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The crystal structures of $2M_1$ phengite and $2M_1$ muscovite

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Die Kristallstrukturen von $2M_1$-Phengit und $2M_1$-Muskowit wurden bis zu $R = 0{,}045$ für Phengit und $R = 0{,}035$ für Muskowit verfeinert. Beide Minerale haben die Raumgruppe $C2/c$. Die Gitterkonstanten von Phengit sind: $a = 5{,}2112 \pm 0{,}0003$ Å, $b = 9{,}0383 \pm 0{,}0004$ Å, $c = 19{,}9473 \pm 0{,}0006$ Å, $\beta = 95{,}769 \pm 0{,}005°$, die für Muskowit: $a = 5{,}1906 \pm 0{,}0002$ Å, $b = 9{,}0080 \pm 0{,}0003$ Å, $c = 20{,}0470 \pm 0{,}0006$ Å, $\beta = 95{,}757 \pm 0{,}002°$. Im $2M_1$-Muskowit sind die Kation-Sauerstoff-Abstände in den Tetraedern T_1 und T_2 einander gleich, $T_1{-}O = T_2{-}O = 1{,}643$ Å, also die (Si, Al)-Lagen nicht geordnet. Die Differenz der entsprechenden Abstände im $2M_1$-Phengit, $T_1{-}O = 1{,}622$ und $T_2{-}O = 1{,}633$, weist auf eine mäßige Ordnung hin. Das Anionengerüst ist im $2M_1$-Muskowit etwa doppelt so stark gestört wie im $2M_1$-Phengit.

Abstract

The crystal structures of $2M_1$ phengite and $2M_1$ muscovite have been refined by least-squares methods using single-crystal diffractometer data. Final discrepancy factors were unweighted $R = 0.045$ for $2M_1$ phengite and 0.035 for $2M_1$ muscovite. Both specimens have the space group $C2/c$ and the following cell dimensions at room temperature:

	$2M_1$ phengite	$2M_1$ muscovite
a	5.2112 ± 0.0003 Å	5.1906 ± 0.0002 Å
b	9.0383 ± 0.0004	9.0080 ± 0.0003
c	19.9473 ± 0.0006	20.0470 ± 0.0006
β	$95.769 \pm 0.005°$	$95.757 \pm 0.002°$.

In $2M_1$ muscovite tetrahedral cation-oxygen distances $T_1{-}O = T_2{-}O = 1.643$ Å show that there is no ordering of (Si, Al) over the tetrahedral sites. In the structure of $2M_1$ phengite, however, the corresponding values, $T_1{-}O = 1.622$ and $T_2{-}O = 1.633$ Å, indicate a very slight ordering. The framework of anions is distorted twice as much in $2M_1$ muscovite than in $2M_1$ phengite.

Introduction

The muscovite-celadonite series of dioctahedral potassic micas can be represented by the following general formulae as suggested by FOSTER (1956):

$$KR^{3+}R^{3+}(Si_3Al)O_{10}(OH)_2 - KR^{2+}R^{3+}(Si_4)O_{10}(OH)_2,$$

where Al^{3+}, Fe^{3+} form the major trivalent cations (R^{3+}) and Mg^{2+}, Fe^{2+} the principal divalent cations (R^{2+}).

Phengite is a dioctahedral mica intermediate in the series muscovite—MgAl celadonite with the formal composition $K(Mg_{0.5}Al_{1.5})(Si_{3.5}Al_{0.5})O_{10}(OH)_2$. Unlike the muscovite end member, dioctahedral micas in other compositions display in nature and in laboratory synthesis a wider variety of stacking sequences, specifically $1M$, $3T$, $2M_1$ (HEINRICH and LEVINSON, 1955; CROWLEY and ROY, 1964; WISE and EUGSTER, 1964). It seems promising, therefore, to study the structural differences in this mica group in order to determine the effect of compositional changes in the formation of different stacking sequences. Similar comparison between dioctahedral and trioctahedral micas is complicated because of octahedral vacancies. Furthermore, the relationship between compositional range of dioctahedral micas and environmental factors of pressure and temperature have been well established through the studies of various investigators such as YODER and EUGSTER (1955), ERNST (1963), CROWLEY and ROY (1964), WISE and EUGSTER (1964), and VELDE (1965).

In the following, the crystal-structure analysis of $2M_1$ phengite will be presented for the first time and as a comparison the refinement of the crystal structure of $2M_1$ muscovite from a Georgia pegmatite is also carried out under the same conditions. At this time the only modern crystallographic refinement of $2M_1$ muscovite was done by BURNHAM and RADOSLOVICH (1964); however, the composition of that mica was not a typical K muscovite but a Na-rich muscovite. Their study showed certain significant errors in the previous refinement of the $2M_1$ muscovite structure by RADOSLOVICH (1960). To avoid any doubts concerning the $2M_1$ muscovite structure, a sample with a typical muscovite composition from a Georgia pegmatite has been refined using counter data and the results are presented together with those of $2M_1$ phengite.

Description of specimens

The samples of $2M_1$ phengite and $2M_1$ muscovite have been previously described by ERNST (1963). The phengite is from a low-grade glaucophane + actinolite + chlorite + aragonite + quartz schist, Tiburon Peninsula, California, with the chemical formula (on the basis of 22 negative charges):

$$(K_{.87}Na_{.07}Ba_{.01}Ca_{.02})(Si_{3.39}Al_{.61})(Al_{1.43}Ti_{.01}Fe^{3+}{}_{.05}Fe^{2+}{}_{.09}Mg_{.50})O_{10.08}(OH)_{1.92}.$$

The muscovite which is from a pegmatite in Georgia, U.S. National Museum No. 105100, has the composition:

$$[K_{.86}Na_{.10}(H_3{}^+O)_{.01}](Si_{3.02}Al_{.98})(Al_{1.90}Ti_{.01}Fe^{3+}{}_{.02}Fe^{2+}{}_{.05}Mg_{.06})O_{10}(OH_{1.99}F_{.01}).$$

ERNST (1963) also reported the following optical properties:

	α	β	γ	$2V_\alpha$
Phengite	1.563	1.600	1.601	33°
Muscovite	1.559	1.597	1.600	27°

Theoretical densities are 2.859 g/cm³ for $2M_1$ phengite and 2.838 g/cm³ for $2M_1$ muscovite; $Z = 4$ for both micas.

Space group and unit cell

The x-ray diffraction symbol for phengite and muscovite determined from precession photographs is $2/mC\text{-}/c$ with possible space groups Cc and $C2/c$.

Precise unit-cell dimensions were determined by least-squares refinement (BURNHAM, 1962) of the data obtained with a precision back-reflection Weissenberg camera using Cu$K\alpha$ radiation (Cu$K\alpha_1$ = 1.54051, Cu$K\alpha_2$ = 1.54433 Å) with 67 and 94 independent observations in the back-reflection region for phengite and Georgia muscovite, respectively. The unit-cell parameters are given in Table 1.

Table 1. *Unit-cell dimensions of $2M_1$ phengite and $2M_1$ muscovite*

	Phengite	*Muscovite*
a	5.2112 ± 0.0003 Å	5.1906 ± 0.0002 Å
b	9.0383 ± 0.0004	9.0080 ± 0.0003
c	19.9473 ± 0.0006	20.0470 ± 0.0006
β	95.769 ± 0.005°	95.757 ± 0.002°
Volume	934.77 ± 0.10 Å³	932.614 ± 0.075 Å³

Intensity measurement and stucture refinement

Intensities were measured by counter methods using a Super-Pace automated single-crystal diffractometer at the Geophysical Laboratory, Carnegie Institution of Washington, Washington, D. C. Nickel-filtered Cu$K\alpha$ radiation was used and the diffracted x-ray energy was collected by a scintillation counter with a Th-activated NaI crystal. The pulse-height analyzer circuitry was set to accept 90% of the incoming radiation. The intensity collection and subsequent data processing have been described by BURNHAM (1966*a*). A single crystal of $2M_1$ phengite with dimensions $0.40 \times 0.25 \times 0.01$ mm and a single crystal of $2M_1$ muscovite with dimensions $0.50 \times 0.25 \times 0.007$ mm were used for intensity collection. Intensity data were converted to observed structure factors by applying the standard Lorentz and polarization correction, and a precise absorption correction (BURNHAM, 1966*b*). If the computed value of integrated intensity are less than 2σ, where σ represents the estimated standard deviation computed from counting statistics (CETLIN and ABRAHAMS, 1963), the intensity is assumed to be below the minimum observable value. For $2M_1$ phengite there were 740 reflections with integrated intensities above 2σ from the 1010 possible reflections. Only 557 of these reflections were independent. For $2M_1$ muscovite there were 567 independent reflections with integrated intensities above 2σ from the 736 possible reflections.

Full-matrix three-dimensional least-squares refinements were carried out for both micas with the observed reflections using an IBM 7094 program written by PREWITT (1962). All atoms were considered to be fully ionized and the scattering curves for them were obtained by the techniques described by PREWITT and BURNHAM (1966).

Two models in space groups $C2/c$ and Cc have been derived from the atomic coordinates and isotropic temperature factors of the $2M_1$ Na-rich muscovite (BURNHAM and RADOSLOVICH, 1964) for the least-squares refinement. In the space group $C2/c$ with 10 atoms in the asymmetric unit, varying only scale factor and atomic coordinates, the discrepancy indices for observed reflections converged after three cycles to an R value $[\Sigma||F_o| - |F_c||/\Sigma|F_o|]$ of 0.051 for phengite, and 0.044 for Georgia muscovite. The next three cycles of least squares were carried out varying isotropic temperature factors in addition to the scale factor and atomic parameters and using the site-occupancy multiplier obtained from the chemical formula. Discrepancy indices

Table 2. *Atomic coordinates and isotropic temperature factors in $2M_1$ phengite* (Standard deviations are given in parentheses)

Atom	Equipoint	x	y	z	B
K	4*e*	0.0	0.0964(5)	1/4	1.76(3) Å²
Al	8*f*	0.2467(3)	0.0825(3)	0.0001(1)	0.74(3)
O_a	8*f*	0.9568(6)	0.4396(7)	0.0544(2)	1.03(8)
O_b	8*f*	0.3933(6)	0.2496(9)	0.0537(2)	1.07(8)
OH	8*f*	0.9531(7)	0.0656(8)	0.0526(2)	1.21(8)
T_1	8*f*	0.9632(3)	0.4297(4)	0.1355(1)	0.60(3)
T_2	8*f*	0.4525(3)	0.2581(3)	0.1354(1)	0.60(3)
O_c	8*f*	0.4426(5)	0.0931(8)	0.1678(1)	1.30(6)
O_d	8*f*	0.7372(7)	0.3257(5)	0.1601(2)	1.41(0.10)
O_e	8*f*	0.2326(7)	0.3574(6)	0.1682(2)	1.23(9)

Table 3. *Atomic coordinates and isotropic temperature factors in $2M_1$ muscovite* (Standard deviations are given in parentheses)

Atom	Equipoint	x	y	z	B
K	4*e*	0.0	0.0985(3)	1/4	1.60(4) Å²
Al	8*f*	0.2496(3)	0.0834(2)	−0.0001(1)	0.47(2)
O_a	8*f*	0.9613(7)	0.4435(5)	0.0540(2)	0.84(7)
O_b	8*f*	0.3850(5)	0.2519(5)	0.0537(2)	0.77(6)
OH	8*f*	0.9564(7)	0.0630(5)	0.0505(2)	0.75(7)
T_1	8*f*	0.9648(2)	0.4295(2)	0.1355(1)	0.54(3)
T_2	8*f*	0.4510(3)	0.2584(2)	0.1355(1)	0.54(2)
O_c	8*f*	0.4174(6)	0.0930(6)	0.1685(2)	1.07(6)
O_d	8*f*	0.7513(7)	0.3110(5)	0.1575(2)	1.34(8)
O_e	8*f*	0.2522(7)	0.3705(5)	0.1689(2)	1.17(7)

Table 4*a*. *Anisotropic thermal parameters in $2M_1$ muscovite* (Standard errors are given in parentheses)

Atom	β_{11}	β_{22}	β_{33}	β_{12}	β_{13}	β_{23}
K	0.0161(7)	0.0050(3)	0.0009 (1)	0.0	0.0004(1)	0.0
Al	0.0044(4)	0.0009(2)	0.00037(3)	−0.00003(4)	0.0002(1)	0.00014 (9)
O_a	0.006 (1)	0.0027(7)	0.0006 (1)	0.0004 (7)	0.0001(3)	0.0003 (1)
O_b	0.007 (1)	0.0020(6)	0.0006 (1)	0.0002 (8)	0.0001(3)	0.0(0.0002)
OH	0.008 (2)	0.002 (1)	0.0004 (1)	0.0002 (7)	−0.0002(3)	−0.0003 (2)
T_1	0.0047(5)	0.0015(2)	0.00037(3)	0.0002 (3)	0.0001(1)	0.0(0.0001)
T_2	0.0049(5)	0.0015(2)	0.00041(3)	−0.0001 (4)	0.0002(1)	0.0(0.0001)
O_c	0.012 (1)	0.0031(5)	0.0007 (1)	0.0006 (8)	0.0005(3)	0.0(0.0002)
O_d	0.013 (2)	0.0049(7)	0.0007 (1)	0.0010 (8)	0.0008(3)	0.0003 (2)
O_e	0.013 (2)	0.0034(7)	0.0006 (1)	0.0004 (7)	−0.0002(3)	−0.0005 (2)

Table 4*b*. *Root-mean-square component of thermal displacement along principal axes of thermal ellipsoids and the orientation of principal axes in $2M_1$ muscovite*

Atom	Axis	Root-mean-square displacement	Angle with respect to		
			$+a$	$+b$	$+c^*$
Al	r_1	0.058 ± 0.008 Å	72 ± 9°	19 ± 12°	97 ± 19°
	r_2	0.077 ± 0.004	96 ± 17	80 ± 17	11 ± 13
	r_3	0.089 ± 0.004	161 ± 10	74 ± 10	99 ± 15
O_a	r_1	0.088 ± 0.011	111 ± 29	115 ± 36	147 ± 48
	r_2	0.098 ± 0.011	58 ± 32	50 ± 30	124 ± 48
	r_3	0.120 ± 0.010	140 ± 22	50 ± 22	90 ± 16
O_b	r_1	0.091 ± 0.013	85 ± 38	23 ± 1	67 ± 99
	r_2	0.096 ± 0.010	79 ± 37	113 ± 1	26 ± 91
	r_3	0.109 ± 0.009	168 ± 32	90 ± 37	78 ± 32
OH	r_1	0.076 ± 0.014	134 ± 23	45 ± 26	97 ± 20
	r_2	0.096 ± 0.011	60 ± 30	54 ± 26	50 ± 26
	r_3	0.114 ± 0.009	121 ± 17	113 ± 22	40 ± 26
T_1	r_1	0.076 ± 0.006	87 ± 21	36 ± 42	55 ± 42
	r_2	0.081 ± 0.005	76 ± 41	125 ± 42	39 ± 42
	r_3	0.086 ± 0.004	166 ± 39	96 ± 33	77 ± 32
T_2	r_1	0.078 ± 0.006	83 ± 21	33 ± 57	122 ± 60
	r_2	0.082 ± 0.005	96 ± 25	121 ± 58	149 ± 60
	r_3	0.091 ± 0.004	170 ± 24	80 ± 23	88 ± 20
O_c	r_1	0.11 ± 0.010	103 ± 15	27 ± 46	67 ± 92
	r_2	0.113 ± 0.009	25 ± 71	70 ± 19	104 ± 36
	r_3	0.131 ± 0.008	111 ± 19	73 ± 23	153 ± 21
O_d	r_1	0.110 ± 0.010	154 ± 12	104 ± 17	69 ± 20
	r_2	0.128 ± 0.009	100 ± 23	125 ± 18	143 ± 19
	r_3	0.151 ± 0.009	113 ± 10	39 ± 18	119 ± 17
O_e	r_1	0.092 ± 0.011	142 ± 12	52 ± 13	96 ± 11
	r_2	0.125 ± 0.009	66 ± 18	51 ± 15	49 ± 20
	r_3	0.143 ± 0.008	118 ± 11	119 ± 17	42 ± 20
K	r_1	0.135 ± 0.004	175 ± 12	90	85 ± 12
	r_2	0.144 ± 0.005	90	0	90
	r_3	0.148 ± 0.003	95 ± 12	90	175 ± 12

Table 5*a*. *Interatomic distances in* $2M_1$ *phengite and in* $2M_1$ *muscovite*

	Phengite	Muscovite
T_1 tetrahedron:		
T_1-O_a (apical)	1.618 ± 0.004 Å	1.637 ± 0.004 Å
T_1-O_c	1.620 ± 0.007	1.644 ± 0.004
T_1-O_d	1.621 ± 0.005	1.632 ± 0.004
T_1-O_e	1.629 ± 0.004	1.661 ± 0.004
Mean T_1-O	1.622 ± 0.003	1.643 ± 0.002
O_a-O_c	2.662 ± 0.006	2.691 ± 0.005
O_a-O_d	2.702 ± 0.006	2.716 ± 0.005
O_a-O_e	2.671 ± 0.006	2.707 ± 0.006
O_c-O_d	2.642 ± 0.008	2.685 ± 0.007
O_c-O_e	2.615 ± 0.008	2.653 ± 0.006
O_d-O_e	2.592 ± 0.006	2.642 ± 0.006
Mean O−O	2.647 ± 0.003	2.682 ± 0.002
T_2 tetrahedron:		
T_2-O_b (apical)	1.630 ± 0.004	1.642 ± 0.004
T_2-O_c	1.629 ± 0.007	1.647 ± 0.005
T_2-O_d	1.634 ± 0.004	1.647 ± 0.004
T_2-O_e	1.639 ± 0.005	1.635 ± 0.004
Mean T_2-O	1.633 ± 0.003	1.643 ± 0.002
O_b-O_c	2.671 ± 0.007	2.702 ± 0.006
O_b-O_d	2.725 ± 0.006	2.728 ± 0.005
O_b-O_e	2.692 ± 0.006	2.698 ± 0.005
O_c-O_d	2.617 ± 0.008	2.643 ± 0.006
O_c-O_e	2.626 ± 0.008	2.642 ± 0.007
O_d-O_e	2.661 ± 0.006	2.678 ± 0.006
Mean O−O	2.665 ± 0.003	2.682 ± 0.002
Al octahedron:		
Al−O_a	1.985 ± 0.004	1.931 ± 0.004
Al−$O_{\bar{a}}$	1.950 ± 0.005	1.951 ± 0.004
Al−O_b	1.956 ± 0.007	1.950 ± 0.005
Al−$O_{\bar{b}}$	1.961 ± 0.007	1.923 ± 0.005
Al−OH	1.938 ± 0.006	1.919 ± 0.004
Al−$O\overline{H}$	1.946 ± 0.004	1.920 ± 0.004
Mean Al−O	1.956 ± 0.002	1.932 ± 0.002
Unshared:		
$O_{\bar{a}}-O_b$	2.918 ± 0.008	2.956 ± 0.005
$O_a-O\overline{H}$	2.863 ± 0.004	2.860 ± 0.004
$O_{\bar{b}}-OH$	2.874 ± 0.008	2.856 ± 0.005
Mean O−O	2.885 ± 0.004	2.891 ± 0.005

Table 5*a*. *(Continued)*

	Phengite	Muscovite
Shared:		
OH−$O\overline{H}$	2.499 ± 0.009 Å	2.402 ± 0.007 Å
$O_a-O_{\bar{a}}$	2.509 ± 0.008	2.461 ± 0.007
$O_b-O_{\bar{b}}$	2.484 ± 0.006	2.447 ± 0.007
Mean O−O	2.497 ± 0.005	2.434 ± 0.004
Interlayer cation:		
K−O_c	2.961 ± 0.003	2.842 ± 0.003
K−O_d	2.982 ± 0.005	2.879 ± 0.005
K−O_e	2.966 ± 0.005	2.845 ± 0.005
Mean K−O_{inner}	2.970 ± 0.003	2.855 ± 0.002
K−O_c	3.189 ± 0.003	3.290 ± 0.003
K−O_d	3.344 ± 0.006	3.511 ± 0.005
K−O_e	3.179 ± 0.006	3.284 ± 0.005
Mean K−O_{outer}	3.237 ± 0.003	3.362 ± 0.003
K−OH	3.931 ± 0.004	3.997 ± 0.003
K−K	10.125 ± 0.002	10.179 ± 0.001

Table 5*b*. *Tetrahedral interatomic angles in* $2M_1$ *phengite and in* $2M_1$ *muscovite* (central atom is vertex)

	Phengite	Muscovite
T_1 tetrahedron:		
$O_c-T_1-O_d$	109.24 ± 0.23°	110.12 ± 0.21°
$O_e-T_1-O_c$	107.20 ± 0.25	106.81 ± 0.21
$O_e-T_1-O_d$	105.77 ± 0.32	106.74 ± 0.24
$O_a-T_1-O_e$	110.66 ± 0.23	110.34 ± 0.21
$O_a-T_1-O_c$	110.64 ± 0.31	110.21 ± 0.22
$O_a-T_1-O_d$	113.07 ± 0.26	112.41 ± 0.22
Mean O−T_1−O	109.43 ± 0.11	109.44 ± 0.09
T_2 tetrahedron:		
$O_c-T_2-O_d$	106.63 ± 0.24	106.71 ± 0.21
$O_e-T_2-O_c$	106.93 ± 0.25	107.25 ± 0.21
$O_d-T_2-O_e$	108.79 ± 0.31	109.37 ± 0.25
$O_b-T_2-O_c$	110.12 ± 0.33	110.45 ± 0.23
$O_b-T_2-O_d$	113.21 ± 0.24	112.07 ± 0.20
$O_b-T_2-O_e$	110.88 ± 0.26	110.79 ± 0.22
Mean O−T_2−O	109.43 ± 0.11	109.44 ± 0.09

converged to the following values for the observed reflections: $R = 0.045$ for $2M_1$ phengite, and $R = 0.036$ for $2M_1$ muscovite. Atomic parameters after these three cycles are given in Table 2 for phengite. The isotropic temperature factors for muscovite (Table 3) were next converted to anisotropic thermal parameters by three more cycles of refinement resulting in $R = 0.035$. Atomic parameters after the total of nine refinement cycles for muscovite are listed in Table 3 while the anisotropic thermal parameters are given in Table 4a. Anisotropic refinement of phengite was not possible owing to negative β_{ii}'s for some atoms. In both structures it was also not possible to vary the occupancy multiplier for cations during any stage of refinement, for it resulted in negative occupancy multipliers.

An attempt was made to refine the second model with space group Cc having 19 atoms in the asymmetric unit. In this case some atoms gave negative isotropic temperature factors and the least-squares correlation matrix showed very high correlation coefficients between the atoms which are centrosymmetrically related to each other in the space group $C2/c$. On this evidence the space group $C2/c$ is proposed for both mica structures.

The results of the least-squares refinement together with the variance-covariance matrix were used as input data for the crystallographic function and error program (ORFEE) (BUSING *et al.*, 1964) to compute interatomic distances and angles of phengite and Georgia muscovite. The bond lengths and tetrahedral interatomic angles are listed in Tables 5*a* and 5*b*; the root-mean-square components of thermal displacement along principal axes are given in Table 4*b* for $2M_1$ muscovite.

The thermal ellipsoids, representing 75% probability distribution, of the atoms in $2M_1$ muscovite structure are plotted in Fig. 1 using the OR TEP computer program (JOHNSON, 1965). This plot shows that the thermal vibrations of the atoms in $2M_1$ muscovite structure are almost isotropic except for basal oxygen atoms. The largest thermal vibrations of these basal oxygen atoms are in the (001) plane and they seem somewhat oriented parallel to the [110] direction. The reader may use Fig. 1 to follow interatomic distances and angles listed in Table 5*a* and 5*b*.

Subsequent three-dimensional difference-Fourier synthesis (using an IBM 7090 program written by SLY *et al.*, 1962) of both micas showed that no appreciable differences exist between calculated and observed electron densities except in the vacant octahedral sites

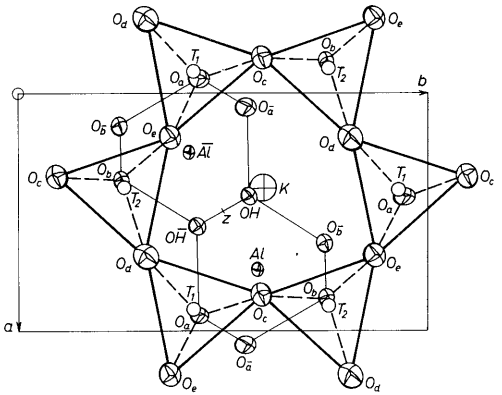

Fig. 1. Thermal-ellipsoid representation of $2M_1$ muscovite projected on (001), ellipsoids enclose 75% probability distribution (JOHNSON, 1965). Thick solid and dashed lines: upper tetrahedral sheets. Thin solid lines: octahedral polyhedra. Letters with a bar, e.g., $O_{\bar{a}}$, indicate that this atom is related by the inversion center, Z, to the atom O_a

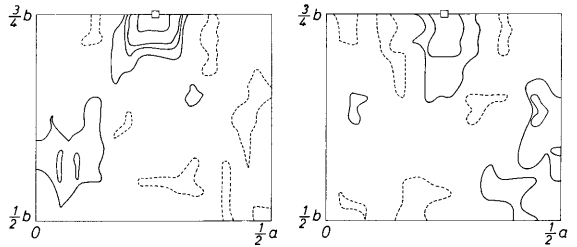

Fig. 2. Three-dimensional ($F_c - F_o$) map at $z = 0$, showing electron densities in vacant octahedral sites of $2M_1$ muscovite and $2M_1$ phengite. (Countours plotted at intervals of 0.1 e/Å^3)

(Fig. 2) which, in phengite, amounts to an electron density of 0.25 e/Å^3, possibly due to the excess of octahedral Mg^{2+}. In the difference electron-density map of Georgia muscovite there is 0.4 e/Å^3 left in this site indicating that most likely the excess of octahedral iron occupies this site.

Table 6. *Observed and calculated structure factors of 2 M_1 phengite*

h	k	l	F_o	F_c
0	0	4	73.8	-63.8
		6	174.3	173.0
		8	71.2	68.1
		10	223.8	-219.7
		14	85.9	90.3
		16	133.6	133.4
		20	63.1	60.5
		22	94.5	88.9
		24	63.2	60.7
2	0	0	133.4	132.3
-2	0	2	189.3	-190.1
2	0	2	92.2	90.2
-2	0	4	151.9	-150.1
2	0	4	43.6	-44.1
-2	0	6	160.7	-159.3
2	0	6	130.9	-131.6
-2	0	8	44.5	-47.1
2	0	8	91.5	91.4
-2	0	10	220.1	-222.3
2	0	10	149.7	-152.1
-2	0	12	74.2	-74.3
2	0	12	208.4	-212.1
-2	0	14	70.6	67.0
2	0	14	66.6	-67.0
-2	0	16	48.1	47.6
2	0	16	60.1	60.9
-2	0	18	132.2	-133.0
2	0	18	101.4	-98.5
-2	0	20	9.4*	9.9
2	0	20	35.9	-38.1
-2	0	22	19.1	21.5
2	0	22	44.3	41.4
4	0	0	168.7	171.2
-4	0	2	152.3	-154.2
4	0	2	141.2	146.2
-4	0	4	10.4*	15.8
4	0	4	10.5*	- 1.7
-4	0	6	125.5	125.5
4	0	6	35.2	31.3
-4	0	8	10.6*	15.4
4	0	8	172.7	174.8
-4	0	10	56.0	-59.7
4	0	10	11.0*	11.5
-4	0	12	145.8	144.8
4	0	12	19.2*	-21.6
-4	0	14	99.4	102.3
4	0	14	9.6*	-10.8
-4	0	16	39.6	37.5
4	0	16	71.7	68.6
-4	0	18	13.4*	-16.4
-4	0	20	64.2	63.4
6	0	0	53.2	-50.3
-6	0	2	121.2	-118.7
6	0	2	28.9	31.0
-6	0	4	9.2*	- 0.9
6	0	4	9.4*	- 8.1
-6	0	6	13.3	-14.7
-6	0	8	35.8	-35.4
-6	0	10	76.4	-70.5
1	1	0	63.8	-65.4
-1	1	1	99.3	101.4
1	1	1	47.2	-50.3
-1	1	2	8.3*	8.5
1	1	2	37.7	-36.5
-1	1	3	92.4	94.4
1	1	3	27.1	23.3
-1	1	4	127.3	124.9
1	1	4	138.3	136.9
-1	1	5	51.1	-44.9
1	1	5	127.4	-127.3
-1	1	6	126.1	-122.2
1	1	6	76.3	-77.1
-1	1	7	64.1	64.1
1	1	7	10.5*	5.6
-1	1	8	25.6	23.4
1	1	8	11.1*	- 4.2
-1	1	9	21.7	27.5
1	1	9	11.4*	- 5.6
-1	1	10	20.3	23.4
1	1	10	11.0*	3.1
-1	1	11	34.1	34.5
1	1	11	11.0*	-13.4
-1	1	12	23.4	25.9
1	1	12	54.6	56.0
-1	1	13	24.4	-24.0
1	1	13	54.0	-56.4
-1	1	14	52.7	-55.6
1	1	14	48.2	-49.2
-1	1	15	55.3	54.3
1	1	15	10.9*	-13.7
-1	1	16	21.0	15.6
1	1	16	10.7*	- 8.6
-1	1	17	44.3	43.5
1	1	17	33.7	-32.5
-1	1	18	10.0*	3.1
1	1	18	9.9*	6.4
-1	1	19	9.7*	19.5
1	1	19	9.5*	- 3.7
-1	1	20	26.9	27.6
1	1	20	33.1	35.4
-1	1	21	9.1*	- 6.8
1	1	21	46.1	-45.8
-1	1	22	38.4	-36.5
1	1	22	42.9	-39.4
-1	1	23	49.9	49.1
1	1	23	8.0*	-13.5
-1	1	24	8.0*	9.2
3	1	0	25.8	-25.9
-3	1	1	9.5*	- 0.2
3	1	1	19.7	-17.1
-3	1	2	30.5	30.5
3	1	2	76.3	-79.0
-3	1	3	62.3	-63.2
3	1	3	68.6	74.7
-3	1	4	38.8	38.5
3	1	4	97.9	99.2
-3	1	5	108.2	-111.4
-3	1	6	78.4	-80.2
3	1	6	23.6	-24.1
-3	1	7	10.1*	9.6
3	1	7	10.7*	- 2.3
-3	1	8	24.9	25.6
3	1	8	28.7	-34.3
-3	1	9	49.4	-47.9
3	1	9	34.6	32.8
-3	1	10	10.8*	2.3
3	1	10	11.8*	- 1.7
-3	1	11	35.4	-37.8
3	1	11	74.9	76.5
-3	1	12	25.0	23.0
3	1	12	45.4	48.0
-3	1	13	12.1*	-19.6
3	1	13	11.2*	5.1
-3	1	14	50.0	-53.0
3	1	14	35.3	-37.3
-3	1	15	25.7	23.5
3	1	15	26.1	25.1
-3	1	16	10.7*	7.8
3	1	16	9.7*	- 6.3
-3	1	17	19.8	-21.4
3	1	17	30.8	28.4
-3	1	18	16.4	19.2
3	1	18	8.9*	-11.0
-3	1	19	13.9	-13.8
3	1	19	26.1	27.5
-3	1	20	8.9*	7.6
3	1	20	27.8	25.6
-3	1	21	33.7	-33.6
-3	1	22	45.3	-45.5
-5	1	1	9.7*	4.4
-5	1	2	27.4	30.4
5	1	2	53.3	-54.0
-5	1	3	21.2	-19.1
-5	1	4	20.3	18.8
5	1	4	52.0	47.8
-5	1	5	9.8*	- 6.7
-5	1	6	47.8	-49.5
-5	1	7	49.6	51.2
5	1	7	47.4	-49.7
-5	1	8	26.7	31.8
5	1	8	14.6	-14.5
-5	1	9	10.0*	16.3
5	1	9	39.7	-39.5
-5	1	10	10.1*	15.0
5	1	10	21.2	-17.9
-5	1	11	29.4	30.3
5	1	11	9.5*	5.8
-5	1	12	10.3*	3.2
5	1	12	48.0	45.8
-5	1	13	21.4	22.2
-5	1	14	31.6	-30.5
-5	1	15	49.7	48.6
-5	1	16	25.0	26.2
0	2	4	112.8	108.0
		5	158.0	-153.4
		6	18.1*	-15.5
		7	51.0	48.9
		8	22.1	17.3
		9	25.4	24.9
		10	33.9	33.4
		11	10.4*	11.8
		12	40.0	42.9
		13	68.6	-69.5
		14	10.8*	- 1.2
		15	43.2	44.4
		16	36.5	36.1
		17	10.3*	7.1
		18	28.5	31.3
		19	9.5*	7.7
		20	28.1	31.4
		21	35.5	-36.5
		22	8.6*	5.5
		23	25.5	26.8
2	2	0	45.3	44.9
-2	2	1	87.2	-89.0
2	2	1	85.8	-87.0
-2	2	2	27.3	-29.7
2	2	2	50.4	-51.2
-2	2	3	86.4	84.9
2	2	3	57.5	54.9
-2	2	4	9.4*	- 1.6
2	2	4	31.8	-32.6
-2	2	5	39.5	-37.0
2	2	5	9.8*	13.2
-2	2	6	41.0	-43.1
2	2	6	16.2	-23.2
-2	2	7	37.0	-33.5
2	2	7	56.4	-55.0
-2	2	8	71.3	-71.4
2	2	8	67.8	-68.7
-2	2	9	45.4	42.0
2	2	9	16.6*	-22.3
-2	2	10	55.2	-55.9
2	2	10	83.0	-87.8
-2	2	11	49.1	51.9
2	2	11	102.7	103.4
-2	2	12	12.1*	-13.3
2	2	12	17.3	14.5
-2	2	13	110.2	-112.7
2	2	13	98.3	-95.3
-2	2	14	69.0	-70.7
2	2	14	26.6	-28.5
-2	2	15	70.1	65.8
2	2	15	10.5*	- 9.8
-2	2	16	10.8*	- 9.7
2	2	16	33.3	-33.8
-2	2	17	32.7	34.2
2	2	17	51.5	52.0
-2	2	18	9.9*	12.9
2	2	18	9.5*	3.0
-2	2	19	39.2	-37.1
2	2	19	9.0*	1.9
-2	2	20	9.2*	-12.9
2	2	20	13.4*	11.4
-2	2	21	21.4	-23.0
2	2	21	50.7	-54.1
-2	2	22	27.2	-29.1
-2	2	23	53.4	55.2
4	2	0	51.3	51.9
-4	2	1	40.8	38.3
4	2	1	10.5*	2.6
-4	2	2	55.6	55.1
-4	2	3	10.5*	11.2
-4	2	4	27.7	29.4
-4	2	5	93.3	-95.7
-4	2	6	40.6	-42.4
4	2	6	18.3	25.5
-4	2	7	66.8	66.4
4	2	7	10.5*	- 5.3
-4	2	8	10.7*	15.1
4	2	8	10.8*	9.2
-4	2	9	10.5*	13.5
4	2	9	10.8*	- 2.6
-4	2	10	10.6*	19.2
4	2	10	20.7	-20.4
-4	2	11	38.9	-38.4
4	2	11	32.0	35.2
-4	2	12	10.8*	0.2
4	2	12	10.6*	9.9
-4	2	13	21.7	-25.8
4	2	13	24.6	-24.2
-4	2	14	11.1*	13.7
4	2	14	16.6	13.5
-4	2	15	50.6	54.9
4	2	15	8.9*	- 5.8
-4	2	16	64.6	66.0
4	2	16	16.5	15.[illegible]
-4	2	17	23.0	-26.7
-4	2	18	27.7	27.3
-4	2	19	8.4*	- 7.8
-6	2	1	9.2*	- 4.7
6	2	1	33.1	33.1
-6	2	2	29.0	-29.4
6	2	3	20.6	20.2
-6	2	4	43.3	-42.9
6	2	4	9.4*	- 3.5
-6	2	6	42.7	-45.1
-6	2	8	9.5*	-15.6
-6	2	9	13.6*	12.8
-1	3	2	7.4*	7.9
1	3	2	7.8*	8.6
1	3	3	161.3	-160.6
-1	3	4	8.3*	10.8
1	3	4	8.9*	11.8
-1	3	5	53.2	52.1
1	3	5	163.7	-163.4
-1	3	6	18.0	15.1
1	3	6	10.2*	4.9
-1	3	7	129.2	124.8
1	3	7	32.8	-33.9
-1	3	8	36.1	-38.4
1	3	8	22.9	-26.5
-1	3	9	101.7	-100.4
1	3	9	218.7	-223.5
-1	3	10	22.7	23.4
1	3	10	24.4	23.5
-1	3	11	168.1	168.9
1	3	11	83.3	-82.1
-1	3	12	15.9*	21.5
1	3	12	10.9*	4.8
-1	3	13	215.0	215.8
1		13	77.8	72.9
-1		14	29.0	-23.4
1		14	10.6*	- 4.4
-1		15	48.2	48.8
1		15	47.8	44.9
-1		16	21.7	-20.1
1	3	16	13.7*	-14.1
-1	3	17	47.6	-50.1
1	3	17	129.7	-130.7
-1	3	18	35.9	35.0
1	3	18	9.3*	8.5
-1	3	19	108.2	108.1
1	3	19	9.1*	11.9
-1	3	20	13.1*	-10.3
1	3	20	8.6*	3.2
-1	3	21	21.4	24.0
1	3	21	8.3*	15.6
-1	3	22	15.8	-16.6
1	3	22	7.9*	- 2.2
-1	3	23	42.0	-40.3
3	3	0	20.2	-25.9
-3	3	1	248.5	-251.2
3	3	1	76.8	78.1
-3	3	2	21.7	25.1
3	3	2	9.8*	- 8.1
-3	3	3	58.2	-58.8
3	3	3	9.9*	- 3.3
-3	3	4	9.7*	7.7
3	3	4	10.1*	5.4
-3	3	5	9.8*	- 2.0
3	3	5	20.1	21.2
-3	3	6	15.1	-17.0
-3	3	7	39.5	-37.4
3	3	7	134.2	136.8
-3	3	8	10.4*	- 8.0
3	3	8	27.0	-24.9
-3	3	9	128.6	-127.9
3	3	9	70.2	-68.2
-3	3	10	29.1	32.7
3	3	10	11.5*	- 2.4
-3	3	11	83.4	80.9
3	3	11	38.0	-40.2
-3	3	12	11.4*	-15.6
3	3	12	24.3	22.6
-3	3	13	26.9	28.4
3	3	13	91.9	90.6
-3	3	14	11.1*	-10.4
3	3	14	10.0*	2.7
-3	3	15	97.2	-98.8
3	3	15	123.0	120.6
-3	3	16	10.1*	4.0
3	3	16	29.5	-28.3
-3	3	17	109.1	-111.8
3	3	17	22.6	-27.6
-3	3	18	9.2*	8.0
3	3	18	19.7	15.4
-3	3	19	26.4	30.6
-3	3	20	8.3*	- 7.3
-3	3	21	61.3	-58.3
5	3	0	9.5*	- 9.6
-5	3	1	59.0	-60.1
5	3	1	9.4*	-10.9
-5	3	2	9.6*	16.9
-5	3	3	90.6	88.3
5	3	3	58.7	-55.4
-5	3	4	9.7*	- 0.6
-5	3	5	97.6	97.4
5	3	5	71.9	-65.6
-5	3	6	9.6*	- 6.1
-5	3	7	9.5*	13.0
5	3	7	36.9	34.3
-5	3	8	9.5*	- 5.8
5	3	8	9.9*	-11.5
-5	3	9	9.6*	-10.0
5	3	9	52.5	-51.3
-5	3	10	14.0	19.1
5	3	10	9.3*	- 1.0
-5	3	11	144.2	142.7
-5	3	12	10.0*	- 5.4
-5	3	13	32.0	29.6
-5	3	14	13.3*	-14.9
0	4	4	75.7	-74.5
		5	9.2*	- 8.4
		6	63.7	-60.3
		7	46.9	-43.4
		8	15.4*	-13.5
		9	21.1	14.4
		10	34.8	-32.6
		11	67.5	62.4
		12	131.2	-130.7
		13	92.6	-89.7
		14	51.3	44.3
		15	16.0	17.0
		16	9.9*	4.5
		17	44.6	46.3
		18	44.2	-45.0
		19	18.0	-15.4
		20	12.8	-16.0
		21	35.1	-36.0
0	4	22	32.1	35.[illegible]
2	4	0	67.4	69.5
-2	4	1	39.3	42.1
2	4	1	13.1	18.0
-2	4	2	8.9*	7.1
2	4	2	88.3	88.7
-2	4	3	44.7	45.1
2	4	3	60.9	61.0
-2	4	4	70.3	-69.7
2	4	4	10.1*	-19.2
-2	4	5	95.2	-94.2
2	4	5	65.5	-68.1
-2	4	6	85.0	87.9
2	4	6	75.0	76.2
-2	4	7	39.6	39.5
2	4	7	10.4*	- 1.6
-2	4	8	10.5*	5.6
2	4	8	38.9	42.8
-2	4	9	33.9	36.5
2	4	9	11.6*	14.2
-2	4	10	11.3*	- 6.4
2	4	10	32.3	31.8
-2	4	11	17.4	-16.8
2	4	11	17.6*	19.6
-2	4	12	20.3*	22.5
2	4	12	39.6	-39.0
-2	4	13	39.1	-43.6
2	4	13	47.0	-47.9
-2	4	14	89.6	92.6
2	4	14	23.7	25.6
-2	4	15	46.4	50.4
2	4	15	9.7*	6.4
-2	4	16	10.0*	5.0
2	4	16	22.0	23.5
-2	4	17	9.5*	0.8
2	4	17	9.1*	11.9
-2	4	18	12.8*	13.9
2	4	18	14.3*	19.6
-2	4	19	8.9*	- 7.3
2	4	19	8.3*	11.4
-2	4	20	12.1*	10.8
2	4	20	11.7*	-14.1
-2	4	21	8.1*	-11.6
4	4	0	62.5	-62.3
-4	4	1	10.2*	- 8.9
4	4	1	19.0	-20.5
-4	4	2	33.6	-32.3
4	4	2	10.2*	16.3
-4	4	3	21.3	20.1
4	4	3	30.4	36.6
-4	4	4	56.7	-57.0
4	4	4	23.2	-29.0
-4	4	5	39.8	-41.2
-4	4	6	9.8*	14.6
4	4	6	38.5	-37.2
-4	4	7	9.8*	4.8
4	4	7	21.0	19.8
-4	4	8	10.0*	-11.3
4	4	8	10.2*	0.0
-4	4	9	28.8	22.4
4	4	9	10.6*	-11.4
-4	4	10	28.6	-27.7
4	4	10	40.9	43.8
-4	4	11	10.2*	- 4.8
4	4	11	57.7	56.6
-4	4	12	10.6*	-19.7
4	4	12	67.1	-65.3
-4	4	13	48.6	-50.9
4	4	13	34.0	-33.1
-4	4	14	42.9	43.8
4	4	14	15.5*	-21.3
-4	4	15	41.8	42.3
-4	4	16	56.1	-52.8
-4	4	17	8.6*	6.6
1	5	2	6.9*	7.6
1	5	4	90.1	-92.2
-1	5	5	8.6*	-21.8
-1	5	6	85.3	86.7
1	5	6	68.1	67.0
-1	5	7	10.2*	-26.1
1	5	7	44.8	-46.8
-1	5	8	11.2*	7.4
1	5	8	11.9*	- 7.2
-1	5	9	25.8	33.4
1	5	9	28.1	-30.7
-1	5	10	12.0*	-21.7
1	5	10	11.7*	8.3
-1	5	11	11.7*	20.5
1	5	11	11.5*	- 0.2
-1	5	12	32.0	-34.6
1	5	12	36.6	-36.2
-1	5	13	39.8	38.8
1	5	13	23.3	-18.1
-1	5	14	59.0	59.4
1	5	14	30.8	30.0
-1	5	15	47.7	48.2
1	5	15	9.8*	-15.7
-1	5	16	15.0*	-19.9
1	5	16	9.4*	1.9
-1	5	17	19.3	19.5

Table 6. *(Continued)*

h	k	l	F_o	F_c
1	5	17	9.3*	- 2.8
-1	5	18	9.2*	-11.9
1	5	18	8.9*	5.6
-1	5	19	20.9	21.9
1	5	19	17.3	-17.1
-1	5	20	18.8	-18.2
1	5	20	38.9	-41.9
-1	5	21	8.1*	9.0
3	5	0	10.5*	11.6
-3	5	1	34.1	-37.8
3	5	1	11.6*	- 8.3
-3	5	2	37.2	-36.3
3	5	2	73.7	77.3
-3	5	3	71.3	-73.6
-3	5	4	17.4	-18.8
3	5	4	89.2	-89.8
-3	5	5	56.1	-56.1
-3	5	6	70.5	75.3
3	5	6	14.7*	11.4
-3	5	7	18.4	-26.8
-3	5	8	36.3	-35.9
3	5	8	40.1	38.7
-3	5	9	24.1	-26.5
3	5	9	15.1*	15.3
-3	5	10	10.7*	6.9
3	5	10	11.2*	7.4
-3	5	11	10.9*	- 2.3
3	5	11	30.0	31.3
-3	5	12	11.2*	-13.0
3	5	12	50.0	-48.5
-3	5	13	11.1*	- 1.5
3	5	13	35.7	34.6
-3	5	14	32.6	31.9
3	5	14	37.0	40.0
-3	5	15	9.9*	4.7
3	5	15	32.1	36.1
-3	5	16	9.5*	-10.0
3	5	16	8.5*	3.4
-3	5	17	8.9*	- 7.2
3	5	17	12.3*	20.1
-3	5	18	8.6*	- 6.5
-3	5	19	31.2	-31.2
-5	5	1	9.3*	-11.0
5	5	2	43.2	40.7
-5	5	4	21.5	-18.7
5	5	4	40.1	-39.1
-5	5	5	9.3*	4.8
5	5	5	22.7	-22.5
-5	5	6	44.2	44.6
5	5	6	13.2*	- 8.1
-5	5	7	38.9	39.3
5	5	7	43.1	-42.4
-5	5	8	15.1	-24.2
5	5	8	9.4*	3.0
-5	5	9	26.5	27.3
-5	5	10	9.7*	-13.8
-5	5	11	31.5	29.8

* Observed intensity is less than $2\sigma(I_0)$; I_0 is assigned the value of $2\sigma(I_0)$.

The observed and calculated structure factors for 2 M_1 phengite and 2 M_1 muscovite are listed in Tables 6 and 7, respectively.

Characteristic features of 2 M_1 phengite and 2 M_1 muscovite structures

Tetrahedral sheets

In the structure of phengite the two average tetrahedral metal-oxygen distances with $T_1 - O = 1.622 \pm 0.003$ and $T_2 - O = 1.633 \pm 0.003$ Å indicate a slight partial ordering of (Si,Al) although isotropic temperature factors for both tetrahedral sites show no difference. As seen on Table 5*a*, the individual $T - O$ distances display no significant differences from the mean value for each tetrahedron, indicating that the tetrahedra are quite regular. In the structure of Georgia muscovite the two average $T_1 - O$ and $T_2 - O$ distances are equal showing the absence of ordering of (Si,Al) over tetrahedral sites. This is in contrast to the results of RADOSLOVICH (1960) but in agreement with those of BURNHAM and RADOSLOVICH (1964) for Na-rich muscovite.

Octahedral sheets

The average octahedral metal-oxygen distance for phengite (1.956 Å) is greater than that for Georgia muscovite (1.932 Å), as would be expected with the increased amount of large cations in the octahedral sites of the former. The shared octahedral edges listed in Table 5*a* show that the OH—$\overline{\mathrm{OH}}$ edge is shorter than the other two shared edges in 2 M_1 muscovite but not in 2 M_1 phengite.

Interlayer region

The interlayer cation is in six-coordination with the basal oxygen atoms from the upper and lower tetrahedral layers, with an average distance of 2.970 Å for phengite and 2.855 Å for Georgia muscovite.

Table 7. *Observed and calculated structure factors of 2 M_1 muscovite*

h	k	l	F_o	F_c
0	0	6	170.2	175.9
		8	75.4	67.9
		10	222.2	-225.0
		12	32.5	31.0
		14	82.6	86.4
		16	122.5	130.4
		18	25.0	23.9
		20	70.2	68.1
		22	95.0	94.4
		24	63.9	65.4
2	0	0	120.0	118.5
-2	0	2	204.4	-203.9
2	0	2	118.6	119.9
2	0	4	55.8	-57.6
-2	0	6	162.5	-162.1
2	0	6	136.2	-134.7
-2	0	8	63.0	-63.2
2	0	8	114.3	111.1
-2	0	10	199.4	-202.5
2	0	10	163.6	-158.8
-2	0	12	84.7	-84.0
2	0	12	220.1	-218.8
-2	0	14	51.1	49.5
2	0	14	63.0	-62.9
-2	0	16	58.4	57.6
2	0	16	47.1	50.4
-2	0	18	131.0	-134.3
2	0	18	104.9	-103.8
-2	0	20	7.0*	4.6
2	0	20	31.5	-32.1
-2	0	22	27.9	29.8
2	0	22	40.1	39.3
4	0	0	161.0	163.0
-4	0	2	123.6	-124.6
4	0	2	134.4	136.9
-4	0	4	7.5*	10.1
4	0	4	7.8*	13.7
-4	0	6	119.1	118.7
4	0	6	28.0	24.2
-4	0	8	36.8	36.9
4	0	8	167.4	168.1
-4	0	10	69.1	-71.3
4	0	10	26.7	25.5
-4	0	12	130.5	129.0
4	0	12	20.9	-24.9
-4	0	14	118.6	117.8
4	0	14	18.4	-13.5
-4	0	16	35.2	33.2
4	0	16	75.8	76.3
-4	0	18	19.3	-21.0
-4	0	20	87.0	85.2
6	0	0	54.7	-54.3
-6	0	2	118.2	-116.0
6	0	2	39.5	39.6
-6	0	4	6.6*	3.9
6	0	4	7.0*	- 9.7
-6	0	6	25.5	-25.0
-6	0	8	47.9	-45.6
1	1	2	35.7	-34.5
-1	1	3	91.9	93.8
1	1	3	22.8	21.8
-1	1	4	123.5	122.3
1	1	4	137.1	132.6
-1	1	5	43.8	-39.8
1	1	5	130.7	-128.1
-1	1	6	118.3	-116.4
1	1	6	72.6	-69.2
-1	1	7	55.7	55.0
1	1	7	7.6*	11.6
-1	1	8	16.9	18.3
1	1	8	8.4*	- 4.6
-1	1	9	16.6	18.5
1	1	9	9.0*	- 5.3
-1	1	10	21.8	20.2
-1	1	11	36.8	38.0
1	1	11	15.2	-18.9
1	1	12	54.8	54.4
-1	1	12	24.5	22.9
-1	1	13	27.3	-27.8
1	1	13	48.9	-52.3
-1	1	14	57.6	-60.0
1	1	14	52.1	-53.4
-1	1	15	51.2	53.5
1	1	15	14.7	-12.9
-1	1	16	14.1	12.9
1	1	16	7.9*	-13.9
-1	1	17	50.7	53.0
1	1	17	36.5	-39.4
-1	1	18	7.6*	2.5
1	1	18	7.3*	6.6
-1	1	19	21.0	21.8
1	1	19	7.2*	0.5
-1	1	20	25.9	29.5
1	1	20	33.0	37.4
-1	1	21	6.9*	- 8.1
1	1	21	42.8	-43.8
-1	1	22	35.8	-34.5
1	1	22	39.7	-39.2
-1	1	23	56.1	56.5
1	1	23	16.0	-18.1
-1	1	24	6.2*	11.0
3	1	0	17.5	-18.1
-3	1	1	7.0*	- 6.9
3	1	1	28.0	-30.3
-3	1	2	35.1	35.0
3	1	2	81.4	-82.8
-3	1	3	72.6	-74.4
3	1	3	74.4	75.9
-3	1	4	27.8	30.8
3	1	4	104.6	105.3
-3	1	5	107.7	-109.9
3	1	5	20.7	-18.6
-3	1	6	64.2	-65.8
3	1	6	15.0	-14.1
-3	1	7	7.3*	3.8
3	1	7	19.6	-16.1
-3	1	8	26.0	27.4
3	1	8	36.6	-37.2
-3	1	9	49.9	-52.3
3	1	9	32.0	34.0
-3	1	10	13.7	- 5.6
3	1	10	8.6*	6.1
-3	1	11	35.2	-36.8
3	1	11	85.8	84.2
-3	1	12	34.4	32.6
3	1	12	51.8	51.0
-3	1	13	16.5	-16.7
3	1	13	8.4*	0.6
-3	1	14	51.2	-50.1
3	1	14	42.7	-43.7
-3	1	15	31.9	29.9
3	1	15	29.6	29.8
-3	1	16	7.8*	0.5
3	1	16	7.2*	- 5.5
-3	1	17	23.5	-22.4
3	1	17	36.2	35.0
-3	1	18	28.2	28.0
3	1	18	6.7*	-10.6
-3	1	19	12.7	-15.5
3	1	19	23.0	24.5
-3	1	20	13.9	14.7
3	1	20	22.1	23.6
-3	1	21	29.2	-32.0
-3	1	22	49.5	-49.2
5	1	0	13.1	6.0
-5	1	1	7.2*	- 6.0
5	1	1	46.6	-49.3
-5	1	2	15.2	15.5
5	1	2	53.1	-54.9
-5	1	3	17.6	-19.2
5	1	3	7.2*	5.8
-5	1	4	18.0	19.9
5	1	4	35.1	36.0
-5	1	5	7.2*	- 1.0
5	1	5	25.8	-30.2
-5	1	6	45.3	-43.0
5	1	6	18.6	21.0
-5	1	7	48.3	48.9
5	1	7	51.1	-52.8
-5	1	8	7.2*	14.4
5	1	8	7.9*	-16.7
-5	1	9	20.4	20.6
5	1	9	51.1	-50.9
5	1	10	25.0	-24.8
-5	1	11	39.1	39.1
5	1	11	7.1*	3.4
-5	1	12	7.7*	8.3
5	1	12	54.9	52.8
-5	1	13	22.0	23.5
-5	1	14	48.9	-45.2
-5	1	15	52.5	51.5
-5	1	16	29.1	26.0
0	2	5	153.5	-148.3
		6	13.0	-12.3
		7	41.7	41.9
		8	14.4	7.3
		9	23.1	24.4
		11	17.4	11.9
		12	37.8	40.1
		13	73.5	-74.3
		14	13.4	-10.3
		15	46.1	46.9
		16	38.7	37.1
		17	7.8*	10.6
		18	34.4	35.6
		19	7.3*	8.2
		20	26.2	28.1
		21	34.3	-35.5
		22	12.1	10.7
		23	31.8	29.8
2	2	0	51.5	49.4
-2	2	1	77.1	-74.2
2	2	1	83.6	-76.7
-2	2	2	6.8*	-10.2
2	2	2	43.1	-43.8
-2	2	3	76.0	75.2
2	2	3	62.2	63.3
-2	2	4	6.9*	0.1
2	2	4	29.6	-30.9
-2	2	5	46.6	-47.4
2	2	5	7.2*	4.7
-2	2	6	44.0	-47.8
2	2	6	23.8	-25.0
2	2	7	50.3	-50.7
-2	2	8	66.5	-67.0
2	2	8	69.3	-70.0
-2	2	9	35.1	33.9
2	2	9	22.5	-16.0
-2	2	10	65.6	-63.2
2	2	10	96.6	-93.0
-2	2	11	46.0	42.7
2	2	11	99.1	97.3
-2	2	12	31.4	-28.4
2	2	12	8.8*	8.2
-2	2	13	110.6	-105.5
2	2	13	95.6	-94.4
-2	2	14	68.4	-66.6
2	2	14	19.6	-24.2
-2	2	15	66.6	64.2
2	2	15	7.7*	- 4.6
-2	2	16	8.0*	- 9.0
2	2	16	36.8	-34.9
-2	2	17	27.4	29.9
2	2	17	50.9	51.5
-2	2	18	12.8	10.9
2	2	18	7.1*	1.4
2	2	19	6.8*	5.5
-2	2	20	6.9*	- 4.3
2	2	20	17.8	16.8
-2	2	21	20.9	-25.3
2	2	21	49.4	-50.5
-2	2	22	20.4	-24.3
-2	2	23	49.4	49.9
4	2	0	53.9	55.2
-4	2	1	47.7	45.5
4	2	1	16.8	16.5
-4	2	2	57.2	58.0
4	2	2	45.8	45.8
-4	2	3	24.1	25.4
4	2	3	56.9	55.4
-4	2	4	27.6	29.8
4	2	4	65.4	65.5
-4	2	5	105.9	-107.9
4	2	5	52.9	-51.1
-4	2	6	53.0	-51.6
4	2	6	22.5	26.7
-4	2	7	71.6	69.3
4	2	7	13.4	14.5
-4	2	8	7.8*	7.3
4	2	8	7.8*	11.7
-4	2	9	25.0	26.5
4	2	9	14.1	-14.2
4	2	10	24.9	-25.7
-4	2	11	45.0	-45.7
4	2	11	25.1	28.8
-4	2	12	14.9	- 6.6
4	2	12	8.0*	0.6
-4	2	13	20.4	-21.4
4	2	13	20.6	-18.6
-4	2	14	9.5*	14.2
4	2	14	15.0	13.5
-4	2	15	66.8	65.8
4	2	15	15.0	-14.9
-4	2	16	81.2	78.8
4	2	16	12.9	14.9
-4	2	17	28.8	-30.0
-4	2	18	33.5	32.3
-4	2	19	6.3*	- 3.7
6	2	0	12.3	11.5
-6	2	1	6.7*	5.3
6	2	1	37.4	-35.0
-6	2	2	24.6	-26.4
6	2	2	10.3	-14.1
-6	2	3	6.7*	- 9.5
6	2	3	42.8	41.4
-6	2	4	59.9	-59.6
6	2	4	7.3*	3.0
-6	2	8	7.4*	- 8.7
1	3	2	6.9*	11.9
1	3	3	135.3	-132.4
-1	3	4	14.2	11.9
-1	3	5	64.8	63.1
1	3	5	170.7	-168.1
-1	3	6	22.8	20.6
1	3	6	7.6*	3.5
-1	3	7	135.4	133.8
-1	3	8	40.1	-40.0
1	3	8	22.0	-21.7
-1	3	9	125.6	-122.3
1	3	9	209.0	-211.0
-1	3	10	22.1	23.3
1	3	10	27.1	27.6
-1	3	11	171.9	169.8
1	3	11	93.5	-91.3
-1	3	12	25.4	21.8
1	3	12	8.1*	0.3
1	3	13	62.0	63.2
-1	3	14	27.1	-25.4
1	3	14	7.9*	- 1.7
-1	3	15	41.8	41.9
1	3	15	52.4	53.0
-1	3	16	23.8	-25.8
1	3	16	7.8*	-13.8
-1	3	17	42.0	-42.7
1	3	17	128.4	-129.4
-1	3	18	37.1	37.5
1	3	18	7.2*	5.7
-1	3	19	120.7	120.1
1	3	19	12.5	12.3
1	3	21	19.6	20.4
-1	3	22	16.8	-18.0
1	3	22	6.3*	2.2
-1	3	23	39.6	-38.4
3	3	0	26.5	-28.2
-3	3	1	260.3	-265.4
3	3	1	67.3	69.0
-3	3	2	27.6	27.5
3	3	2	7.7*	- 8.8
-3	3	3	48.7	-49.4
3	3	3	7.7*	-11.7
-3	3	4	13.6	9.9
3	3	4	7.8*	4.9
-3	3	5	7.5*	9.0
3	3	5	41.6	39.6
-3	3	6	16.2	-17.5
3	3	6	22.9	24.1
-3	3	7	60.7	-62.2
3	3	7	133.2	133.1
-3	3	8	7.8*	- 8.0
3	3	8	29.1	-27.5
-3	3	9	125.1	-126.6
3	3	9	73.5	-72.2
-3	3	10	37.2	37.2
3	3	10	8.7*	- 1.2
-3	3	11	86.0	86.1
3	3	11	31.0	-33.5
-3	3	12	23.1	-20.6
3	3	12	24.6	24.5
-3	3	13	9.3*	11.8
3	3	13	89.1	86.5
-3	3	14	9.5*	-11.1
3	3	14	7.5*	0.1
-3	3	15	96.2	-94.1
3	3	15	116.4	117.6
3	3	16	29.0	-31.5
-3	3	17	101.1	-100.3
-3	3	18	7.1*	6.7
3	3	18	18.3	18.1
3	3	19	53.2	52.8
-3	3	20	12.0	- 8.3
-3	3	21	59.8	-59.2
-5	3	0	15.1	-13.0
5	3	1	19.1	-20.2
-5	3	2	17.9	18.8
5	3	2	7.2*	- 7.2
-5	3	3	88.1	88.0
5	3	3	62.4	-61.5
-5	3	4	7.3*	- 1.6
5	3	4	7.2*	2.3
-5	3	5	98.6	98.7
5	3	5	67.3	-65.5
-5	3	6	7.2*	- 6.7
5	3	6	7.3*	10.4
-5	3	8	7.1*	- 4.6
-5	3	9	7.4*	-10.2
5	3	9	52.0	-51.2
5	3	10	7.2*	1.6
5	3	11	100.1	-98.2
-5	3	12	8.4*	- 6.8
-5	3	14	12.8	-11.8
-5	3	15	35.4	-36.0
0	4	5	17.4	-16.1
		6	57.5	-56.8
		7	40.1	-40.2
		9	7.9*	10.2
		10	45.6	-45.7
		11	55.8	55.8
		12	130.5	-131.1
		13	81.6	-79.6
		14	51.2	48.9
		15	7.8*	16.7
		16	7.5*	- 1.6
		17	44.0	47.3
		18	41.9	-41.3
		19	6.9*	- 6.1
		21	35.2	-36.2
		22	32.5	30.1
2	4	0	68.3	68.5
-2	4	1	32.4	30.6
2	4	3	51.7	51.1
-2	4	4	78.1	-78.0
2	4	4	7.6*	- 1.1
-2	4	5	99.9	-99.8
2	4	5	60.7	-60.1
-2	4	6	83.2	84.7
2	4	6	76.5	77.2
-2	4	7	21.9	23.5
2	4	7	7.9*	0.9
-2	4	8	7.7*	8.6
2	4	8	34.3	32.5
-2	4	9	48.6	48.4
2	4	9	8.7*	8.1
-2	4	10	8.2*	- 7.6
2	4	10	41.9	43.8
-2	4	11	19.6	-20.5
-2	4	12	28.8	27.6
2	4	12	42.6	-40.3
-2	4	13	55.0	-52.1
2	4	13	49.9	-48.7
-2	4	14	100.8	99.9
2	4	14	16.2	16.7
-2	4	15	58.7	58.1
2	4	15	7.4*	5.7
-2	4	16	7.5*	5.6
2	4	16	28.9	31.7
-2	4	17	7.3*	1.4
2	4	17	15.5	19.8
-2	4	18	20.3	20.0
2	4	18	20.7	24.5
-2	4	19	12.7	-14.6
2	4	19	6.5*	13.1
-2	4	20	6.6*	10.9
2	4	20	18.2	-19.0
-2	4	21	6.4*	- 7.6
4	4	0	53.8	-57.1
-4	4	1	7.7*	9.6
4	4	1	15.3	-13.2
-4	4	2	47.9	-48.1
4	4	2	21.8	18.6
-4	4	3	14.1	14.2
4	4	3	40.1	42.7
-4	4	4	55.9	-54.6
4	4	4	42.2	-43.7
-4	4	5	42.6	-42.2
4	4	5	7.7*	- 4.8
-4	4	6	23.3	23.3
4	4	6	31.1	-32.6
-4	4	7	20.2	20.0
4	4	7	19.3	-18.5
-4	4	8	22.4	-25.1
4	4	8	7.7*	2.0
-4	4	9	7.5*	17.9
4	4	9	8.0*	- 7.7
-4	4	10	27.8	-27.0
4	4	10	29.7	32.8
-4	4	11	7.7*	- 6.0
-4	4	12	8.0*	-12.0
4	4	12	63.4	-61.3
-4	4	13	33.4	-34.6
4	4	13	34.1	-34.6
-4	4	14	38.9	34.3
4	4	14	15.7	-17.6
-4	4	15	36.6	35.3
-4	4	16	58.6	-57.9
-4	4	17	6.6*	7.4
-1	5	2	26.5	26.1
1	5	2	7.6*	- 2.2
-1	5	3	20.1	18.4
1	5	3	58.3	-58.1
-1	5	4	115.5	-115.3
1	5	4	80.1	-79.2
-1	5	5	26.9	-25.9
1	5	5	60.1	-60.7
-1	5	6	79.3	78.6
1	5	6	70.7	68.5
-1	5	7	8.2*	13.7
1	5	7	47.8	-49.2
-1	5	8	20.6	20.0
1	5	8	9.8*	-14.3
-1	5	9	28.9	33.7
1	5	9	31.9	-32.6
-1	5	10	23.4	-23.5
1	5	10	15.2	14.9
-1	5	11	8.7*	15.9
1	5	11	8.4*	- 0.2
-1	5	12	42.3	-40.3
1	5	12	32.9	-32.9
-1	5	13	35.1	38.9
1	5	13	7.9*	-13.1
-1	5	14	69.6	69.1
1	5	14	24.6	25.4
-1	5	15	53.8	54.7
1	5	15	14.8	-15.9
-1	5	16	17.9	-18.2
1	5	16	7.3*	5.6
-1	5	17	26.0	26.0
1	5	17	7.0*	0.6
-1	5	18	17.3	-17.5
1	5	18	6.9*	9.8
-1	5	19	20.5	21.8
1	5	19	12.5	-15.2
-1	5	20	16.7	-16.3
1	5	20	43.9	-46.4
-1	5	21	14.4	13.4
3	5	0	7.8*	5.7
-3	5	1	34.2	-36.4
3	5	1	8.0*	3.4
-3	5	2	52.2	-53.0
3	5	2	87.8	87.6
-3	5	3	90.9	-90.2

Table 7. *(Continued)*

h	k	l	F_o	F_c
3	5	3	20.0	23.5
-3	5	4	7.8*	- 9.9
3	5	4	101.4	-102.2
-3	5	5	60.4	-59.1
3	5	5	8.0*	-12.3
-3	5	6	69.6	72.5
3	5	6	7.9*	5.2
-3	5	7	28.5	-27.9
3	5	7	19.6	-20.1
-3	5	8	46.2	-45.0
3	5	8	52.7	51.7
-3	5	9	32.6	-33.1
3	5	9	8.3*	14.0
-3	5	10	7.9*	14.8
3	5	10	8.7*	- 1.0
-3	5	11	8.1*	- 1.3
3	5	11	32.6	30.6
-3	5	12	8.7*	-12.1
3	5	12	57.1	-54.9
-3	5	13	9.8*	11.6
3	5	13	38.4	39.2
-3	5	14	30.1	26.1
3	5	14	48.5	48.7
-3	5	15	7.5*	7.3
3	5	15	38.2	39.6
-3	5	16	7.2*	- 7.6
3	5	16	6.5*	- 2.8
-3	5	17	6.8*	- 3.6
3	5	17	23.9	24.2
-3	5	18	12.0	- 8.2
-3	5	19	28.4	-29.7
5	5	0	16.3	-17.7
-5	5	1	24.8	-23.6
5	5	1	13.1	-12.6
-5	5	2	7.0*	- 0.4
5	5	2	35.7	36.7
-5	5	3	24.9	-23.3
5	5	3	18.3	-19.7
-5	5	4	21.2	-19.2
5	5	4	22.4	-23.4
5	5	5	16.5	-17.9
-5	5	6	35.4	35.7
5	5	6	7.4*	-16.2
-5	5	7	34.5	35.4
5	5	7	52.7	-51.5
-5	5	8	7.5*	- 3.8
-5	5	9	35.6	35.5
-5	5	10	7.8*	-12.7
-5	5	11	36.0	36.2
0	6	4	9.2*	3.7
		5	22.3	-22.8
		6	56.8	-55.3
		7	30.6	-30.0
		8	112.8	-113.4
		10	67.9	67.5
		11	18.5	-18.0
		13	35.0	-33.6
		14	77.2	-78.3
		16	110.9	-111.7
		17	38.2	38.8
		18	6.7*	9.9
		19	24.7	-23.8
2	6	0	105.5	-106.8
-2	6	1	70.9	70.9
2	6	1	30.4	34.5
-2	6	2	162.5	165.7
-2	6	3	13.5	-16.7
2	6	3	26.7	27.1
-2	6	4	122.5	126.4
-2	6	6	10.5	13.3
2	6	6	39.1	40.2
-2	6	7	8.0*	6.2
2	6	7	27.3	-29.4
-2	6	8	38.3	38.1
2	6	8	60.7	-58.3
-2	6	9	30.9	31.0
2	6	9	37.6	35.4
-2	6	10	166.5	163.9
2	6	10	121.6	119.6
-2	6	11	33.1	-32.9
2	6	11	8.5*	- 2.4
-2	6	12	24.4	26.9
2	6	12	116.9	115.0
-2	6	13	8.1*	- 6.0
2	6	13	14.3	-12.2
-2	6	14	27.6	-26.2
2	6	14	45.9	47.6
-2	6	15	7.3*	- 3.5
2	6	15	27.4	-27.6
-2	6	16	7.2*	- 1.2
2	6	16	6.8*	- 9.8
-2	6	17	28.6	29.7
2	6	17	28.8	28.3
-2	6	18	84.9	84.0
-2	6	19	9.9	-13.6
4	6	0	73.0	-72.0
-4	6	1	40.0	40.4
4	6	1	7.4*	- 3.9
-4	6	2	61.4	63.4
4	6	2	108.9	-110.5
4	6	3	26.1	30.1
-4	6	4	36.0	-37.8
4	6	4	20.9	-19.6
-4	6	5	15.9	-10.5
4	6	5	14.6	9.9
-4	6	6	68.1	-68.4
4	6	6	15.2	14.5
-4	6	7	7.5*	4.3
4	6	7	45.3	-44.0
-4	6	8	47.8	-44.7
4	6	8	136.1	-133.7
-4	6	9	31.6	28.9
4	6	9	29.6	28.7
-4	6	10	25.7	20.8
4	6	10	53.5	-48.1
-4	6	11	28.5	-28.9
4	6	11	20.2	14.4
-4	6	12	68.8	-66.5
-4	6	13	7.5*	-10.8
-4	6	14	91.9	-87.0
1	7	0	29.8	29.1
-1	7	1	108.9	-109.8
1	7	1	34.7	35.4
-1	7	2	32.4	-34.2
1	7	2	30.0	25.9
-1	7	3	68.6	-69.1
-1	7	4	23.4	-19.8
1	7	4	74.9	-75.7
1	7	5	74.2	73.5
-1	7	6	38.6	38.7
1	7	6	23.4	21.1
-1	7	7	88.4	-86.2
1	7	7	9.4*	4.9
-1	7	8	10.3*	- 7.1
1	7	8	35.5	37.3
1	7	10	27.8	-23.9
-1	7	11	8.0*	- 3.0
1	7	11	7.8*	5.3
-1	7	12	7.7*	-10.9
1	7	12	20.3	-18.7
-1	7	13	38.3	36.9
1	7	13	99.6	100.3
-1	7	14	14.7	12.8
1	7	14	39.3	39.1
-1	7	15	16.9	-15.9
1	7	15	12.8	14.4
-1	7	16	10.6	13.2
1	7	16	6.8*	- 3.0
-1	7	17	23.9	-25.6
1	7	17	24.6	26.0
-1	7	18	6.4*	-11.9
3	7	0	18.4	18.0
-3	7	1	19.7	-19.8
-3	7	2	7.5*	- 0.5
-3	7	3	7.5*	- 4.9
3	7	3	61.9	-63.6
3	7	4	27.9	-31.3
-3	7	5	77.2	78.6
3	7	5	7.6*	- 0.6
-3	7	6	29.0	30.6
3	7	6	7.7*	0.5
-3	7	7	7.5*	3.6
3	7	7	17.8	-22.5
-3	7	8	16.6	17.1
-3	7	9	18.3	22.4
3	7	9	34.5	-34.6
-3	7	10	21.5	-21.1
3	7	10	14.9	7.8
-3	7	11	49.5	45.1
3	7	11	76.4	-73.7
-3	7	12	8.8*	-14.8
3	7	12	24.5	-23.2
-3	7	13	72.7	69.3
3	7	13	6.6*	7.6
-3	7	14	35.0	34.2
-3	7	15	34.4	-33.6
0	8	4	20.1	-19.6
		5	46.5	44.0
		6	20.7	-21.9
		7	8.3*	11.0
		8	14.6	-12.6
		9	16.1	-18.2
		10	7.7*	- 4.7
		11	32.8	-32.0
		12	7.4*	- 1.5
		13	60.7	59.7
		14	26.8	-28.8
		15	27.1	-27.7
		16	6.6*	-10.6
		17	18.6	-19.5
2	8	0	8.0*	- 3.0
-2	8	1	7.7*	- 3.1
2	8	1	16.1	7.6
-2	8	2	7.6*	- 5.7
2	8	2	7.9*	6.4
-2	8	3	28.7	-29.7
2	8	3	33.4	-34.3
-2	8	4	17.7	21.8
2	8	4	22.0	20.7
-2	8	5	59.3	59.4
2	8	5	26.6	30.0
-2	8	6	26.2	27.5
2	8	6	16.6	16.4
-2	8	7	15.4	-15.0
2	8	7	8.2*	8.5
-2	8	8	44.9	45.8
2	8	8	46.1	47.1
-2	8	9	21.7	-23.6
2	8	9	8.5*	6.2
-2	8	10	29.0	30.4
2	8	10	34.0	35.3
-2	8	11	8.4*	- 2.8
2	8	11	42.4	-43.5
-2	8	12	42.8	40.6
2	8	12	30.6	29.4
-2	8	13	41.6	41.4
2	8	13	35.3	34.6
-2	8	14	26.9	26.5
2	8	14	15.5	18.2
-2	8	15	42.2	-43.5
-2	8	16	6.5*	- 1.0
4	8	0	46.3	-46.2
-4	8	1	7.0*	- 6.5
4	8	1	6.9*	11.8
-4	8	2	33.5	-34.1
4	8	2	44.2	-44.9
-4	8	3	6.9*	- 5.3
4	8	3	31.1	-31.5
-4	8	4	7.0*	9.3
4	8	4	19.8	-24.9
-4	8	5	51.5	48.4
4	8	5	16.0	16.3
-4	8	6	8.4*	7.1
-4	8	7	30.0	-30.0
-4	8	8	7.9*	- 0.2
-4	8	9	9.6*	-13.7

* Observed intensity is less than $2\sigma(I_0)$; I_0 is assigned the value of $2\sigma(I_0)$.

Another set of six outer oxygen atoms surrounds the interlayer cation with an average distance of 3.237 and 3.362 Å for phengite and muscovite, respectively.

Distortions

Atomic planes in micas are distorted in the following ways:

(*a*) by rotations in the plane,

(*b*) by tilting in elevations.

(*a*) In ideal atomic configurations, both anions and cations form hexagonal arrays with interatomic angles of 120°. Deviations[1] (2α) from this value give the distortions in the plane. The values of 2α for both micas are given in Table 8. The displacements of basal oxygen atoms are almost twice as much in Georgia muscovite (average $2\alpha = 22.7°$) as in phengite (average $2\alpha = 12.1°$). Displacements of

[1] Half of 2α for the basal oxygen atoms is usually referred to as the tetrahedral rotation, α.

Table 8. *Deviations* (2α) *of interatomic angles from* 120° *in* $2M_1$ *phengite,* $2M_1$ *and* 3T *muscovites*

(Angles are measured counterclockwise starting from first two atoms whose coordinates are listed in Tables 2 and 3 for phengite and $2M_1$ muscovite. Standard errors are given in parentheses.)

$2M_1$ Phengite			$2M_1$ Muscovite		3T Muscovite (GÜVEN and BURNHAM, 1967)	
Angles between basal oxygen atoms:		2α		2α		2α
$O_e-O_d-O_e$	107.1(2)	12.9°	96.3(2)	23.7°	95.0(4)	25.0°
$O_d-O_c-O_e$	131.8(1)	11.8	142.5(1)	22.5	141.2(9)	21.2
$O_e-O_e-O_d$	108.1(2)	11.9	97.2(2)	22.8	95.0(4)	25.0
$O_e-O_d-O_e$	132.3(2)	12.3	142.3(2)	22.3	145.5(6)	25.5
$O_d-O_e-O_e$	108.1(1)	11.9	97.3(1)	22.7	97.2(4)	22.8
$O_e-O_e-O_d$	131.5(2)	11.5	142.2(2)	22.2	143.8(6)	23.8
		Mean 12.1		Mean 22.7		Mean 23.9
		± 0.1		± 0.1		± 0.2
Angles between apical oxygen atoms:						
$O_b-O_a-O_b$	112.7(2)	7.3	111.9(2)	8.1	$O_a-O_b-O_a$ 111.3(7)	8.7
$O_a-O_b-O_a$	133.7(2)	13.7	136.2(2)	16.2	$O_b-O_a-O_b$ 111.8(8)	8.2
$O_b-O_a-O_b$	113.6(2)	6.4	111.9(2)	8.1	$O_a-O_b-O_a$ 137.0(8)	17.0
		Mean 9.2		Mean 10.8		Mean 11.3
		± 0.1		± 0.1		± 0.3
Angles between tetrahedral cations:						
$T_2-T_1-T_2$	119.2(1)	0.8	118.6(1)	1.4	$T_1-T_2-T_1$ 117.5(3)	2.5
$T_1-T_2-T_1$	122.4(1)	2.4	122.8(1)	2.8	$T_2-T_1-T_2$ 122.7(5)	2.7
$T_2-T_1-T_2$	118.5(1)	1.5	118.6(1)	1.4	$T_1-T_2-T_1$ 119.8(4)	0.2
		Mean 1.6		Mean 1.9		Mean 2.5
		± 0.1		± 0.1		± 0.3
Angles between octahedral cation:						
Al–Al′–Al	120.8(1)	0.8	120.2(1)	0.2	120.0	

apical oxygen atoms are, however, quite similar in both structures; the displacement in one direction is distinctly greater ($2\alpha = 16.2°$ for muscovite and $2\alpha = 13.7°$ for phengite) than others.

The tetrahedral cations, however, show smaller displacements from their ideal sites; whereas the octahedral cations show practically no displacement from their ideal positions in both mica structures.

(*b*) Tilting of the tetrahedral sheets gives rise to differences in coordinates of the basal oxygen atoms. One of the basal oxygen atoms, O_d, is displaced off the plane of O_c and O_e oxygen atoms by an amount

$$\Delta z = \left[\frac{z_{O_e} + z_{O_e}}{2} - z_{O_d}\right] c \sin\beta = 0.22 \pm 0.01 \text{ Å}$$

for Georgia muscovite and 0.16 ± 0.01 Å for phengite. This corrugation of the basal-oxygen layers, usually referred to as tetrahedral tilt, is characteristic of dioctahedral $2M_1$ micas.

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