7	18.1
0	21.7	-23.8	-2	4.3	3.3	9	2.9	- 0.6	1	38.7	-42.1	2	7.4	- 8.2
1	8.7	8.7	-1	43.5	41.2	-2 2 -9	2.8	1.8	2	14.3	-14.3	3	26.2	23.8
2	7.5	8.0	0	21.7	21.0	-8	15.3	15.1	3	5.0	- 4.5	4	17.9	15.7
3	38.0	41.0	1	27.7	29.6	-7	6.8	- 7.0	4	46.6	-44.8	-2 15 -3	9.4	- 9.0
4	19.9	-21.5	2	2.3	- 1.5	-6	30.3	-29.4	5	58.4	-57.6	-2	6.6	- 8.0
5	7.2	- 7.0	3	20.2	-21.2	-5	9.4	- 8.2	6	28.0	26.5	-1	15.6	-14.3
6	26.9	-26.3	4	18.7	19.1	-4	16.2	-15.6	7	36.5	34.4	0	33.4	-32.3
7	38.6	-38.2	5	2.7	- 0.6	-3	47.4	-44.0	8	16.4	16.3	1	13.7	-13.9
8	21.1	-20.2	6	16.7	15.2	-2	32.8	33.6	-2 8 -8	11.6	11.7	2	15.6	12.5
9	21.2	-20.0	7	5.5	2.4	-1	132.0	140.6	-7	59.8	-60.4	3	21.8	18.6
-3 4 -8	41.3	-39.2	-3 10 -7	16.9	17.1	0	78.9	-84.1	-6	4.2	3.6	-2 16 -2	7.5	8.3
-7	40.4	-38.5	-6	2.9	2.6	1	5.6	3.0	-5	14.6	14.7	-1	15.4	-15.1
-6	42.2	-41.7	-5	13.1	-10.6	2	17.1	-16.8	-4	29.0	-29.1	0	16.8	-15.8
-5	9.8	- 9.0	-4	36.6	-33.9	3	1.9	- 0.7	-3	15.4	-14.3	1	7.6	7.8
-4	44.7	42.2	-3	77.1	-74.6	4	23.4	24.1	-2	13.6	13.3	-1 1 -9	23.3	-25.8
-3	20.8	-18.8	-2	23.7	23.0	5	13.6	13.0	-1	12.3	-12.4	-8	2.7	2.5
-2	16.5	15.3	-1	22.1	21.6	6	87.6	-88.0	0	37.5	37.4	-7	18.9	18.8
-1	7.2	- 4.8	0	13.2	-13.6	7	36.4	-34.5	1	119.8	134.1	-6	10.3	- 9.4
0	61.8	-64.5	1	7.3	- 6.4	8	45.3	45.5	2	61.0	-65.7	-5	13.8	13.2
1	8.7	5.1	2	42.8	-46.0	9	15.2	-13.4	3	36.1	-35.5	-4	19.5	-17.7
2	57.6	60.8	3	8.2	- 7.1	-2 3 -9	18.2	18.6	4	13.7	-12.9	-3	7.3	- 6.6
3	37.0	39.0	4	18.3	18.3	-8	27.5	27.4	5	23.2	-22.5	-2	141.0	141.1
4	3.5	0.7	5	39.3	37.8	-7	28.3	27.4	6	6.4	7.4	-1	29.2	36.8
5	49.1	49.1	6	33.3	31.8	-6	76.8	-75.7	7	12.0	10.0	0	43.5	45.8
6	27.6	27.1	7	2.9	1.3	-5	43.0	-40.1	8	2.9	0.6	1	4.0	0.5
7	33.2	33.3	-3 11 -6	13.9	14.3	-4	2.3	- 0.6	-2 9 -7	28.1	29.5	2	54.2	-54.1
8	9.5	- 7.6	-5	17.1	-17.8	-3	6.3	5.0	-6	18.8	17.4	3	17.6	-15.7
-3 5 -8	4.8	3.5	-4	20.0	-18.5	-2	24.0	-22.5	-5	6.0	4.2	4	2.3	- 0.2
-7	2.8	2.9	-3	73.9	72.0	-1	39.6	-38.3	-4	27.8	-25.4	5	19.7	19.9
-6	9.6	10.4	-2	60.4	57.0	0	8.9	7.3	-3	89.4	-85.3	6	17.4	15.7
-5	16.6	14.9	-1	4.8	- 6.0	1	39.1	39.7	-2	30.0	-27.9	7	16.7	-16.1
-4	16.3	14.4	0	6.1	- 5.6	2	5.8	- 3.0	-1	12.9	12.2	8	36.1	-36.0
-3	18.0	17.6	1	28.5	-31.2	3	88.9	91.4	0	29.9	30.9	9	24.3	-21.9

Table 2. *(Continued)*

h	k	l	$\|F_o\|$	F_c
-1	2	-9	12.4	11.8
		-8	8.4	7.0
		-7	2.7	2.6
		-6	6.4	- 5.3
		-5	31.4	30.2
		-4	93.6	-89.0
		-3	2.3	- 1.2
		-2	35.8	34.4
		-1	11.4	-11.4
		0	16.1	-16.3
		1	64.9	-65.4
		2	17.6	-16.4
		3	19.0	18.1
		4	51.8	50.5
		5	14.1	13.1
		6	12.4	11.0
		7	30.2	29.3
		8	10.6	9.4
		9	2.9	2.1
-1	3	-9	2.8	- 4.1
		-8	32.7	33.1
		-7	17.0	16.4
		-6	15.8	-16.1
		-5	29.7	-30.0
		-4	19.9	20.7
		-3	60.1	54.3
		-2	7.4	- 5.5
		-1	43.8	38.8
		0	42.7	-42.6
		1	25.1	-24.7
		2	4.2	- 1.9
		3	40.9	-37.0
		4	71.4	-69.1
		5	43.7	-42.8
		6	67.4	65.9
		7	34.4	32.8
		8	12.7	12.1
		9	16.0	15.4
-1	4	-9	25.1	22.4
		-8	29.6	-30.0
		-7	29.3	-30.0
		-6	12.4	12.7
		-5	9.1	- 9.8
		-4	51.5	-49.5
		-3	10.0	- 9.9
		-2	7.6	- 6.9
		-1	35.8	-33.0
		0	160.7	200.8
		1	116.4	121.3
		2	48.7	-46.5
		3	19.1	-17.7
		4	14.8	-14.2
		5	21.2	-19.7
		6	15.5	14.3
		7	4.4	1.7
		8	17.2	-17.2
		9	26.5	-25.1
-1	5	-8	18.3	19.3
		-7	35.4	36.8
		-6	39.2	40.2
		-5	11.6	11.3
		-4	141.7	-143.6
		-3	117.4	-116.7
		-2	33.3	-29.7
		-1	36.3	33.9
		0	4.8	5.6
		1	36.4	-36.0
		2	63.5	60.0
		3	11.1	-10.5
		4	2.3	0.9
		5	5.7	2.4
		6	24.7	24.2
		7	2.7	1.8
		8	19.1	17.1
-1	6	-8	16.6	16.4
		-7	38.4	38.7
		-6	49.4	51.9
		-5	2.5	1.5
		-4	11.7	11.4
		-3	59.4	59.0
		-2	15.5	-14.9
		-1	48.2	42.8
		0	28.0	-27.4
		1	15.8	-15.6
		2	14.7	-12.6
		3	14.4	13.8
		4	8.0	- 6.8
		5	57.1	-55.6
		6	21.4	-21.6
		7	44.4	-43.8
		8	9.2	6.0
-1	7	-8	28.7	-27.7
		-7	16.5	-17.1
		-6	11.3	-11.8
		-5	13.4	-12.8
		-4	23.2	23.1
		-3	23.2	22.3
		-2	5.8	- 5.3
		-1	20.3	-19.7
		0	3.5	2.7
		1	6.5	5.0
		2	41.0	38.1
		3	117.8	118.1
		4	38.1	-36.8
		5	25.3	-24.6
		6	13.4	-13.0
		7	14.5	-14.6
		8	31.0	29.9
-1	8	-8	28.4	-28.9
		-7	2.7	- 3.2
		-6	19.7	20.6
		-5	20.0	18.8
		-4	12.9	12.8
		-3	29.6	31.0
		-2	41.8	-40.2
		-1	76.3	-78.9
		0	9.2	9.0
		1	10.1	9.3
		2	14.6	13.8
		3	36.7	-37.3
		4	17.4	-16.5
		5	9.9	11.7
		6	23.3	24.0
		7	68.0	65.3
		8	3.0	- 0.8
-1	9	-7	10.3	-10.8
		-6	19.8	18.8
		-5	40.8	42.2
		-4	5.3	4.7
		-3	18.2	-18.8
		-2	2.4	- 0.5
		-1	57.8	62.6
		0	13.3	-13.1
		1	43.3	-42.7
		2	24.4	21.8
		3	47.6	-46.4
		4	24.1	-23.2
		5	4.6	3.3
		6	9.3	- 7.6
		7	48.7	-44.1
-1	10	-7	15.7	15.7
		-6	9.0	- 6.9
		-5	42.1	-44.0
		-4	2.6	- 0.1
		-3	8.6	7.9
		-2	26.3	-27.7
		-1	6.1	6.5
		0	18.0	19.1
		1	3.8	- 1.8
		2	25.2	22.9
		3	78.2	74.5
		4	15.4	13.1
		5	31.5	-28.4
		6	2.8	- 1.6
		7	12.3	-11.1
-1	11	-7	9.8	9.0
		-6	8.7	- 7.8
		-5	8.8	10.3
		-4	5.3	6.4
		-3	2.6	- 0.5
		-2	28.4	-28.8
		-1	20.7	-21.1
		0	57.2	-58.5
		1	34.7	-32.1
		2	29.1	26.7
		3	5.6	2.9
		4	8.0	7.8
		5	6.0	6.3
		6	44.1	-41.1
-1	12	-6	7.6	- 6.7
		-5	17.9	15.8
		-4	29.8	29.6
		-3	49.0	51.9
		-2	5.8	- 6.1
		-1	9.9	-10.4
		0	8.9	- 8.6
		1	45.3	43.7
		2	36.3	35.5
		3	10.0	8.2
		4	14.2	-14.2
		5	29.5	-28.0
		6	9.8	- 8.0
-1	13	-5	10.8	12.1
		-4	21.5	19.8
		-3	65.1	-67.8
		-2	25.2	-26.0
		-1	28.6	30.4
		0	11.4	-10.7
		1	13.1	12.9
		2	7.4	7.0
		3	9.7	- 9.3
		4	22.6	19.4
		5	60.5	56.2
-1	14	-5	8.5	-10.1
		-4	10.8	10.8
		-3	15.5	15.9
		-2	17.9	17.6
		-1	6.5	4.5
		0	8.0	- 7.3
		1	79.3	-74.0
		2	34.1	-31.4
		3	24.2	22.0
		4	25.5	22.8
		5	34.5	33.5
		-2	40.0	41.1
		-1	2.6	2.3
		0	22.5	-21.9
		1	10.5	11.7
		2	8.2	- 7.5
		3	40.3	-37.6
-1	16	-1	29.8	30.4
		0	16.4	-15.8
0	0	1	55.2	50.0
		2	56.0	-51.8
		3	25.3	-24.0
		4	34.2	-33.6
		5	11.1	- 9.7
		6	19.3	18.1
		7	11.9	-13.3
		8	43.2	-44.3
		9	4.1	2.8
0	1	-9	2.9	- 0.6
		-8	24.5	26.2
		-7	25.9	25.4
		-6	35.2	34.4
		-5	14.3	-13.4
		-4	137.8	-142.6
		-3	103.9	-102.5
		-2	9.4	- 7.4
		-1	16.5	16.4
		0	31.6	-30.1
		1	3.5	- 1.7
		2	53.8	45.3
		3	59.7	-53.6
		4	86.8	82.3
		5	5.1	- 2.4
		6	11.3	-11.6
		7	10.5	-11.2
		8	25.8	22.8
		9	22.4	22.2
0	2	-9	2.8	- 0.5
		-8	4.8	5.4
		-7	34.7	34.5
		-6	44.3	45.1
		-5	2.4	2.8
		-4	64.0	63.5
		-3	57.8	55.9
		-2	70.5	-67.0
		-1	17.0	-13.9
		0	20.0	-17.7
		1	21.9	-20.9
		2	14.9	12.2
		3	25.4	24.5
		4	61.9	-57.6
		5	23.0	-19.6
		6	9.4	8.9
		7	38.0	-36.8
		8	25.9	24.2
		9	26.9	26.7
0	3	-9	8.3	- 7.2
		-8	17.2	-15.7
		-7	15.0	-16.6
		-6	7.5	- 5.5
		-5	21.4	22.0
		-4	18.8	18.9
		-3	10.4	-10.9
		-2	19.2	-17.8
		-1	31.4	-32.4
		0	31.2	29.6
		1	29.9	-20.6
		2	19.5	17.8
		3	32.2	29.2
		4	39.7	-37.4
		5	8.6	8.0
		6	15.0	-14.1
		7	7.5	5.2
		8	17.3	16.7
		9	14.6	-15.4
0	4	-9	5.7	5.5
		-8	25.2	-24.6
		-7	7.6	7.5
		-6	31.2	31.3
		-5	2.5	- 4.5
		-4	68.3	68.0
		-3	10.1	- 8.1
		-2	120.2	-129.1
		-1	40.6	-42.2
		0	38.9	40.3
		1	17.6	-15.1
		2	8.2	6.7
		3	45.1	-41.8
		4	9.2	8.9
		5	10.4	11.0
		6	54.8	54.5
		7	37.2	35.8
0	5	-9	22.9	-22.4
		-8	14.2	-13.4
		-7	4.3	- 5.6
		-6	56.9	58.4
		-5	27.0	27.4
		-4	12.1	-11.9
		-3	22.7	-23.4
		-2	70.5	73.7
		-1	5.0	5.4
		0	16.4	15.7
		1	20.2	17.5
		2	14.0	-12.4
		3	63.3	-58.6
		4	9.6	- 8.7
		5	6.4	6.4
		6	55.4	-54.0
		7	62.4	-59.2
		8	41.1	37.2
0	6	-8	14.2	-13.3
		-7	30.1	31.0
		-6	79.4	-83.3
		-5	73.4	-78.3
		-4	23.1	24.1
		-3	2.6	- 0.7
		-2	2.1	0.8
		-1	12.0	12.8
		0	6.8	6.7
		1	28.3	-26.8
		2	133.9	130.3
		3	96.9	91.5
		4	2.5	0.1
		5	6.7	6.8
		6	24.5	-23.9
		7	18.3	-16.9
		8	2.9	- 0.9
0	7	-8	4.8	- 0.6
		-7	3.6	- 5.2
		-6	7.9	-10.4
		-5	21.8	22.5
		-4	9.7	8.9
		-3	17.2	16.9
		-2	59.2	-62.1
		-1	61.7	-66.0
		0	61.9	-62.1
		1	15.8	-15.0
		2	51.6	48.9
		3	8.7	- 8.1
		4	20.8	19.6
		5	34.4	-34.7
		6	32.0	-30.0
		7	21.0	21.9
0	8	-8	3.2	1.6
		-7	9.3	- 7.1
		-6	2.6	- 0.7
		-5	12.2	11.9
		-4	52.2	55.3
		-3	33.7	35.3
		-2	13.1	-14.5
		-1	13.5	-14.0
		0	3.0	- 4.1
		1	54.1	54.3
		2	24.3	23.3
		3	27.8	-28.3
		4	26.5	-26.0
		5	21.7	-20.4
		6	4.4	4.2
		7	18.6	-17.0
0	9	-7	13.4	-14.8
		-6	2.7	- 3.3
		-5	15.8	15.7
		-4	26.1	27.5
		-3	44.0	-47.0
		-2	14.5	15.8
		-1	7.6	- 7.8
		0	20.0	-20.6
		1	11.1	11.3
		2	3.7	3.5
		3	19.2	-18.9
		4	62.4	54.3
		5	67.2	65.3
		6	22.3	-20.7
		7	34.2	-32.0
0	10	-7	35.0	36.4
		-6	17.3	-17.7
		-5	3.0	0.4
		-4	20.5	21.7
		-3	22.8	24.7
		-2	27.3	28.8
		-1	2.2	0.4
		0	62.7	-64.5
		1	98.8	-98.0
		2	6.6	5.6
		3	19.8	18.8
		4	13.4	12.1
		5	8.7	- 9.0
		6	18.8	17.8
		7	13.0	14.9
0	11	-7	37.0	-37.5
		-6	31.8	-30.8
		-5	8.2	- 8.0
		-4	14.1	13.0
		-3	63.0	67.5
		-2	40.0	43.7
		-1	8.9	- 9.1
		0	7.6	- 5.9
		1	37.3	37.8
		2	21.8	-21.5
		3	25.5	-24.2
		4	19.4	17.2
		5	10.0	- 9.9
		6	6.8	- 7.0
0	12	-6	41.5	-41.8
		-5	15.9	-16.9
		-4	6.4	- 5.2
		-3	46.3	-50.3
		-2	2.4	0.1
		-1	6.0	- 4.8
		0	9.1	- 8.3
		1	21.8	22.6
		2	7.4	8.1
		3	2.8	- 2.7
		4	4.9	5.1
		5	20.6	19.0
0	13	-5	26.6	26.8
		-4	22.4	-23.3
		-3	14.1	-14.2
		-2	9.4	9.4
		-1	5.5	- 7.9
		0	23.5	24.6
		1	4.7	- 2.5
		2	16.7	-15.7
		3	55.0	-50.5
		4	5.5	- 6.7
		5	11.6	8.9
0	14	-4	32.1	-30.9
		-3	6.8	5.4
		-2	20.8	21.4
		-1	43.0	44.7
		0	12.1	11.5
		1	21.0	-20.3
		2	8.0	- 7.4
		3	22.1	22.0
		4	32.6	30.1
0	15	-3	11.1	12.0
		-2	19.3	19.2
		-1	30.1	-31.0
		0	24.2	-22.9
		1	25.5	24.3
		2	15.4	-14.5
1	0	-9	21.5	-20.6
		-8	15.9	-16.0
		-7	8.1	8.6
		-6	46.7	46.6
		-5	6.1	- 5.2
		-4	15.8	14.1
		-3	132.1	-138.6
		-2	134.8	-132.7
		-1	23.8	23.7
		0	14.0	14.9
		1	33.0	-30.4
		2	33.4	-30.2
		3	3.4	- 2.5
		4	5.5	- 5.1
		5	3.3	4.6
		6	87.6	88.6
		7	10.6	11.2
		8	3.6	- 0.2
		9	17.2	16.2
1	1	-9	10.4	- 9.9
		-8	23.7	-23.4
		-7	15.5	15.5
		-6	70.1	71.1
		-5	3.4	2.6
		-4	5.9	- 5.6
		-3	30.6	31.4
		-2	118.3	129.7
		-1	46.9	46.8
		0	19.2	-14.4
		1	30.6	-27.6
		2	60.0	-56.8
		3	17.7	-11.7
		4	14.2	13.1
		5	10.9	- 8.1
		6	116.2	-115.2
		7	25.6	-24.6
		8	43.6	42.2
		9	2.9	- 2.4
1	2	-9	21.5	-20.9
		-8	2.6	- 1.0
		-7	2.6	- 0.3
		-6	93.4	-97.5
		-5	45.8	-45.5
		-4	40.2	39.1
		-3	4.5	4.9
		-2	19.4	18.8
		-1	23.3	23.5
		0	36.2	-38.9
		1	18.7	17.6
		2	145.7	148.7
		3	66.1	60.5
		4	48.2	-44.8
		5	10.4	- 8.8
		6	50.5	-48.8

Table 2. *(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	2	7	11.9	-11.6	1	8	3	20.1	-19.2	2	1	-9	22.5	-21.7	2	6	3	47.1	48.1	3	0	-9	2.9	- 2.5
		8	6.1	6.6			4	21.5	20.1			-8	10.5	-10.3			4	12.5	-12.0			-8	6.0	6.0
		9	26.2	24.2			5	27.9	25.1			-7	11.7	-10.3			5	15.7	14.0			-7	15.2	-14.6
1	3	-9	14.6	16.2			6	11.0	- 9.1			-6	51.4	-52.7			6	19.8	-19.2			-6	27.2	29.1
		-8	7.8	- 7.0			7	27.0	25.4			-5	5.0	- 2.9			7	21.6	-21.6			-5	20.7	-20.6
		-7	5.9	- 5.7	1	9	-7	4.4	4.6			-4	36.2	-38.7	2	7	-8	7.1	5.8			-4	111.0	-123.2
		-6	25.8	27.5			-6	16.5	18.0			-3	8.5	9.8			-7	4.6	- 1.2			-3	18.7	19.2
		-5	20.0	19.1			-5	8.4	9.0			-2	25.2	25.9			-6	25.9	-27.5			-2	23.5	26.2
		-4	19.8	19.7			-4	20.8	-22.3			-1	19.9	-19.3			-5	22.6	-24.4			-1	2.9	- 2.2
		-3	38.8	-38.6			-3	4.8	5.6			0	25.8	-25.6			-4	12.3	-12.3			0	20.5	21.0
		-2	8.6	- 9.4			-2	2.2	- 0.8			1	13.8	-14.3			-3	28.9	32.4			1	12.0	11.0
		-1	11.6	-14.7			-1	7.1	- 6.8			2	21.7	-20.7			-2	72.6	-80.0			2	60.0	-58.6
		0	41.1	-43.0			0	40.1	42.6			3	96.0	93.2			-1	87.2	-94.9			3	32.8	31.3
		1	15.2	15.7			1	33.2	-32.6			4	178.2	182.0			0	24.3	25.1			4	110.6	106.5
		2	12.4	11.6			2	35.0	-32.1			5	29.6	27.8			1	2.2	- 1.6			5	13.1	-13.6
		3	15.7	15.0			3	28.9	-28.1			6	29.0	-26.7			2	9.3	10.6			6	24.2	22.2
		4	22.0	19.6			4	25.6	23.6			7	12.9	-12.2			3	28.7	27.7			7	10.0	- 8.0
		5	34.8	-32.6			5	9.2	8.5			8	33.8	-32.8			4	19.3	-18.4			8	9.1	- 7.8
		6	13.5	-11.5			6	11.3	10.5	2	2	-9	15.6	16.2			5	10.2	10.9	3	1	-9	45.8	44.6
		7	36.0	34.5			7	12.7	-12.9			-8	54.5	55.8			6	74.5	71.2			-8	44.8	46.1
		8	7.3	6.6	1	10	-7	5.7	4.0			-7	20.9	-20.3			7	58.7	55.3			-7	18.7	19.5
1	4	-9	21.8	-22.4			-6	2.8	- 1.5			-6	38.7	-39.6	2	8	-7	24.6	-24.3			-6	6.9	8.7
		-8	15.3	-15.2			-5	13.3	-11.5			-5	2.3	- 0.2			-6	73.7	77.1			-5	18.7	-19.9
		-7	6.0	- 3.9			-4	10.9	-10.8			-4	21.7	22.4			-5	48.5	53.0			-4	2.1	- 3.4
		-6	20.8	20.9			-3	6.8	- 6.9			-3	66.3	69.6			-4	24.3	-26.4			-3	7.4	7.9
		-5	18.0	17.3			-2	45.2	48.3			-2	28.5	31.1			-3	11.7	-12.8			-2	3.2	4.7
		-4	60.3	62.0			-1	29.8	30.6			-1	40.5	-43.1			-2	2.2	1.0			-1	44.7	48.1
		-3	16.1	-17.5			0	14.1	-15.1			0	166.1	-213.8			-1	30.7	32.7			0	112.2	-124.5
		-2	3.3	1.4			1	13.9	-13.4			1	45.0	-44.0			0	8.3	8.3			1	111.1	-118.5
		-1	30.0	-30.2			2	9.5	- 9.4			2	16.2	14.9			1	3.5	- 3.2			2	73.2	-72.4
		0	8.5	- 8.2			3	19.0	18.0			3	10.5	10.0			2	56.7	-56.1			3	25.8	24.5
		1	50.4	-45.9			4	17.7	14.5			4	13.9	-12.9			3	76.7	-72.9			4	7.3	7.1
		2	43.2	38.8			5	14.2	-13.4			5	2.5	1.1			4	10.0	- 9.3			5	6.2	5.1
		3	8.5	7.9			6	4.8	- 6.0			6	2.7	- 2.3			5	13.6	12.8			6	2.7	- 0.0
		4	28.1	-26.7	1	11	-6	10.4	- 9.8			7	16.3	16.4			6	17.1	15.6			7	24.4	-22.8
		5	4.1	2.8			-5	17.8	-18.4			8	41.8	41.2			7	13.5	12.9			8	8.6	7.5
		6	27.8	-26.4			-4	6.3	- 6.2	2	3	-9	2.8	- 2.3	2	9	-7	9.8	11.6	3	2	-9	16.4	16.5
		7	22.9	-20.9			-3	25.4	27.1			-8	22.9	-23.4			-6	10.2	-12.2			-8	8.8	7.0
		8	17.4	-15.9			-2	10.0	-11.7			-7	24.7	-23.7			-5	49.2	-51.4			-7	12.6	-13.9
1	5	-8	17.2	-17.5			-1	52.7	-55.6			-6	40.4	-42.1			-4	6.4	- 4.1			-6	21.8	-20.8
		-7	2.6	- 3.2			0	17.9	18.1			-5	19.1	-20.5			-3	8.6	- 9.2			-5	15.2	16.9
		-6	11.0	-10.1			1	3.8	- 2.1			-4	55.8	58.9			-2	34.0	36.2			-4	22.0	-23.4
		-5	37.6	39.3			2	28.3	-26.5			-3	67.3	70.9			-1	49.8	53.2			-3	70.5	75.6
		-4	13.1	-14.0			3	20.0	19.7			-2	31.0	31.0			0	41.2	42.8			-2	70.5	76.3
		-3	42.1	-43.6			4	10.8	9.8			-1	1.8	1.9			1	7.7	- 4.6			-1	9.9	-10.0
		-2	26.8	28.9			5	5.2	2.8			0	57.1	59.1			2	13.5	-13.4			0	19.9	19.6
		-1	48.7	-51.0			6	38.0	35.8			1	65.8	65.6			3	19.5	18.9			1	38.7	37.8
		0	11.2	-10.6	1	12	-6	21.8	21.1			2	49.6	-48.1			4	37.0	-33.8			2	4.9	5.9
		1	4.3	- 2.4			-5	60.4	64.5			3	23.6	-22.6			5	2.7	2.1			3	74.8	73.0
		2	23.1	-21.4			-4	4.9	- 4.3			4	68.0	-66.3			6	26.0	22.6			4	10.5	-10.5
		3	13.4	11.8			-3	6.0	- 6.9			5	18.2	-16.9	2	10	-7	11.9	10.5			5	20.3	-20.0
		4	151.4	150.9			-2	2.4	0.8			6	22.9	22.1			-6	2.7	3.8			6	30.3	-29.9
		5	43.5	41.8			-1	11.9	12.2			7	11.7	11.4			-5	27.2	-26.5			7	5.9	- 5.6
		6	39.0	-36.7			0	11.4	11.5			8	50.2	-47.0			-4	34.4	-37.3			8	2.8	1.0
		7	2.8	- 1.2			1	11.3	-12.4	2	4	-9	4.1	4.5			-3	2.4	- 1.7	3	3	-8	16.9	15.9
		8	19.9	-18.5			2	32.8	-31.6			-8	12.9	13.0			-2	10.2	-10.3			-7	10.0	-10.0
1	6	-8	42.0	43.8			3	59.8	-56.9			-7	30.9	-30.1			-1	7.6	7.4			-6	31.9	-33.5
		-7	16.4	17.7			4	22.0	-20.1			-6	5.7	- 4.3			0	32.2	33.5			-5	30.0	-30.4
		-6	32.8	-33.5			5	11.7	9.5			-5	2.4	- 0.9			1	7.5	- 8.6			-4	16.7	18.6
		-5	2.5	- 4.4	1	13	-5	43.6	-45.2			-4	67.1	-73.5			2	5.5	6.2			-3	16.5	-16.6
		-4	24.3	25.7			-4	2.7	- 1.5			-3	12.9	-13.4			3	3.8	1.8			-2	118.3	-131.7
		-3	38.1	40.1			-3	10.1	- 9.3			-2	54.4	57.6			4	2.7	- 0.6			-1	1.9	0.4
		-2	32.9	35.2			-2	2.5	- 3.1			-1	3.9	- 1.1			5	9.7	9.3			0	38.4	39.6
		-1	17.3	17.9			-1	37.3	38.0			0	9.9	11.0			6	16.1	-14.9			1	20.9	21.6
		0	164.6	-185.0			0	49.9	49.8			1	29.7	29.7	2	11	-6	25.4	24.4			2	16.3	16.1
		1	132.5	-133.9			1	22.3	22.7			2	19.7	-19.1			-5	19.6	-20.1			3	6.4	- 6.1
		2	16.4	15.9			2	13.8	-12.6			3	3.8	- 1.4			-4	4.6	- 4.2			4	23.8	-22.1
		3	12.5	11.1			3	2.7	2.3			4	43.3	40.5			-3	20.2	21.5			5	42.6	41.6
		4	6.4	6.1			4	7.3	- 5.5			5	7.2	- 2.3			-2	20.3	-21.6			6	76.2	73.2
		5	2.7	- 3.5	1	14	-4	32.9	-34.5			6	2.7	- 2.6			-1	12.8	13.7			7	10.0	8.4
		6	10.8	11.2			-3	28.7	-29.7			7	2.8	1.5			0	2.5	0.7			8	27.2	-25.4
		7	2.8	- 2.2			-2	7.5	6.1			8	21.8	-19.9			1	5.6	4.8	3	4	-8	31.7	-33.0
		8	23.4	23.7			-1	11.8	-11.4	2	5	-8	43.5	43.1			2	18.8	19.0			-7	14.3	-15.0
1	7	-8	16.5	-18.1			0	25.5	23.0			-7	2.7	- 1.2			3	6.3	4.0			-6	79.4	83.5
		-7	60.3	-61.3			1	23.1	-23.7			-6	23.8	24.0			4	64.6	-60.9			-5	2.4	1.9
		-6	17.8	-16.2			2	18.2	-17.7			-5	11.4	-11.6			5	48.2	-45.5			-4	22.3	-24.3
		-5	17.1	-18.4			3	11.5	12.0			-4	2.2	- 1.5	2	12	-5	19.8	20.6			-3	8.9	10.5
		-4	50.2	53.7	1	15	-2	2.7	- 0.2			-3	12.8	13.3			-4	5.5	4.3			-2	20.9	21.8
		-3	73.5	82.3			-1	11.4	- 9.8			-2	3.1	2.7			-3	45.3	-46.5			-1	17.0	18.4
		-2	43.2	46.8			0	12.5	11.5			-1	9.8	10.3			-2	11.1	-10.4			0	47.1	48.4
		-1	14.3	-15.9			1	7.6	- 8.7			0	24.0	-24.1			-1	10.9	-10.0			1	29.6	-30.2
		0	43.4	43.3	2	0	-9	26.6	-26.5			1	36.3	-35.4			0	20.5	20.7			2	103.0	-104.4
		1	74.5	74.3			-8	16.1	-15.5			2	61.8	-58.5			1	64.3	65.1			3	21.8	-19.0
		2	44.3	-42.8			-7	21.9	23.4			3	3.7	2.6			2	13.1	12.7			4	15.4	14.1
		3	21.8	20.4			-6	40.4	40.1			4	9.7	9.4			3	2.7	- 2.4			5	16.6	15.7
		4	21.4	-21.5			-5	47.3	48.4			5	5.0	- 3.9			4	2.8	- 2.0			6	13.6	13.0
		5	39.3	-38.3			-4	25.9	25.6			6	14.6	13.0	2	13	-4	9.3	9.1			7	7.0	6.4
		6	2.8	- 0.2			-3	17.7	-18.5			7	10.7	- 9.6			-3	35.8	-37.9			8	9.9	8.7
		7	17.4	15.9			-2	47.0	49.4			8	9.8	- 7.5			-2	38.8	-40.6	3	5	-8	7.1	6.0
1	8	-8	2.9	4.9			-1	45.9	-44.2	2	6	-8	10.9	11.3			-1	2.6	4.4			-7	11.0	11.3
		-7	23.4	-23.5			0	6.9	- 5.6			-7	13.1	12.9			0	4.4	- 5.0			-6	49.3	-52.1
		-6	42.8	-43.5			1	9.3	6.6			-6	18.1	-19.4			1	72.8	-74.8			-5	10.2	- 9.9
		-5	2.6	1.8			2	30.6	28.6			-5	27.3	-27.2			2	14.8	13.3			-4	24.9	-26.3
		-4	28.3	-30.5			3	17.7	-16.7			-4	2.3	- 3.3			3	10.5	10.1			-3	2.1	- 2.6
		-3	90.0	-102.2			4	18.8	-17.0			-3	27.0	28.7	2	14	-3	42.4	45.2			-2	63.4	68.3
		-2	27.8	30.1			5	19.3	17.3			-2	89.2	97.3			-2	19.4	21.9			-1	49.6	51.9
		-1	3.8	4.7			6	43.1	-40.7			-1	4.6	3.6			-1	2.7	- 0.9			0	28.0	27.7
		0	33.1	34.2			7	28.9	-27.5			0	25.0	-24.6			0	11.4	-10.7			1	18.5	-18.7
		1	36.1	37.9			8	53.5	-52.1			1	8.3	7.0			1	6.5	- 6.9			2	21.2	20.7
		2	3.5	- 1.4			9	11.8	-12.0			2	3.8	4.1			2	6.4	- 7.5			3	21.6	-21.2

Table 2. *(Continued)*

h	k	l	$\|F_o\|$	F_c
3	5	4	50.6	-49.7
		5	7.0	7.1
		6	2.7	- 0.9
		7	17.4	-15.6
3	6	-8	15.2	15.5
		-7	12.2	11.4
		-6	10.3	-10.4
		-5	33.6	-35.4
		-4	23.7	-24.4
		-3	19.3	21.3
		-2	78.6	-87.0
		-1	43.0	45.3
		0	29.1	29.9
		1	11.8	-13.2
		2	3.7	2.1
		3	16.9	-16.8
		4	5.1	3.2
		5	2.7	- 1.7
		6	5.6	5.3
		7	24.5	22.2
3	7	-7	16.3	14.2
		-6	29.8	30.1
		-5	12.4	13.6
		-4	36.0	39.3
		-3	4.6	5.0
		-2	45.5	-49.2
		-1	6.9	6.0
		0	5.8	- 7.1
		1	47.0	49.5
		2	2.3	0.2
		3	12.7	-13.5
		4	88.8	-85.9
		5	* 10.7	-39.8
		6	11.8	10.1
		7	3.0	- 2.3
3	8	-7	2.8	- 3.0
		-6	34.4	36.2
		-5	* 2.7	15.1
		-4	* 2.3	- 9.7
		-3	* 46.8	-54.4
		-2	* 34.5	-32.5
		-1	* 2.3	- 8.1
		0	* 64.3	69.8
		1	* 71.4	72.1
		2	* 2.6	5.1
		3	* 2.7	- 6.5
		4	11.0	10.2
		5	48.9	47.0
		6	12.3	-10.7
3	9	-7	33.1	33.2
		-6	9.7	8.6
		-5	9.4	9.4
		-4	10.2	- 9.8
		-3	41.7	-44.9
		-2	25.3	-25.9
		-1	20.6	21.9
		0	50.1	-51.5
		1	63.8	-66.6
		2	30.3	30.3
		3	2.5	0.2
		4	24.8	25.1
		5	39.3	37.6
		6	8.6	- 7.2
3	10	-6	5.4	- 5.5
		-5	2.6	- 4.6
		-4	40.7	42.7
		-3	33.1	35.3
		-2	13.9	-12.5
		-1	2.4	- 1.8
		0	8.0	- 7.4
		1	7.4	6.2
		2	16.1	-17.1
		3	5.8	5.1
		4	10.5	- 9.1
		5	34.3	-32.1
3	11	-5	2.7	- 2.4
		-4	2.6	- 0.6
		-3	2.6	- 4.9
		-2	7.3	8.9
		-1	2.5	- 0.1
		0	2.6	- 3.3
		1	39.3	39.2
		2	32.9	31.9
		3	2.7	- 1.6
		4	20.5	-19.6
3	12	-5	22.6	21.6
		-4	7.4	7.8
		-3	5.6	- 4.8
		-2	30.1	-30.6
		-1	17.7	-18.6
		0	6.8	- 6.3
		1	21.6	19.9
		2	5.1	5.1
		3	29.6	-29.3
3	13	-3	16.6	-17.3
		-2	19.2	20.7
		-1	48.1	47.5
		0	14.9	-14.2
		1	2.7	- 2.1
		2	2.7	0.8
3	14	-1	37.7	-36.9
		0	20.1	-18.8
4	0	-8	41.1	-40.5
		-7	37.1	36.3
		-6	54.1	57.0
		-5	25.1	-27.6
		-4	8.0	- 7.9
		-3	23.8	24.9
		-2	47.6	50.2
		-1	11.3	12.6
		0	54.7	58.2
		1	91.0	-95.6
		2	114.6	-118.2
		3	5.2	- 5.4
		4	2.6	0.0
		5	2.6	- 0.7
		6	11.9	11.7
		7	15.9	15.1
		8	8.7	7.6
4	1	-8	16.4	16.8
		-7	10.2	8.7
		-6	47.2	-48.5
		-5	33.2	-36.6
		-4	48.2	-52.3
		-3	67.7	73.7
		-2	105.0	114.8
		-1	50.4	53.4
		0	6.4	- 4.4
		1	9.2	- 9.3
		2	75.6	76.2
		3	40.9	-39.9
		4	41.7	-40.0
		5	10.8	9.1
		6	10.2	- 9.0
		7	5.2	- 5.1
		8	16.9	15.7
4	2	-8	8.2	7.2
		-7	10.3	8.8
		-6	18.7	-19.4
		-5	42.1	-44.6
		-4	12.4	-12.0
		-3	33.7	-36.3
		-2	95.4	-104.9
		-1	4.3	3.8
		0	17.5	-18.0
		1	19.1	20.1
		2	35.5	36.2
		3	5.0	3.8
		4	13.6	-12.7
		5	22.4	-21.0
		6	28.5	27.5
		7	39.6	37.8
		8	39.4	36.9
4	3	-8	12.0	10.7
		-7	44.1	44.4
		-6	32.5	34.1
		-5	35.1	37.3
		-4	29.3	32.3
		-3	41.7	-45.4
		-2	38.1	-41.6
		-1	2.1	- 2.5
		0	17.0	18.3
		1	21.7	23.0
		2	31.3	30.7
		3	38.1	-36.9
		4	87.1	-86.4
		5	7.6	- 8.0
		6	6.0	5.8
		7	9.4	9.0
4	4	-8	42.2	-43.2
		-7	15.6	15.8
		-6	25.5	26.3
		-5	2.4	0.5
		-4	29.8	-31.6
		-3	12.8	-13.3
		-2	39.1	-42.8
		-1	3.5	3.0
		0	74.1	76.5
		1	17.7	16.9
		2	12.9	12.6
		3	6.9	- 7.7
		4	40.2	39.2
		5	7.9	7.3
		6	6.3	- 7.2
		7	21.5	-20.7
4	5	-8	19.7	20.5
		-7	20.9	20.1
		-6	13.0	13.1
		-5	8.1	9.7
		-4	18.8	-19.8
		-3	31.2	-33.8
		-2	16.8	18.4
		-1	25.5	27.3
		0	101.0	-106.4
		1	10.4	10.6
		2	48.5	49.1
		3	17.0	-16.9
		4	38.3	38.2
		5	7.2	7.2
		6	13.3	-12.5
4	5	7	6.9	6.5
4	6	-7	4.3	5.3
		-6	19.0	-18.8
		-5	8.0	5.7
		-4	58.7	63.2
		-3	12.3	12.3
		-2	11.6	-12.7
		-1	13.4	13.8
		0	8.6	7.6
		1	12.7	-11.5
		2	8.4	- 9.7
		3	17.4	17.0
		4	69.2	-68.0
		5	32.6	-30.3
		6	4.9	4.5
4	7	-7	16.7	-18.2
		-6	16.2	-16.2
		-5	22.0	24.2
		-4	9.2	- 9.8
		-3	13.6	-15.4
		-2	9.6	10.9
		-1	10.5	-10.4
		0	15.6	16.3
		1	53.0	54.6
		2	39.4	38.9
		3	12.1	-10.4
		4	10.8	11.4
		5	6.5	- 7.2
		6	30.4	-27.9
4	8	-7	14.0	14.5
		-6	12.6	13.4
		-5	21.9	22.0
		-4	2.5	- 2.0
		-3	23.9	-26.3
		-2	47.4	-50.0
		-1	14.4	-14.7
		0	6.1	- 7.7
		1	2.4	- 1.8
		2	18.4	-19.1
		3	40.7	-42.1
		4	14.2	13.6
		5	5.1	- 0.3
		6	11.3	11.5
4	9	-6	17.8	19.5
		-5	32.0	32.9
		-4	13.5	-15.2
		-3	11.6	-12.0
		-2	65.6	70.1
		-1	31.8	33.1
		0	30.2	-29.8
		1	9.9	-10.3
		2	6.4	- 7.7
		3	17.8	18.6
		4	28.4	26.6
		5	17.7	-17.2
4	10	-5	21.7	-23.9
		-4	12.0	13.1
		-3	11.6	11.3
		-2	21.9	-22.3
		-1	24.2	-24.9
		0	23.9	-24.0
		1	4.6	- 4.4
		2	47.0	47.7
		3	53.1	52.5
		4	13.8	13.4
4	11	-5	43.7	44.5
		-4	8.5	- 9.9
		-3	18.5	18.7
		-2	16.5	-15.9
		-1	41.3	-42.4
		0	18.1	-18.0
		1	16.5	15.8
		2	29.5	-29.2
		3	2.7	1.0
4	12	-3	7.3	5.8
		-2	25.7	26.0
		-1	16.5	16.2
		0	19.0	-18.6
		1	2.7	- 1.0
		2	13.8	-12.8
4	13	-1	2.8	3.7
		0	14.6	13.8
5	0	-8	17.2	-16.6
		-7	21.4	21.3
		-6	3.2	0.2
		-5	2.4	- 0.6
		-4	4.4	- 4.2
		-3	32.3	-35.2
		-2	36.3	-38.4
		-1	42.0	44.0
		0	53.9	56.3
		1	4.0	- 2.3
		2	14.6	15.0
		3	16.2	-16.9
		4	50.4	48.7
		5	20.0	-18.7
		6	7.7	- 6.9
		7	25.8	-23.9
5	1	-8	21.4	21.7
		-7	18.6	17.0
		-6	5.9	6.1
		-5	17.7	-18.4
		-4	10.6	-10.4
		-3	2.2	3.7
		-2	20.4	21.6
		-1	43.2	-45.2
		0	81.5	-85.4
		1	32.8	33.0
		2	3.4	3.0
		3	14.1	-13.4
		4	37.3	36.8
		5	2.6	- 0.6
		6	15.7	-13.0
		7	32.7	30.0
5	2	-8	2.8	0.1
		-7	7.6	- 9.2
		-6	25.8	-27.5
		-5	66.9	71.9
		-4	84.6	94.5
		-3	9.1	7.8
		-2	13.9	-14.9
		-1	13.6	-15.0
		0	2.3	- 1.3
		1	4.9	5.7
		2	23.1	23.0
		3	39.1	-39.8
		4	88.4	-88.5
		5	20.2	-19.6
		6	6.8	- 6.7
		7	10.7	8.3
5	3	-8	45.8	-46.4
		-7	21.6	-23.3
		-6	5.9	4.8
		-5	10.0	10.7
		-4	6.2	- 6.1
		-3	26.4	-29.4
		-2	11.0	-12.7
		-1	9.2	10.1
5	4	-7	2.7	2.2
		-6	8.1	8.2
		-5	2.4	0.2
		-4	6.8	6.9
		-3	39.5	-42.6
		-2	28.3	-29.6
		-1	35.7	-38.0
		0	7.0	5.7
		1	2.3	3.6
		2	36.6	-37.6
		3	8.2	- 8.6
		4	25.4	26.8
		5	14.0	13.0
		6	13.2	11.9
		7	18.7	-16.9
5	5	-7	9.4	9.6
		-6	7.8	5.5
		-5	21.4	23.1
		-4	17.5	-18.4
		-3	8.6	- 9.4
		-2	56.9	60.6
		-1	29.5	-31.0
		0	9.8	-10.2
		1	3.8	3.7
		2	12.0	11.8
		3	10.0	10.7
		4	27.1	25.1
		5	23.7	-22.6
		6	63.3	-60.7
5	6	-7	8.1	7.1
		-6	46.0	-48.1
		-5	4.7	5.0
		-4	11.5	12.1
		-3	11.2	12.3
		-2	27.9	-29.1
		-1	28.0	-29.3
		0	22.1	-22.7
		1	15.1	15.5
		2	77.7	78.7
		3	24.6	24.9
		4	2.6	- 2.6
		5	13.3	-13.2
		6	23.2	21.4
5	7	-6	32.3	33.3
		-5	33.9	34.5
		-4	10.4	8.5
		-3	24.4	26.5
		-2	33.5	-35.0
		-1	48.0	-49.7
		0	4.2	- 3.6
		1	2.4	1.0
		2	57.7	-58.0
		3	6.7	7.4
		4	38.1	37.6
5	7	5	9.5	- 8.6
5	8	-6	2.7	- 3.1
		-5	9.6	10.1
		-4	23.4	23.9
		-3	14.3	14.8
		-2	60.0	63.0
		-1	21.2	21.7
		0	4.8	4.5
		1	8.9	- 9.1
		2	18.3	-18.7
		3	7.4	- 7.6
		4	6.3	- 5.7
		5	13.7	12.5
5	9	-5	35.7	-38.6
		-4	37.4	-39.8
		-3	14.8	16.0
		-2	32.4	32.3
		-1	6.4	- 5.7
		0	6.2	5.7
		1	28.6	-29.1
		2	13.6	-12.9
		3	9.7	9.7
		4	42.2	40.6
5	10	-4	6.0	6.8
		-3	36.6	36.9
		-2	2.6	2.2
		-1	6.8	- 6.6
		0	29.8	-30.1
		1	34.0	-33.7
		2	13.2	12.3
		3	13.6	13.1
5	11	-3	11.9	12.1
		-2	6.0	- 6.1
		-1	19.5	-18.8
		0	36.7	35.9
		1	28.6	28.7
		2	20.1	-19.7
5	12	-1	5.2	5.0
6	0	-7	2.7	- 0.3
		-6	8.0	7.7
		-5	3.7	- 0.2
		-4	3.4	- 0.9
		-3	42.5	-45.8
		-2	3.2	4.8
		-1	17.9	-20.7
		0	2.9	- 0.1
		1	16.4	17.9
		2	5.7	- 3.8
		3	17.7	17.5
		4	5.0	5.3
		5	5.3	3.6
		6	14.4	-13.7
		7	2.9	- 0.5
6	1	-7	2.7	- 1.4
		-6	7.4	7.1
		-5	10.3	11.3
		-4	18.4	-20.2
		-3	23.1	24.3
		-2	28.5	30.4
		-1	26.9	-29.7
		0	12.1	12.4
		1	2.3	- 1.7
		2	2.4	4.7
		3	37.5	37.8
		4	10.1	9.1
		5	62.5	-60.3
		6	61.4	-59.1
6	2	-7	40.2	-42.0
		-6	32.9	-34.1
		-5	28.7	31.0
		-4	21.0	23.3
		-3	8.0	- 7.9
		-2	16.8	-16.5
		-1	43.7	-47.2
		0	38.7	-40.4
		1	71.2	73.2
		2	74.0	76.0
		3	22.0	23.6
		4	2.5	- 0.4
		5	7.1	6.5
		6	18.9	17.2
6	3	-7	8.6	- 6.8
		-6	58.0	59.9
		-5	15.2	16.6
		-4	24.8	27.2
		-3	5.9	- 6.9
		-2	47.8	-50.8
		-1	35.6	-38.0
		0	17.5	17.4
		1	63.2	-66.7
		2	70.6	-71.6
		3	16.3	17.0
		4	4.0	4.7
		5	17.2	17.5
		6	24.4	23.5
6	4	-7	20.1	-20.4
		-6	2.6	1.4
		-5	27.4	28.8
		-4	3.7	- 6.2
		-3	35.1	37.8

Table 2. *(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
6	4	-2	87.7	94.6	6	9	-3	18.2	18.3	7	3	-4	14.4	14.7	7	8	1	10.7	8.9	8	4	2	42.8	-42.9
		-1	11.8	11.7			-2	4.5	3.1			-3	5.7	5.7			2	39.6	-38.4			3	14.8	-15.8
		0	7.1	7.9			-1	17.1	17.1			-2	17.3	-17.7	7	9	-1	26.9	26.6	8	5	-4	7.1	- 7.6
		1	39.6	-41.5			0	8.9	- 9.1			-1	53.9	56.8			0	4.2	- 0.7			-3	4.2	- 4.2
		2	31.4	-32.8			1	43.9	-44.0			0	68.4	70.3	8	0	-6	20.3	20.6			-2	6.4	6.4
		3	6.9	- 6.9			2	26.1	-26.4			1	11.8	-12.7			-5	58.2	-60.9			-1	25.4	25.0
		4	24.3	24.7			3	11.5	-12.2			2	7.5	- 7.9			-4	23.2	-24.4			0	23.3	-21.6
		5	2.7	- 2.2	6	10	-3	15.6	15.7			3	2.6	- 1.2			-3	6.4	6.5			1	38.7	39.3
		6	13.2	-12.3			-2	27.6	27.2			4	19.1	-18.7			-2	3.1	3.0			2	66.7	65.7
6	5	-6	22.1	-22.9			-1	13.7	13.6			5	16.2	16.4			-1	2.4	4.7			3	10.3	- 9.0
		-5	33.7	-35.6			0	8.5	8.9	7	4	-6	30.5	31.6			0	30.5	-31.4	8	6	-3	17.8	-18.5
		-4	20.2	-21.5			1	2.7	2.9			-5	55.1	-58.8			1	11.6	-13.0			-2	53.0	-53.8
		-3	18.5	19.8	7	0	-7	16.6	-16.0			-4	59.8	-62.9			2	7.8	- 7.1			-1	12.5	-12.8
		-2	5.0	- 4.4			-6	3.2	- 3.2			-3	4.5	- 1.5			3	34.3	33.4			0	2.9	- 2.6
		-1	17.4	18.7			-5	4.5	4.8			-2	24.5	26.0			4	34.7	34.8			1	21.0	21.2
		0	2.4	- 2.3			-4	18.4	-19.0			-1	9.9	10.6			5	2.8	3.4			2	19.0	-16.5
		1	23.7	-24.7			-3	59.2	64.2			0	33.0	-32.9	8	1	-6	19.9	-19.4	8	7	-1	23.3	-23.2
		2	2.5	0.3			-2	47.4	49.2			1	13.5	-14.8			-5	31.9	31.6			0	5.0	- 3.6
		3	21.7	20.6			-1	15.8	-16.9			2	13.6	-12.1			-4	17.1	17.4	9	0	-4	18.2	-18.4
		4	31.8	32.1			0	6.1	- 6.3			3	17.4	17.4			-3	2.5	2.5			-3	13.1	12.3
		5	4.7	- 2.8			1	19.8	-21.5			4	48.7	49.6			-2	8.1	7.6			-2	8.8	10.5
6	6	-6	9.5	6.2			2	13.3	-13.9			5	24.4	24.8			-1	10.4	- 8.5			-1	7.6	8.2
		-5	24.0	-24.4			3	2.6	- 1.7	7	5	-5	4.1	- 1.5			0	28.6	-28.9			0	18.1	18.5
		-4	8.3	7.8			4	14.4	14.3			-4	51.7	52.6			1	14.5	-14.9			1	30.1	-29.3
		-3	15.1	16.2			5	18.0	-16.9			-3	2.6	0.5			2	2.6	- 2.8			2	8.3	- 8.1
		-2	4.2	- 0.8			6	5.0	- 4.5			-2	10.0	10.2			3	20.5	-21.2			3	6.0	- 8.1
		-1	9.9	- 9.3	7	1	-7	25.2	-24.8			-1	2.5	1.7			4	13.0	-12.9	9	1	-4	18.3	-19.8
		0	23.5	-23.3			-6	19.7	-21.0			0	34.2	-35.1	8	2	-5	2.6	0.3			-3	2.6	- 1.2
		1	4.8	- 5.0			-5	32.2	-34.2			1	37.5	-37.7			-4	10.5	10.5			-2	14.6	14.1
		2	5.0	4.6			-4	6.4	- 6.5			2	2.6	- 4.2			-3	4.6	2.6			-1	14.6	-12.6
		3	16.9	17.1			-3	18.1	19.9			3	7.1	- 6.9			-2	8.0	- 7.3			0	25.2	-23.1
		4	33.7	-32.8			-2	15.7	-16.9			4	31.7	-30.7			-1	45.5	48.4			1	61.4	62.3
		5	8.1	7.2			-1	21.7	22.5	7	6	-5	5.1	- 4.1			0	10.2	9.7			2	24.0	23.7
6	7	-5	4.7	- 5.2			0	6.2	- 6.4			-4	2.7	- 3.7			1	2.6	- 2.5			3	21.1	-21.0
		-4	14.7	14.9			1	2.4	- 2.8			-3	24.2	23.8			2	8.0	- 8.3	9	2	-4	9.3	8.4
		-3	10.1	- 9.0			2	10.0	8.9			-2	11.6	11.3			3	10.7	-11.6			-3	41.8	-43.7
		-2	9.4	- 9.0			3	31.6	32.1			-1	9.4	9.7			4	2.8	2.1			-2	26.5	-27.2
		-1	4.3	1.6			4	2.6	1.0			0	14.8	14.8	8	3	-5	29.1	-29.4			-1	3.8	- 0.8
		0	58.7	58.1			5	2.7	3.6			1	8.5	- 7.8			-4	10.3	-10.4			0	4.1	- 3.0
		1	3.8	- 2.7			6	11.6	10.1			2	5.1	2.3			-3	43.9	-45.8			1	7.2	- 4.2
		2	20.4	-19.9	7	2	-6	9.6	-10.0			3	10.5	- 9.9			-2	14.2	-14.1			2	6.0	4.1
		3	18.6	17.3			-5	6.8	- 7.3			4	12.1	-12.6			-1	30.0	31.6	9	3	-3	14.7	13.7
		4	5.6	- 5.1			-4	17.2	17.6	7	7	-4	2.7	- 0.6			0	12.1	13.0			-2	6.4	6.3
6	8	-5	13.0	-13.0			-3	15.1	16.7			-3	8.0	- 7.5			1	16.0	15.7			-1	16.3	-17.1
		-4	51.3	-53.1			-2	8.7	- 8.8			-2	26.6	-25.6			2	13.8	-15.1			0	15.9	17.0
		-3	19.8	-19.7			-1	31.2	-31.1			-1	25.5	25.1			3	29.0	-28.9			1	2.8	- 3.9
		-2	10.5	10.2			0	20.3	-20.9			0	4.9	- 4.9			4	2.9	- 4.0			2	22.7	-22.0
		-1	11.8	12.1			1	12.9	11.8			1	10.8	10.8	8	4	-5	2.7	- 3.2	9	4	-2	10.8	10.4
		0	2.6	- 1.6			2	2.5	0.3			2	11.2	10.7			-4	34.5	-34.7			-1	26.2	24.2
		1	28.2	-28.3			3	14.4	-13.6			3	29.4	-29.1			-3	2.6	- 3.5			0	4.9	4.7
		2	11.9	10.7			4	32.4	-31.9	7	8	-5	28.2	-28.3			-2	39.9	40.4			1	14.3	15.9
		3	5.7	- 5.7			5	16.2	16.3			-2	31.3	30.1			-1	9.0	10.6	10	0	-2	9.7	8.2
		4	36.9	37.3	7	3	-6	2.7	2.5			-1	19.0	18.2			0	26.3	26.4			-1	16.6	14.4
6	9	-4	35.0	34.6			-5	2.6	- 1.7			0	11.8	11.8			1	17.8	-17.2			0	12.1	12.7

1.9387—2.2060 Å, the average distance being 2.0477 Å; in the other, from 2.0660—2.2386 Å, the average being 2.1687 Å. These interatomic distances indicate that the iron is trivalent in the former octahedron and divalent in the latter. This conclusion is supported by the Mössbauer spectra, which indicates a simple pattern of separated single peaks for Fe^{3+} and Fe^{2+}. As shown in Fig. 3, the ratio of Fe^{3+} to the total Fe content is about 0.60, which is close to that indicated in the chemical formula of NAMBU *et al.* (1969). The iron and the substituting Mn and Mg atoms in these slightly distorted octahedra are coordinated with nonbridging oxygen atoms. Similarly, there are two types of Ca-coordination polyhedra. The first has six nonbridging oxygen atoms at a wide range of cation-anion distances and two bridging oxygen atoms at longer distances. The second has four nonbridging oxygen atoms at nearly equal distances and four bridging oxygen atoms at longer distances. The Fe and Ca polyhedra are linked together by common edges and corner oxygen atoms. Pairs of alternating Ca, Fe

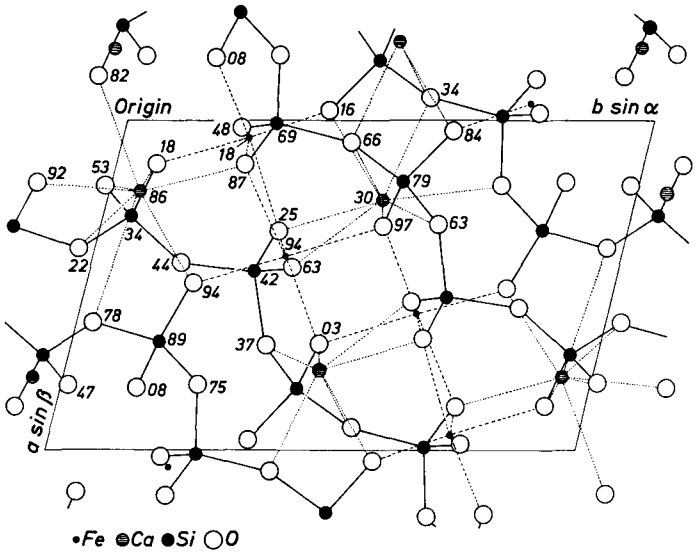

Fig. 2a. Structure of babingtonite as projected along the c axis. Numbers indicate the relative heights of the atomic positions in terms of percentages of the c translation

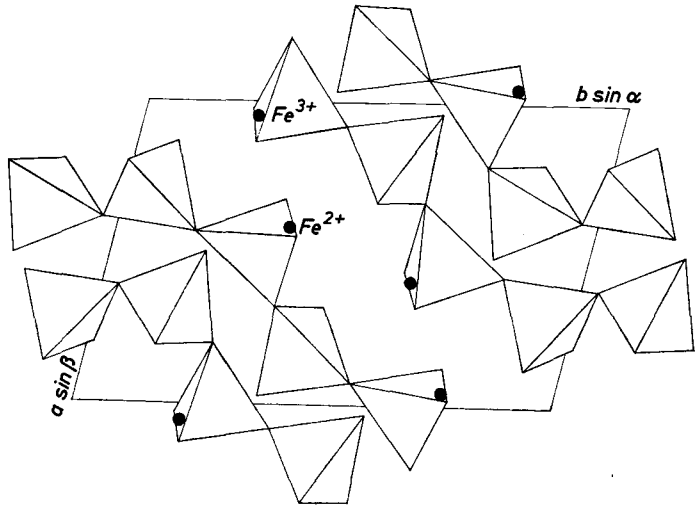

Fig. 2b. Illustration of the location and orientation of the silica chains. The position of the types of Fe ions are also shown

and Fe, Ca polyhedra are bond together to form bands between the silica chains.

The silica tetrahedra are linked by sharing bridging oxygen atoms. The average Si—O—Si angle is 137.3° with a range of 131.7—144.0°. The average Si—O distance is 1.6518 for bridging oxygen and 1.6139 Å for nonbridging oxygen. The eight distances from Si to bridging

Table 3. *Selected bond distances and their standard deviations*

Si(1) tetrahedron		
Si(1)—O(1)	1.6249 Å	0.0017 Å
Si(1)—O(2)	1.6239	0.0038
Si(1)—O(3)	1.6161	0.0066
Si(1)—O(15)	1.6433	0.0044
O(1)—O(2)	2.6794	0.0057
O(1)—O(3)	2.5534	0.0057
O(1)—O(15)	2.6643	0.0062
O(2)—O(3)	2.7115	0.0076
O(2)—O(15)	2.6455	0.0058
O(3)—O(15)	2.6814	0.0081
Si(2) tetrahedron		
Si(2)—O(4)	1.5369	0.0039
Si(2)—O(5)	1.6029	0.0059
Si(2)—O(6)	1.6682	0.0048
Si(2)—O(3)	1.6324	0.0051
O(3)—O(4)	2.6524	0.0045
O(3)—O(5)	2.7204	0.0080
O(3)—O(6)	2.6553	0.0063
O(4)—O(5)	2.7135	0.0081
O(4)—O(6)	2.7132	0.0080
O(5)—O(6)	2.5488	0.0056
Si(3) tetrahedron		
Si(3)—O(7)	1.6048	0.0037
Si(3)—O(8)	1.6036	0.0036
Si(3)—O(6)	1.6329	0.0012
Si(3)—O(9)	1.6827	0.0067
O(6)—O(7)	2.6726	0.0060
O(6)—O(8)	2.6474	0.0054
O(6)—O(9)	2.6194	0.0065
O(7)—O(8)	2.7478	0.0059
O(7)—O(9)	2.5422	0.0072
O(8)—O(9)	2.7129	0.0076
Si(4) tetrahedron		
Si(4) —O(10)	1.6214 Å	0.0030 Å
Si(4) —O(11)	1.6123	0.0060
Si(4) —O(9)	1.6562	0.0049
Si(4) —O(12)	1.6583	0.0047
O(9) —O(10)	2.7292	0.0047
O(9) —O(11)	2.6511	0.0081
O(9) —O(12)	2.6037	0.0058
O(10)—O(11)	2.7160	0.0081
O(10)—O(12)	2.6347	0.0072
O(11)—O(12)	2.6867	0.0059
Si(5) tetrahedron		
Si(5) —O(13)	1.5854	0.0041
Si(5) —O(14)	1.6231	0.0041
Si(5) —O(12)	1.6645	0.0013
Si(5) —O(15)	1.6635	0.0067
O(12)—O(13)	2.6677	0.0059
O(12)—O(14)	2.6744	0.0050
O(12)—O(15)	2.7385	0.0073
O(13)—O(14)	2.7324	0.0066
O(13)—O(15)	2.6009	0.0066
O(14)—O(15)	2.5815	0.0078
Ca(1) polyhedron		
Ca(1)—O(1)	2.2866	0.0072
O(13)	2.3250	0.0068
O(14)	2.3520	0.0059
O(2)	2.3654	0.0060
O(10)	2.4409	0.0057
O(2)	2.7075	0.0072
O(15)	3.0616	0.0053
O(15)	3.0839	0.0075

Table 3. *(Continued)*

Ca(2) polyhedron		
Ca(2)—O(8)	2.3512	0.0058
O(5)	2.3539	0.0070
O(7)	2.3756	0.0070
O(4)	2.3760	0.0059
O(6)	2.4518	0.0075
O(9)	2.5679	0.0061
O(12)	2.6407	0.0062
O(9)	2.8813	0.0050
Fe^{2+} octahedron		
Fe^{2+}—O(4)	2.2137	0.0052
O(5)	2.1102	0.0052
O(8)	2.2386	0.0054
O(8)	2.2019	0.0067
O(10)	2.1820	0.0060
O(13)	2.0660	0.0047
Fe^{3+} octahedron		
Fe^{3+}—O(2)	2.0574	0.0047
O(4)	2.0982	0.0065
O(7)	1.9814	0.0043
O(10)	2.2060	0.0054
O(11)	2.0044	0.0054
O(14)	1.9387	0.0066
Oxygen-oxygen distances between adjacent Si—O tetrahedra. less than 2.80 A		
O(1)—O(11)	2.5813	0.0072
O(2)—O(14)	2.7544	0.0067

oxygen atoms, averaging 1.6587 Å, involve the same oxygen atoms as those from Ca to bridging oxygen atoms. The shorter bond from Si to bridging oxygen, of 1.6243 Å length, contains O(3) which is not bonded to either Ca or Fe cations. Because of these difference in the

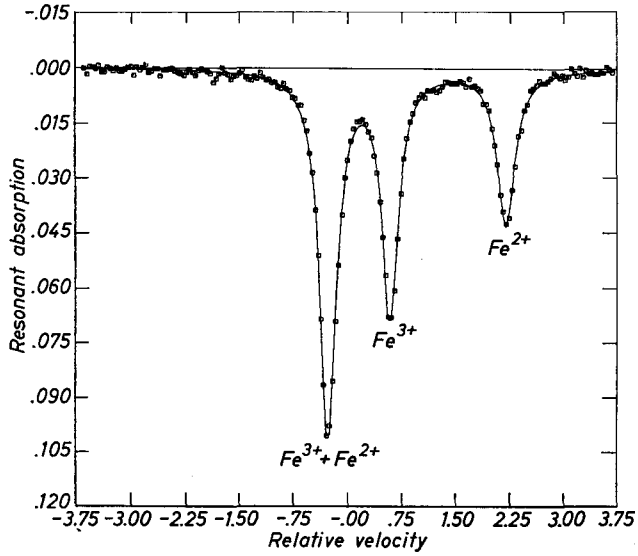

Fig. 3. Resonant absorption diagram of the Mössbauer spectrum of babingtonite

Table 4. *Selected bond angles and their standard deviations*

O(1)—Ca(1)—O(2)		78.1°	0.3°
O(1)	O(2)*	158.5	1.5
O(1)	O(10)	110.7	0.3
O(1)	O(13)	112.8	0.4
O(1)	O(14)	81.4	0.2
O(1)	O(15)	73.6	0.3
O(1)	O(15)*	127.5	0.5
O(2)	O(2)*	80.6	0.2
O(2)	O(10)	95.6	0.2
O(2)	O(13)	167.5	2.8
O(2)	O(14)	65.5	0.3
O(2)	O(15)	136.5	0.7
O(2)	O(15)*	104.3	0.2
O(2)*	O(10)	73.3	0.3
O(2)*	O(13)	88.7	0.2
O(2)*	O(14)	87.9	0.2
O(2)*	O(15)	122.4	0.4
O(2)*	O(15)*	56.6	0.4
O(10)	O(13)	75.0	0.3
O(10)	O(14)	155.6	1.1
O(10)	O(15)	125.0	0.5
O(10)	O(15)*	120.9	0.3
O(13)	O(14)	120.9	0.4
O(13)	O(15)	55.4	0.5
O(13)	O(15)*	74.6	0.2
O(14)	O(15)	78.0	0.2
O(14)	O(15)	55.1	0.4
O(15)	O(15)*	70.1	0.3
O(5)—Ca(2)—O(4)		91.2	0.2
O(5)	O(6)	64.0	0.4
O(5)	O(7)	160.0	1.7
O(5)	O(8)	81.7	0.2
O(5)	O(9)	136.5	0.6
O(5)	O(9)*	112.1	0.3
O(5)	O(12)	82.0	0.2
O(4)	O(6)	120.7	0.4
O(4)	O(7)	73.0	0.3
O(4)	O(8)	75.2	0.2
O(4)	O(9)	131.6	0.5
O(4)	O(9)*	89.6	0.2
O(4)	O(12)	159.9	1.5
O(6)	O(7)	134.6	0.7
O(6)	O(8)	141.1	0.8
O(6)	O(9)	84.0	0.2
O(6)—Ca(2)—O(9)*		58.2°	0.4°
O(6)	O(12)	73.1	0.3
O(7)	O(8)	82.4	0.2
O(7)	O(9)	61.8	0.4
O(7)	O(9)*	80.7	0.2
O(7)	O(12)	108.7	0.3
O(8)	O(9)	112.6	0.3
O(8)	O(9)*	160.0	1.3
O(8)	O(12)	85.1	0.2
O(9)	O(9)*	68.1	0.3
O(9)	O(12)	60.0	0.4
O(9)*	O(12)	110.5	0.3
O(4)—Fe^{2+}—O(5)		170.5	2.8
O(4)	O(8)	80.8	0.2
O(4)	O(8)*	95.0	0.2
O(4)	O(10)	80.5	0.2
O(4)	O(13)	93.0	0.2
O(5)	O(8)	92.9	0.2
O(5)	O(8)*	91.0	0.2
O(5)	O(10)	93.2	0.2
O(5)	O(13)	93.6	0.2
O(8)	O(8)*	81.1	0.2
O(8)	O(10)	95.7	0.2
O(8)	O(13)	173.1	3.8
O(8)*	O(10)	174.8	6.6
O(8)*	O(13)	96.6	0.2
O(10)	O(13)	86.2	0.2
O(2)—Fe^{3+}—O(4)		92.5	0.2
O(2)	O(7)	175.0	4.6
O(2)	O(10)	84.6	0.2
O(2)	O(11)	88.1	0.2
O(2)	O(14)	87.1	0.2
O(4)	O(7)	87.6	0.2
O(4)	O(10)	82.5	0.2
O(4)	O(11)	89.4	0.2
O(4)	O(14)	170.5	3.6
O(7)	O(10)	90.5	0.2
O(7)	O(11)	96.9	0.2
O(7)	O(14)	91.9	0.2
O(10)	O(11)	168.8	2.5
O(10)	O(14)	88.1	0.2
O(11)	O(14)	100.0	0.3

Table 4. *(Continued)*

O(1)—Si(1)—O(2)		111.1	0.2	O(9)—Si(4)—O(10)		112.8°	0.3°
O(1)	O(3)	104.0	0.3	O(9)	O(11)	108.4	0.3
O(1)	O(15)	109.2	0.2	O(9)	O(12)	103.5	0.3
O(2)	O(3)	113.6	0.4	O(10)	O(11)	114.3	0.3
O(2)	O(15)	108.1	0.2	O(10)	O(12)	106.9	0.2
O(3)	O(15)	110.7	0.3	O(11)	O(12)	110.5	0.3
O(3)—Si(2)—O(4)		108.5	0.3	O(12)—Si(5)—O(13)		110.3	0.2
O(3)	O(5)	114.5	0.4	O(12)	O(14)	108.9	0.2
O(3)	O(6)	107.1	0.3	O(12)	O(15)	110.8	0.3
O(4)	O(5)	113.8	0.3	O(13)	O(14)	116.8	0.3
O(4)	O(6)	110.4	0.3	O(13)	O(15)	106.3	0.3
O(5)	O(6)	102.4	0.3	O(14)	O(15)	103.5	0.3
O(6)—Si(3)—O(7)		111.3	0.2	Si(1)—O(3) —Si(2)		136.8	0.7
O(6)	O(8)	109.8	0.2	Si(2)—O(6) —Si(3)		144.0	0.5
O(6)	O(9)	104.4	0.3	Si(3)—O(9) —Si(4)		139.7	0.7
O(7)	O(8)	117.8	0.3	Si(4)—O(12)—Si(5)		131.7	0.3
O(7)	O(9)	101.3	0.3	Si(5)—O(15)—Si(1)		134.4	0.6
O(8)	O(9)	111.3	0.3				

Asterisk denotes position of $-x$, $-y$, $-z$, when different equivalent positions of same species are involved in the group.

Si—O bonds the silica tetrahedron is distorted. The nonbridging oxygen atoms are also shifted a little in the tetrahedra and the distances between bridging and nonbridging oxygen atoms are shorter when the nonbridging oxygen atoms are involved in short Ca—O bonding.

The structure of babingtonite is distinctly similar to that of rhodonite. The fifth tetrahedron, containing Si(1), however, is shifted in babingtonite because of the oxygen atoms' strong bond to the Ca(1) cation located on one side of the tetrahedron. The positions of the Ca and Fe cations correspond roughly to four of the five cation positions in the rhodonite structure. The hydrogen-atom proton is probably in a site close to O(3) or to O(1) and O(11) or both, for these are exceptionally short O—O distances of 2.5534 within a tetrahedron and 2.5813 Å between adjacent tetrahedra.

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