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The crystal structure of taeniolite, $KLiMg_2Si_4O_{10}F_2$

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Auszug

Taeniolith, $KLiMg_2Si_4O_{10}F_2$, wurde aus Gemengen von KF, LiF, MgO und SiO_2 synthetisch dargestellt und seine Kristallstruktur aus dreidimensionalen Röntgendaten verfeinert. Die Verbindung kristallisiert monoklin in der Raumgruppe $C2/m$, $a = 5{,}231(1)$, $b = 9{,}065(2)$, $c = 10{,}140(1)$ Å, $\beta = 99{,}86(2)°$, und $Z = 2$. Die Verfeinerung nach dem (Voll-Matrix-) Kleinste-Quadrate-Verfahren ergab einen R-Wert von 0,024 für 1303 beobachtete Reflexe. Alle Abstände der Si-Atome von den O-Atomen der Schichten sind 1,638(1) Å, dagegen ist der Abstand Si—O zu den freien Tetraederspitzen 1,586(1) Å. Ein Vergleich der Glimmer-Struktur des 1M-Typs zeigte deutlich den Einfluß der Oktaeder-Kationen auf die Verdrehung der $(Si,Al)O_4$-Tetraeder. Die Li^+-Ionen konzentrieren sich mehr über der M(2)-Lage als über der M(1)-Lage, gemäß dem Unterschiede der Großen der beiden Oktaeder. Die Verdrehung der Tetraeder um die Normale der Schichten ist noch kleiner als beim $KMg_{2.5}Si_4O_{10}F_2$; sie beträgt 1,08°. Die Oktaeder-Abplattungswinkel ψ sind 57,8° für die M(1)-Lage und 57,9° für die M(2)-Lage.

Abstract

Taeniolite, $KLiMg_2Si_4O_{10}F_2$, was synthesized from a mixture of KF, LiF, MgO and SiO_2, and the crystal structure was refined with three-dimensional x-ray diffraction data. The crystals are monoclinic (1M type) with the space group $C2/m$, $a = 5.231(1)$, $b = 9.065(2)$, $c = 10.140(1)$ Å, $\beta = 99.86(2)°$, and $Z = 2$. Refinements with the full-matrix least-squares procedure gave the final R value of 0.024 for 1303 observed reflections. All the bridging Si—O distances are 1.638(1) Å, whereas the nonbridging one is 1.586(1) Å. A comparison of several 1M-type micas clearly indicates the effect of octahedral cations on the distortion of $(Si,Al)O_4$ tetrahedra. Li^+ ions are more concentrated at the M(2) site than at M(1) in conformity with the size difference between the coordination octahedra. The ditrigonal distortion of the tetrahedral sheets is still smaller than that of $KMg_{2.5}Si_4O_{10}F_2$, having the tetrahedral rotation angle α of 1.08°. The octahedral flattening angles, ψ, are 57.8° and 57.9° for M(1) and M(2) sites, respectively.

Introduction

Taeniolite, $KLiMg_2Si_4O_{10}F_2$, is one of the rare examples of natural tetrasilicic micas. The mineral was known to have a 1M-type structure and to be closely related to the synthetic silicates, $KMg_{2.5}Si_4O_{10}F_2$ (TORAYA *et al.*, 1976) and $KMg_{2.5}Si_4O_{10}(OH)_2$ (SEIFERT and SCHREYER, 1971), though the details of the structure were not clear. $KMg_{2.5}Si_4O_{10}F_2$ has a very small ditrigonal distortion of tetrahedral layers, with a rotation angle α (DONNAY *et al.*, 1964) of 1.42°. It is of interest to see how the replacement of $\frac{1}{2}Mg^{2+}$ by Li^+ per a formula unit affects the shape of the silicate layers in the mineral.

In fluoropolylithionite, $KLi_2AlSi_4O_{10}F_2$, a half of Li^+ ions occupy $2c$ [M(1)] sites and the remaining half of Li^+ and Al^{3+} ions are at $4h$ [M(2)] sites (TAKEDA and BURNHAM, 1969). In contrast to this ordered arrangement of octahedral cations, the Mg^{2+} ions in $KMg_{2.5}Si_4O_{10}F_2$ are distributed over the two independent octahedral sites in complete disorder. It is also the purpose of the present study to elucidate the distribution of octahedral cations in this crystal.

Experimental

Crystals of $KLiMg_2Si_4O_{10}F_2$ were synthesized from a mixture of KF, LiF, MgO and SiO_2 in the molar ratios of 1:1:2:4 with the same procedure as described in a previous report on $KMg_{2.5}Si_4O_{10}F_2$ (TORAYA *et al.*, 1976). The specimen obtained was an aggregate of flakes of transparent crystals. It was confirmed from Weissenberg photographs that most of the crystals are essentially based on the 1M-type stacking of the double sheets, though stacking disorder and twinnings are quite common. The cell dimensions were determined with the least-squares procedure from fifteen 2θ values obtained by powder diffractometry in the range $5° < 2\theta < 70°$. They are given in Tab. 1 together with other crystal data.

For intensity measurement, a crystal with dimensions $0.30 \times 0.25 \times 0.14$ mm was selected out, which was free from diffuse streaks. Intensities were measured on a four-circle diffractometer (Philips PW 1100) up to $2\theta = 80°$ with Mo$K\alpha$ radiation monochromated with

Table 1. *Crystal data of taeniolite*

monoclinic, $C2/m$

$a = 5.231(1)$, $b = 9.065(2)$, $c = 10.140(1)$ Å

$\beta = 99.86(2)°$

$V = 473.8(1)$ Å^3, $Z = 2$

$D_x = 2.84$ g · cm^{-3}

graphite. The ω-2θ scan technique was employed with the scan speed of $4^\circ\,\mathrm{min}^{-1}$ in ω. The scan range was determined according to the formula $1.30^\circ + 0.20^\circ \times \tan\theta$. Background counts were measured at each limit of a scan range during a time determined by the formula, time $=$ (scantime/2) $\times$ $(I_{\mathrm{back}}/I_{\mathrm{int}})^{1/2}$, where I_{back} represents the background counts per second preliminary measured and I_{int} is the mean counts per second during the scan. When the total counts were less than 100000, the scanning was repeated twice. In all 1303 independent reflection data were obtained, and they were corrected for Lorentz, polarization and absorption factors. Absorption corrections were carried out with the program ACACA (WUENSCH and PREWITT, 1965) by taking into accounts the crystal shape, the correction factors ranging between 0.8462 and 0.7044 ($\mu = 12.66\ \mathrm{cm}^{-1}$ for Mo$K\alpha$).

Refinement of the structure

Structure refinement was started on the assumption of random distribution of two Li^+ and four Mg^{2+} ions over six octahedral sites in the unit cell. Adopting the atomic parameters of tetrasilicic potassium fluoromica (TORAYA *et al.*, 1976) for the initial values, a few cycles of full-matrix least-squares refinements were carried out with a program LINUS (COPPENS and HAMILTON, 1970) in the isotropic mode, yielding a conventional R value of 0.042. Difference Fourier maps synthesized at this stage indicated ordering of metals at octahedral sites. Therefore, refinements were continued by varying the distribution of Li^+ and Mg^{2+} ions over the two independent octahedral sites in the anisotropic thermal mode, reducing the R values to 0.025. Since negative and positive peaks were still observed at the interlayer and octahedral cation sites, respectively, on the difference Fourier maps, populations of K^+, Li^+ and Mg^{2+} ions were varied by restricting the net charge of the crystal to be neutral and by assuming that no vacancy exists at either of the octahedral sites. The refinement reduced the R value to 0.024, giving the population of 0.97 for K^+, and 0.71 and 0.66 for Mg^{2+} ions at M(1) and M(2) sites, respectively. The atomic scattering factors used were those for K^+, Li^+, Mg^{2+}, Si^{4+} and F^- taken from *International tables for x-ray crystallography* (1974) and for O^{2-} given by TOKONAMI (1965). Unit weights were assigned for all the reflections. The final atomic parameters are given in Tab. 2, and the observed and calculated structure factors are compared in Tab. 3. All the computations were carried out on a HITAC 8700 computer at the Computer Center of Tokyo Institute of Technology.

Table 2. *Final atomic parameters*

	α	x	y	z
K	0.967(4)	0	$\frac{1}{2}$	0
M(1)	Mg 0.708 Li 0.292	0	0	$\frac{1}{2}$
M(2)	Mg 0.663(3) Li 0.337	0	0.33442(9)	$\frac{1}{2}$
Si		0.07573(6)	0.16666(3)	0.22829(3)
O(1)		0.0494(3)	0	0.1650(1)
O(2)		0.3075(2)	0.2473(1)	0.1650(1)
O(3)		0.1284(2)	0.1668(1)	0.3871(1)
F		0.6333(2)	0	0.3967(1)

	β_{11}	β_{22}	β_{33}	β_{12}	β_{13}	β_{23}
K	0.0179(2)	0.00573(8)	0.00452(6)	0	0.00160(9)	0
M(1)	0.0063(3)	0.00169(10)	0.00157(9)	0	0.00098(12)	0
M(2)	0.0056(2)	0.00187(8)	0.00155(6)	0	0.00045(9)	0
Si	0.0041(1)	0.00131(3)	0.00112(2)	0.00000(4)	0.00047(3)	— 0.00001(2)
O(1)	0.0115(4)	0.00144(10)	0.00169(9)	0	0.00047(14)	0
O(2)	0.0066(2)	0.00305(8)	0.00161(6)	— 0.00183(11)	0.00070(9)	— 0.00009(6)
O(3)	0.0064(2)	0.00196(7)	0.00116(5)	— 0.00009(10)	0.00050(8)	0.00000(5)
F	0.0090(3)	0.00287(10)	0.00226(8)	0	0.00092(13)	0

α is the population.

Anisotropic temperature factors are expressed in the form exp $[-(h^2\beta_{11} + k^2\beta_{22} + l^2\beta_{33} + 2hk\beta_{12} + 2hl\beta_{13} + 2kl\beta_{23})]$.

Tabelle 3. *The observed and calculated structure factors*

h	k	l	|Fo|	|Fc|	h	k	l	|Fo|	|Fc|	h	k	l	|Fo|	|Fc|	h	k	l	|Fo|	|Fc|	h	k	l	|Fo|	|Fc|
2	0	0	85.1	83.5	-4	4	1	14.9	14.7	3	3	2	6.1	7.1	-2	2	3	15.2	13.9	-1	1	4	16.7	17.8
4	0	0	7.7	8.1	-8	4	1	10.4	10.5	1	3	2	14.2	10.2	-4	2	3	30.1	30.5	-3	1	4	40.8	40.8
6	0	0	4.0	4.5	-7	5	1	7.6	6.9	-1	3	2	102.2	101.4	-6	2	3	13.5	13.0	-5	1	4	38.5	38.7
8	0	0	5.4	4.8	-5	5	1	7.8	7.5	-3	3	2	45.2	45.6	-8	2	3	12.6	12.5	-7	1	4	18.5	18.3
9	1	0	6.8	7.4	-3	5	1	21.6	22.9	-5	3	2	39.6	39.7	-9	3	3	35.5	35.1	-8	2	4	6.1	5.5
7	1	0	22.9	23.0	-1	5	1	13.1	13.3	-7	3	2	27.5	27.6	-7	3	3	30.5	29.9	-6	2	4	17.8	17.7
5	1	0	27.0	26.7	1	5	1	26.5	26.5	-9	3	2	11.6	11.2	-5	3	3	10.3	10.3	-4	2	4	42.9	43.7
1	1	0	36.1	34.8	3	5	1	43.3	44.2	-8	4	2	5.3	4.4	-1	3	3	85.9	88.7	-2	2	4	35.5	35.5
0	2	0	39.5	38.5	5	5	1	27.5	27.7	-6	4	2	17.4	16.9	1	3	3	62.8	60.4	0	2	4	3.8	4.8
2	2	0	50.0	51.7	7	5	1	7.0	7.5	-4	4	2	17.0	17.2	3	3	3	58.7	59.2	4	2	4	3.5	2.9
4	2	0	20.6	20.8	6	6	1	24.7	24.9	-2	4	2	21.3	21.3	5	3	3	69.8	70.5	6	2	4	28.9	29.1
6	2	0	18.9	18.1	4	6	1	25.0	25.6	0	4	2	30.6	29.3	7	3	3	29.6	29.5	8	2	4	11.2	11.5
8	2	0	18.9	17.9	2	6	1	79.3	78.0	2	4	2	57.6	56.4	8	4	3	13.1	13.0	7	3	4	43.5	43.1
7	3	0	19.4	19.9	0	6	1	44.9	45.3	4	4	2	16.7	16.7	6	4	3	8.0	7.7	5	3	4	18.0	18.1
5	3	0	55.4	55.3	-2	6	1	91.1	93.4	6	4	2	5.6	5.8	4	4	3	15.7	15.9	3	3	4	47.5	48.7
3	3	0	45.1	44.7	-4	6	1	39.4	40.0	8	4	2	5.5	4.4	2	4	3	5.9	5.5	1	3	4	39.3	38.5
1	3	0	81.7	79.2	-6	6	1	6.3	6.5	3	5	2	30.3	30.9	0	4	3	22.4	22.5	-1	3	4	17.7	18.3
0	4	0	53.7	56.3	-8	6	1	24.2	23.3	1	5	2	63.2	62.3	-2	4	3	60.3	60.8	-3	3	4	5.4	6.4
2	4	0	12.4	12.6	-7	7	1	6.9	7.3	-1	5	2	39.9	39.9	-4	4	3	24.7	24.8	-5	3	4	24.9	25.4
4	4	0	22.9	22.8	-5	7	1	10.3	10.7	-3	5	2	4.0	3.3	-8	4	3	2.7	3.6	-7	3	4	35.2	35.2
6	4	0	28.6	28.7	-3	7	1	18.3	18.7	-5	5	2	13.3	13.8	-7	5	3	4.6	5.2	-9	3	4	10.6	10.4
7	5	0	20.7	20.1	-1	7	1	9.7	10.5	-7	5	2	13.3	13.2	-5	5	3	14.0	13.9	-8	4	4	9.6	9.8
5	5	0	22.9	23.0	1	7	1	15.3	14.8	-8	6	2	20.0	19.5	-3	5	3	47.1	48.4	-6	4	4	25.2	25.1
3	5	0	3.1	2.4	3	7	1	38.7	37.0	-6	6	2	78.8	79.2	-1	5	3	56.1	56.2	-4	4	4	7.9	7.6
1	5	0	24.3	24.3	5	7	1	24.7	24.7	-4	6	2	44.2	45.0	1	5	3	23.7	23.1	-2	4	4	24.5	23.6
0	6	0	134.4	139.1	8	8	1	9.7	9.3	-2	6	2	9.8	9.1	3	5	3	1.7	2.3	0	4	4	35.6	35.5
2	6	0	94.5	95.6	6	8	1	12.8	12.8	2	6	2	2.4	0.5	5	5	3	7.6	7.7	2	4	4	10.3	10.5
4	6	0	10.1	9.5	4	8	1	12.9	12.9	4	6	2	27.8	27.6	7	5	3	3.2	2.0	4	4	4	18.8	19.1
6	6	0	15.6	15.9	2	8	1	27.7	27.8	6	6	2	20.5	19.9	8	6	3	11.0	10.5	6	4	4	7.2	7.7
8	6	0	9.3	9.3	0	8	1	18.4	18.6	8	6	2	29.4	29.3	6	6	3	31.9	31.5	8	4	4	21.4	20.9
7	7	0	16.4	16.9	-2	8	1	17.3	17.5	7	7	2	5.3	5.9	4	6	3	24.4	24.2	7	5	4	9.6	9.8
5	7	0	18.8	18.6	-4	8	1	6.8	6.3	5	7	2	2.8	3.3	2	6	3	37.3	35.8	5	5	4	5.5	4.8
3	7	0	4.2	2.7	-8	8	1	8.2	8.2	3	7	2	25.2	23.9	0	6	3	5.9	6.6	3	5	4	5.1	5.4
1	7	0	20.3	21.7	-7	9	1	9.1	9.7	1	7	2	46.5	47.7	-2	6	3	58.2	60.0	1	5	4	11.7	11.5
0	8	0	15.4	15.7	-5	9	1	30.6	30.7	-1	7	2	36.1	36.8	-4	6	3	54.9	56.1	-1	5	4	6.8	6.6
2	8	0	7.8	7.8	-3	9	1	73.4	74.0	-3	7	2	1.7	1.6	-6	6	3	8.3	7.6	-3	5	4	30.4	31.3
4	8	0	17.1	17.1	-1	9	1	45.0	45.3	-5	7	2	13.0	13.7	-8	6	3	16.5	16.5	-5	5	4	30.3	30.7
6	8	0	22.3	22.0	1	9	1	10.2	9.7	-7	7	2	7.8	8.8	-7	7	3	4.5	4.3	-7	5	4	16.9	16.4
7	9	0	12.6	12.8	3	9	1	8.7	8.3	-8	8	2	4.8	3.8	-5	7	3	12.5	12.9	-8	6	4	10.3	10.2
5	9	0	34.5	34.6	5	9	1	10.5	10.3	-6	8	2	13.2	13.3	-3	7	3	34.6	35.2	-6	6	4	16.0	16.3
3	9	0	23.4	23.6	7	9	1	12.5	12.5	-4	8	2	10.2	10.6	-1	7	3	43.4	44.7	-4	6	4	22.1	22.1
1	9	0	39.7	40.0	4	10	1	25.6	24.6	-2	8	2	15.6	15.5	1	7	3	17.1	17.8	0	6	4	59.6	59.5
0	10	0	15.6	16.2	2	10	1	19.0	18.7	0	8	2	25.7	25.0	3	7	3	8.3	7.3	2	6	4	96.8	94.9
2	10	0	9.8	9.4	0	10	1	2.1	2.2	2	8	2	35.1	35.0	5	7	3	6.4	6.2	4	6	4	43.1	42.9
4	10	0	10.4	10.3	-2	10	1	7.8	7.7	4	8	2	11.6	10.9	6	8	3	6.5	7.2	8	6	4	19.2	19.2
6	10	0	9.3	9.7	-4	10	1	11.7	11.6	6	8	2	5.1	4.2	4	8	3	13.8	13.2	7	7	4	11.5	11.5
5	11	0	12.2	11.4	-6	10	1	8.7	7.6	7	9	2	14.0	13.7	0	8	3	6.5	6.5	3	7	4	6.0	6.2
3	11	0	1.9	1.1	-5	11	1	8.3	8.6	3	9	2	6.7	6.4	-2	8	3	36.3	36.8	1	7	4	6.5	7.1
1	11	0	16.6	16.6	-3	11	1	13.0	13.0	1	9	2	24.5	25.5	-4	8	3	17.5	17.1	-3	7	4	23.5	24.0
0	12	0	79.0	79.6	-1	11	1	6.4	6.3	-1	9	2	55.0	56.0	-7	9	3	18.8	18.9	-5	7	4	30.2	30.1
2	12	0	30.9	30.4	1	11	1	9.8	9.7	-3	9	2	19.8	20.0	-5	9	3	10.4	9.7	-7	7	4	13.4	13.2
4	12	0	4.9	5.1	3	11	1	24.3	24.3	-5	9	2	27.2	27.3	-3	9	3	4.8	4.3	-8	8	4	8.2	7.9
6	12	0	6.7	4.6	5	11	1	18.1	17.1	-7	9	2	16.9	16.8	-1	9	3	22.0	21.9	-6	8	4	19.8	19.1
5	13	0	11.2	11.3	4	12	1	26.7	26.2	-4	10	2	6.1	7.4	1	9	3	28.4	27.9	-4	8	4	6.1	6.4
3	13	0	4.6	2.3	2	12	1	34.7	34.8	-2	10	2	16.0	15.8	3	9	3	42.1	40.1	-2	8	4	13.2	13.3
1	13	0	11.3	11.2	0	12	1	8.1	7.1	0	10	2	29.3	30.0	5	9	3	44.5	44.1	0	8	4	21.9	21.5
0	14	0	9.4	9.7	-2	12	1	27.5	27.2	2	10	2	5.9	5.6	7	9	3	20.3	19.9	2	8	4	8.7	8.8
2	14	0	5.9	6.0	-4	12	1	36.7	36.6	4	10	2	6.5	6.5	4	10	3	7.9	7.7	4	8	4	13.5	13.1
4	14	0	6.5	7.1	-6	12	1	9.5	9.9	6	10	2	11.4	11.2	2	10	3	15.8	16.1	6	8	4	7.1	6.3
3	15	0	9.3	9.9	-5	13	1	4.6	4.5	3	11	2	13.4	13.4	0	10	3	18.7	19.4	7	9	4	34.8	34.7
1	15	0	17.1	16.7	-3	13	1	13.4	14.0	1	11	2	26.5	26.4	-2	10	3	13.8	13.3	5	9	4	11.6	11.2
8	0	1	13.2	12.4	-1	13	1	8.5	8.1	-1	11	2	21.6	21.6	-4	10	3	16.5	16.6	3	9	4	31.3	29.9
6	0	1	6.4	6.7	1	13	1	9.8	9.5	-5	11	2	12.0	11.9	-6	10	3	7.4	7.6	1	9	4	24.6	24.1
4	0	1	57.9	59.9	3	13	1	16.4	16.3	-6	12	2	35.3	35.1	-5	11	3	9.7	9.7	-1	9	4	3.4	0.6
2	0	1	101.4	101.1	5	13	1	10.4	11.2	-4	12	2	34.3	34.7	-3	11	3	22.3	22.1	-3	9	4	6.0	6.0
-2	0	1	81.5	79.0	4	14	1	13.9	13.2	-2	12	2	9.6	9.5	-1	11	3	27.0	27.1	-5	9	4	19.7	19.7
-4	0	1	92.0	93.6	2	14	1	10.3	10.2	0	12	2	15.9	16.0	1	11	3	11.6	11.4	-7	9	4	23.8	23.8
-6	0	1	19.6	19.1	-4	14	1	8.3	8.9	2	12	2	11.1	10.7	3	11	3	4.6	4.7	-6	10	4	8.4	9.0
-8	0	1	31.2	31.7	-3	15	1	35.1	35.3	6	12	2	15.5	15.2	5	11	3	4.0	4.1	-4	10	4	19.8	20.1
-9	1	1	13.0	12.7	-1	15	1	18.9	19.2	3	13	2	14.0	13.1	4	12	3	11.0	10.7	-2	10	4	12.2	11.6
-7	1	1	8.9	8.4	1	15	1	10.1	10.0	1	13	2	22.4	22.4	0	12	3	24.8	24.8	0	10	4	6.1	6.4
-5	1	1	9.7	10.2	3	15	1	4.9	4.6	-1	13	2	14.4	14.1	-2	12	3	19.7	19.5	2	10	4	6.4	6.0
-3	1	1	26.4	26.7	0	16	1	5.5	6.2	-5	13	2	7.8	8.0	-4	12	3	32.0	32.6	4	10	4	2.2	2.8
-1	1	1	18.4	17.1	-8	0	2	35.4	35.2	-2	14	2	10.6	10.2	-6	12	3	11.9	12.1	6	10	4	18.0	18.1
1	1	1	36.8	36.0	-6	0	2	73.4	73.9	0	14	2	16.9	17.2	-5	13	3	5.7	5.2	3	11	4	6.9	6.9
3	1	1	55.9	56.5	-4	0	2	93.3	94.7	4	14	2	3.6	3.6	-3	13	3	19.5	19.7	1	11	4	6.6	6.2
5	1	1	33.2	33.5	-2	0	2	42.7	43.2	3	15	2	2.1	3.7	-1	13	3	17.9	17.9	-3	11	4	13.4	13.6
7	1	1	7.2	7.2	0	0	2	39.3	30.5	1	15	2	12.4	12.6	1	13	3	6.3	6.2	-5	11	4	20.3	19.9
4	2	1	49.1	50.4	2	0	2	84.1	88.1	-1	15	2	23.6	23.6	5	13	3	7.3	6.3	-6	12	4	5.4	6.2
2	2	1	38.1	37.8	4	0	2	1.5	1.4	-3	15	2	11.3	12.0	4	14	3	5.6	6.0	-4	12	4	4.9	4.4
0	2	1	5.1	5.5	6	0	2	35.9	35.2	0	16	2	7.2	6.9	2	14	3	11.6	11.4	-2	12	4	15.6	16.0
-2	2	1	52.2	54.2	8	0	2	39.3	38.6	6	0	3	26.6	26.4	0	14	3	8.3	8.7	0	12	4	19.9	20.1
-4	2	1	20.0	21.0	9	1	2	5.3	3.8	4	0	3	21.2	23.0	-2	14	3	4.8	5.2	2	12	4	44.7	44.3
-6	2	1	11.8	11.9	7	1	2	6.2	5.7	2	0	3	17.3	18.4	-4	14	3	9.2	9.3	4	12	4	34.7	33.5
-8	2	1	15.3	15.6	3	1	2	39.8	40.4	0	0	3	90.2	87.5	-3	15	3	5.7	6.3	1	13	4	7.8	7.5
-9	3	1	6.0	6.4	1	1	2	91.1	88.6	-2	0	3	13.7	10.1	-1	15	3	9.7	10.0	-3	13	4	12.4	13.0
-7	3	1	9.3	8.8	-1	1	2	65.1	62.6	-4	0	3	78.2	78.9	1	15	3	13.3	12.8	-5	13	4	13.1	12.9
-5	3	1	45.1	45.7	-3	1	2	5.2	5.0	-6	0	3	24.3	24.2	3	15	3	16.1	15.1	-4	14	4	11.6	11.6
-3	3	1	134.9	139.1	-5	1	2	15.3	15.6	-8	0	3	36.3	35.9	-8	0	4	6.9	6.0	-2	14	4	7.8	7.3
-1	3	1	85.0	83.1	-7	1	2	12.9	12.7	-9	1	3	8.2	9.4	-6	0	4	8.7	8.5	0	14	4	3.7	3.6
1	3	1	44.0	42.8	-8	2	2	6.5	6.6	-7	1	3	5.2	5.3	-2	0	4	62.1	60.8	2	14	4	4.3	4.1
5	3	1	22.1	21.1	-6	2	2	6.8	6.7	-5	1	3	16.9	16.6	0	0	4	23.4	16.9	1	15	4	13.8	13.7
7	3	1	14.6	15.2	-4	2	2	11.2	12.7	-3	1	3	59.3	59.4	2	0	4	121.4	125.8	-3	15	4	4.2	3.5
9	3	1	18.0	16.7	-2	2	2	44.2	44.3	-1	1	3	84.5	81.5	4	0	4	80.8	82.9	8	0	5	4.6	4.8
8	4	1	10.2	10.3	0	2	2	88.4	83.8	1	1	3	38.7	39.4	6	0	4	18.3	18.3	6	0	5	34.3	34.6
6	4	1	18.9	18.5	2	2	2	3.7	2.7	3	1	3	2.6	2.4	8	0	4	11.2	10.9	4	0	5	53.4	54.3
4	4	1	18.4	18.4	4	2	2	16.1	16.5	5	1	3	7.5	7.9	7	1	4	13.1	12.6	2	0	5	31.8	32.6
2	4	1	46.1	45.2	6	2	2	16.2	16.0	4	2	3	10.4	11.7	5	1	4	5.9	5.9	0	0	5	117.9	114.5
0	4	1	45.8	47.4	8	2	2	7.9	8.1	2	2	3	41.6	42.1	3	1	4	4.9	4.9	-2	0	5	39.7	38.5
-2	4	1	23.8	24.1	7	3	2	17.8	17.5	0	2	3	62.9	61.2	1	1	4	5.2	4.2	-4	0	5	35.1	35.1

Tabelle 3. *(Continued)*

h	k	l	|Fo|	|Fc|	h	k	l	|Fo|	|Fc|	h	k	l	|Fo|	|Fc|	h	k	l	|Fo|	|Fc|	h	k	l	|Fo|	|Fc|
-6	0	5	5.2	5.8	8	0	6	11.2	11.6	-1	1	7	36.9	36.6	5	3	8	9.5	8.8	-4	4	9	7.0	5.8
-8	0	5	26.0	26.1	7	1	6	5.5	6.0	1	1	7	29.4	29.6	3	3	8	14.2	14.6	-6	4	9	13.6	13.5
-9	1	5	13.4	13.5	5	1	6	7.0	6.9	5	1	7	8.6	8.2	1	3	8	33.3	34.0	-8	4	9	21.6	21.7
-7	1	5	21.2	21.0	3	1	6	28.7	29.4	6	2	7	19.4	19.6	-1	3	8	21.5	21.9	-7	5	9	13.9	13.8
-5	1	5	13.2	11.8	1	1	6	28.0	28.4	4	2	7	6.3	5.8	-3	3	8	55.1	54.7	-5	5	9	14.2	14.1
-3	1	5	6.2	5.8	-1	1	6	8.5	6.9	2	2	7	10.5	10.0	-5	3	8	65.8	65.8	-1	5	9	8.0	8.5
-1	1	5	6.8	6.1	-3	1	6	7.7	7.6	0	2	7	36.5	36.2	-7	3	8	12.0	12.1	1	5	9	3.0	4.2
3	1	5	15.8	16.0	-5	1	6	10.7	11.1	-2	2	7	70.0	68.9	-8	4	8	7.4	7.6	3	5	9	16.5	16.3
5	1	5	22.3	22.6	-9	1	6	8.0	7.5	-4	2	7	7.0	6.3	-6	4	8	8.4	8.8	5	5	9	12.1	12.0
7	1	5	9.1	9.1	-8	2	6	8.6	8.1	-6	2	7	3.9	3.1	-4	4	8	45.5	44.8	6	6	9	22.0	21.7
6	2	5	27.8	27.8	-6	2	6	16.8	16.6	-9	3	7	16.6	15.6	-2	4	8	22.3	22.2	4	6	9	8.1	8.5
4	2	5	20.9	21.2	-4	2	6	7.2	7.2	-7	3	7	44.6	44.4	0	4	8	13.5	14.0	2	6	9	9.5	9.0
2	2	5	51.2	51.4	-2	2	6	39.5	38.5	-5	3	7	42.3	42.6	2	4	8	9.0	8.7	0	6	9	14.1	14.6
0	2	5	6.5	6.0	0	2	6	18.2	18.3	-3	3	7	25.3	25.1	4	4	8	17.5	17.5	-2	6	9	10.5	10.1
-2	2	5	21.4	21.8	2	2	6	66.9	67.9	-1	3	7	53.0	52.7	6	4	8	8.1	8.0	-4	6	9	10.1	9.9
-4	2	5	5.1	4.6	4	2	6	20.4	21.1	1	3	7	29.9	29.6	7	5	8	8.6	8.7	-6	6	9	20.8	20.7
-6	2	5	3.6	3.3	6	2	6	9.2	9.0	3	3	7	65.1	65.5	5	5	8	5.9	6.0	-8	6	9	35.9	35.6
-8	2	5	17.8	17.8	7	3	6	14.1	14.6	5	3	7	40.3	40.6	1	5	8	7.3	7.7	-7	7	9	12.5	12.9
-9	3	5	5.4	4.8	5	3	6	8.8	8.7	7	3	7	20.1	19.9	-1	5	8	10.2	10.1	-5	7	9	13.3	12.7
-7	3	5	11.2	10.8	3	3	6	54.1	54.7	4	4	7	22.5	22.4	-3	5	8	24.9	25.5	-3	7	9	3.2	1.9
-5	3	5	28.9	28.5	1	3	6	117.0	116.4	2	4	7	13.6	13.1	-5	5	8	17.9	17.4	-1	7	9	6.8	7.0
-3	3	5	59.6	59.7	-1	3	6	33.3	33.1	0	4	7	56.4	55.8	-8	6	8	19.0	19.5	3	7	9	11.5	11.1
-1	3	5	125.7	125.9	-3	3	6	48.0	48.5	-2	4	7	24.3	24.5	-4	6	8	34.5	34.4	5	7	9	11.1	11.5
1	3	5	89.9	88.2	-5	3	6	24.5	24.3	-4	4	7	32.1	31.8	-2	6	8	27.4	27.0	4	8	9	5.8	6.0
3	3	5	24.3	24.3	-9	3	6	4.2	3.3	-6	4	7	4.5	4.6	0	6	8	66.9	66.3	2	8	9	7.1	7.0
5	3	5	33.2	34.1	-8	4	6	7.9	8.0	-8	4	7	9.5	9.2	2	6	8	29.9	29.5	0	8	9	25.8	25.7
7	3	5	8.3	7.8	-4	4	6	5.9	5.6	-7	5	7	8.6	8.2	4	6	8	31.6	31.5	-2	8	9	7.7	7.9
6	4	5	17.3	17.2	0	4	6	64.9	63.9	-3	5	7	14.7	14.8	6	6	8	8.7	9.0	-6	8	9	10.6	10.0
4	4	5	45.3	45.4	2	4	6	31.5	31.2	-1	5	7	31.0	30.7	5	7	8	7.3	8.0	-7	9	9	19.6	19.5
2	4	5	6.1	6.5	4	4	6	24.2	23.6	1	5	7	25.6	25.3	3	7	8	4.4	4.0	-5	9	9	8.7	8.8
0	4	5	19.7	19.1	7	5	6	5.4	5.5	5	5	7	6.9	7.4	1	7	8	7.7	7.5	-3	9	9	43.8	44.2
-2	4	5	7.8	8.1	5	5	6	6.2	5.7	6	6	7	7.0	6.0	-1	7	8	10.5	11.3	-1	9	9	41.1	40.9
-4	4	5	22.9	23.0	3	5	6	23.2	23.0	4	6	7	23.4	23.6	-3	7	8	20.8	21.1	1	9	9	31.8	31.3
-6	4	5	18.7	18.6	1	5	6	24.9	24.7	2	6	7	12.1	10.9	-5	7	8	13.4	14.1	3	9	9	22.9	22.9
-8	4	5	6.5	6.4	-1	5	6	7.2	6.9	0	6	7	55.6	54.8	-6	8	8	6.8	7.3	4	10	9	8.1	8.3
-7	5	5	19.8	19.5	-3	5	6	8.8	9.5	-2	6	7	54.4	55.1	-4	8	8	34.2	34.1	2	10	9	7.9	6.8
-5	5	5	9.4	9.7	-5	5	6	10.0	9.9	-4	6	7	19.4	19.2	-2	8	8	15.6	16.1	-2	10	9	17.8	18.2
-3	5	5	6.5	6.8	-8	6	6	13.1	13.1	-6	6	7	31.2	31.6	0	8	8	9.7	9.9	-6	10	9	17.1	16.8
-1	5	5	6.7	6.8	-6	6	6	20.1	20.6	-8	6	7	13.4	13.9	2	8	8	6.7	6.9	-5	11	9	8.7	9.0
3	5	5	14.1	13.8	-4	6	6	70.1	70.8	-7	7	7	6.3	6.3	4	8	8	14.5	13.7	-1	11	9	3.5	3.6
5	5	5	21.6	21.0	-2	6	6	82.6	83.2	-5	7	7	4.0	3.4	6	8	8	6.4	6.2	1	11	9	3.8	3.7
7	5	5	7.2	7.4	0	6	6	25.3	24.8	-3	7	7	13.9	13.7	3	9	8	11.9	11.5	3	11	9	6.9	7.1
6	6	5	20.9	20.6	2	6	6	16.5	16.6	-1	7	7	26.0	26.5	1	9	8	23.9	23.8	0	12	9	6.9	6.6
4	6	5	65.4	64.8	4	6	6	14.7	15.0	1	7	7	16.4	17.0	-1	9	8	9.2	9.5	-2	12	9	14.7	15.1
2	6	5	5.5	5.3	6	6	6	27.4	27.3	5	7	7	6.5	5.8	-3	9	8	35.0	34.6	-4	12	9	6.4	5.5
0	6	5	48.3	48.6	3	7	6	23.8	22.9	4	8	7	18.3	18.4	-5	9	8	44.2	44.2	-1	13	9	4.3	5.0
-2	6	5	21.9	23.2	1	7	6	20.6	20.4	2	8	7	7.1	7.4	-7	9	8	11.5	11.4	-2	14	9	13.9	13.5
-6	6	5	24.6	24.3	-1	7	6	5.4	5.2	0	8	7	37.0	36.6	-6	10	8	18.4	18.9	-8	0	10	10.4	10.9
-8	6	5	12.6	12.6	-3	7	6	4.7	4.8	-2	8	7	18.7	18.6	-4	10	8	14.7	14.4	-6	0	10	41.7	41.3
-7	7	5	13.6	13.9	-5	7	6	9.9	9.7	-4	8	7	21.8	22.1	-2	10	8	16.4	16.6	-4	0	10	29.7	29.7
-5	7	5	9.1	9.1	-8	8	6	6.9	6.6	-6	8	7	5.0	5.0	0	10	8	3.6	2.0	-2	0	10	52.7	52.0
-3	7	5	6.3	6.0	-4	8	6	5.1	4.8	-7	9	7	30.7	29.5	2	10	8	21.5	21.8	0	0	10	26.6	26.0
-1	7	5	10.7	12.0	0	8	6	41.9	41.4	-5	9	7	29.1	29.3	3	11	8	5.6	3.4	4	0	10	12.3	11.8
3	7	5	13.9	12.9	2	8	6	24.6	24.2	-3	9	7	19.5	19.1	1	11	8	6.3	6.5	5	1	10	9.5	9.5
5	7	5	14.8	14.7	4	8	6	18.7	17.9	-1	9	7	34.3	34.3	-1	11	8	4.6	5.9	3	1	10	18.3	18.2
7	7	5	7.5	7.7	5	9	6	7.0	7.6	1	9	7	15.5	15.5	-3	11	8	13.0	12.5	1	1	10	22.9	23.2
6	8	5	12.6	12.9	3	9	6	38.8	38.0	3	9	7	40.9	40.1	-5	11	8	8.3	8.5	-1	1	10	14.9	14.9
4	8	5	34.0	33.4	1	9	6	66.2	65.1	5	9	7	26.3	26.3	-4	12	8	10.6	11.0	-3	1	10	4.7	4.6
2	8	5	4.5	4.7	-1	9	6	19.0	18.8	4	10	7	4.3	4.6	-2	12	8	8.5	8.6	-5	1	10	7.1	6.7
0	8	5	5.5	5.9	-3	9	6	26.1	26.1	2	10	7	4.7	4.1	0	12	8	28.4	27.8	-8	2	10	4.7	5.3
-2	8	5	9.4	9.8	-5	9	6	17.7	17.7	0	10	7	19.9	19.2	2	12	8	26.4	26.5	-6	2	10	7.6	8.6
-4	8	5	16.8	16.8	-7	9	6	4.5	0.9	-2	10	7	34.4	34.2	4	12	8	6.3	5.5	-4	2	10	7.6	7.4
-6	8	5	12.4	13.1	-6	10	6	10.7	10.9	-5	10	7	5.4	4.1	1	13	8	3.3	3.5	-2	2	10	23.6	23.0
-7	9	5	10.4	10.0	-4	10	6	6.4	6.5	-3	11	7	9.4	9.5	-3	13	8	11.0	11.4	0	2	10	21.8	21.8
-5	9	5	15.3	16.0	-2	10	6	12.9	13.5	-1	11	7	17.9	18.1	-2	14	8	9.9	10.2	2	2	10	22.5	22.4
-3	9	5	36.6	36.6	0	10	6	11.7	11.9	1	11	7	10.2	10.2	6	0	9	33.3	32.9	4	2	10	12.4	12.1
-1	9	5	70.3	70.8	2	10	6	34.3	33.5	5	11	7	3.6	3.4	4	0	9	15.4	15.2	6	2	10	17.6	17.0
1	9	5	43.3	42.9	4	10	6	10.6	10.6	4	12	7	5.3	4.7	2	0	9	12.1	11.8	5	3	10	32.0	32.2
3	9	5	19.0	18.5	6	10	6	6.3	7.1	2	12	7	8.5	7.9	0	0	9	19.5	19.3	3	3	10	45.1	45.0
5	9	5	22.7	23.1	3	11	6	14.5	14.6	0	12	7	20.7	20.6	-2	0	9	34.2	34.3	1	3	10	10.2	10.5
6	10	5	18.1	17.7	1	11	6	12.1	12.1	-2	12	7	43.7	44.2	-4	0	9	12.1	11.6	-1	3	10	12.0	11.4
4	10	5	13.5	13.4	-3	11	6	5.3	5.3	-3	13	7	4.6	4.5	-6	0	9	38.2	37.8	-3	3	10	14.3	14.3
2	10	5	22.9	22.4	-5	11	6	7.7	8.3	-1	13	7	11.3	11.6	-8	0	9	25.4	25.9	-5	3	10	24.3	24.2
0	10	5	4.8	5.0	-6	12	6	17.9	17.1	1	13	7	9.9	9.4	-7	0	9	15.9	15.9	-7	3	10	8.2	8.5
-2	10	5	12.7	12.5	-4	12	6	39.3	39.2	0	14	7	11.1	11.0	-5	1	9	16.9	16.9	-8	4	10	9.6	9.9
-5	11	5	6.8	7.3	-2	12	6	29.1	29.3	-2	14	7	20.8	21.2	-1	1	9	9.2	9.2	-6	4	10	2.4	2.4
-3	11	5	2.1	3.0	0	12	6	3.0	1.6	-1	15	7	18.8	19.3	1	1	9	5.7	6.0	-4	4	10	27.6	27.4
-1	11	5	8.5	9.2	2	12	6	23.3	23.4	-8	0	8	33.7	33.2	3	1	9	17.8	18.0	-2	4	10	5.3	4.4
3	11	5	9.3	9.0	4	12	6	11.0	10.3	-6	0	8	19.2	19.3	5	1	9	14.0	14.3	2	4	10	18.9	18.3
5	11	5	10.1	9.7	3	13	6	9.2	8.6	-4	0	8	16.4	16.9	7	1	9	9.1	8.5	4	4	10	24.1	24.3
4	12	5	25.5	25.0	1	13	6	11.0	11.2	-2	0	8	30.3	30.2	6	2	9	16.1	16.4	5	5	10	9.0	8.5
2	12	5	11.2	11.6	-3	13	6	7.7	7.3	0	0	8	71.9	73.6	4	2	9	15.6	15.0	3	5	10	16.2	15.8
0	12	5	31.4	31.7	-5	13	6	5.3	4.7	2	0	8	64.4	66.2	2	2	9	10.9	9.9	1	5	10	18.0	18.1
-2	12	5	17.9	17.6	-4	14	6	4.1	4.6	4	0	8	17.7	17.9	0	2	9	4.4	4.2	-1	5	10	11.3	11.8
-4	12	5	11.3	12.3	-2	14	6	7.7	8.1	6	0	8	20.3	20.0	-2	2	9	31.5	31.9	-3	5	10	3.1	3.9
-6	12	5	3.0	3.3	0	14	6	8.2	8.3	7	1	8	9.7	9.5	-4	2	9	6.5	7.2	-5	5	10	6.8	7.2
-5	13	5	2.5	3.2	2	14	6	22.7	22.1	5	1	8	7.8	8.2	-6	2	9	26.9	27.0	-6	6	10	28.3	28.3
-1	13	5	4.5	5.6	1	15	6	35.8	35.2	3	1	8	4.0	4.2	-8	2	9	7.7	7.6	-4	6	10	41.0	41.1
2	14	5	13.1	12.7	-1	15	6	11.9	11.1	1	1	8	7.3	8.1	-7	3	9	23.6	23.4	-2	6	10	17.8	17.6
-2	14	5	9.1	9.1	6	0	7	12.2	11.7	-1	1	8	16.1	15.4	-5	3	9	16.2	16.1	0	6	10	32.0	32.5
-3	15	5	16.5	17.0	4	0	7	9.7	9.9	-3	1	8	30.5	30.6	-3	3	9	67.8	66.8	4	6	10	23.1	22.5
-1	15	5	29.9	29.4	2	0	7	20.1	21.3	-5	1	8	20.0	19.8	-1	3	9	66.5	66.4	6	6	10	12.6	12.1
1	15	5	19.6	19.9	0	0	7	44.5	43.7	-9	1	8	4.7	4.9	1	3	9	52.4	51.9	5	7	10	6.4	6.7
-6	0	6	40.1	40.6	-2	0	7	117.5	117.1	-6	2	8	30.7	30.6	3	3	9	32.2	32.2	3	7	10	13.1	13.1
-4	0	6	94.3	95.3	-4	0	7	4.5	4.6	-4	2	8	24.8	24.6	7	3	9	16.6	16.0	1	7	10	18.3	18.2
-2	0	6	89.3	88.1	-6	0	7	30.0	29.6	-2	2	8	36.5	35.9	6	4	9	9.6	8.6	-1	7	10	9.5	9.5
0	0	6	27.6	25.5	-8	0	7	11.4	11.2	0	2	8	3.5	2.2	4	4	9	9.7	9.7	-5	7	10	4.0	3.8
2	0	6	51.1	52.6	-9	1	7	4.7	4.4	2	2	8	37.0	37.6	2	4	9	11.6	11.7	-4	8	10	21.0	21.1
4	0	6	26.4	26.2	-7	1	7	8.1	8.3	4	2	8	3.2	3.4	0	4	9	34.9	34.4	2	8	10	14.0	13.9
6	0	6	42.6	42.7	-3	1	7	17.6	17.2	7	3	8	5.3	4.9	-2	4	9	7.9	8.3	4	8	10	19.8	19.7

Tabelle 3. *(Continued)*

h	k	l	|Fo|	|Fc|	h	k	l	|Fo|	|Fc|	h	k	l	|Fo|	|Fc|	h	k	l	|Fo|	|Fc|	h	k	l	|Fo|	|Fc|
3	9	10	30.8	30.5	-4	6	11	8.6	8.5	-2	6	12	12.5	11.8	0	6	13	30.6	30.4	-4	0	15	6.4	5.9
1	9	10	7.9	8.7	-6	6	11	7.1	6.6	0	6	12	5.0	4.0	-2	6	13	24.0	23.9	-6	0	15	21.0	20.7
-1	9	10	8.4	8.6	-7	7	11	7.2	5.9	2	6	12	57.7	57.3	-4	6	13	32.5	32.7	-5	1	15	11.3	10.2
-3	9	10	11.9	11.3	-3	7	11	12.1	12.7	4	6	12	33.1	33.0	-6	6	13	22.8	22.3	-1	1	15	19.9	20.0
-5	9	10	14.6	15.1	-1	7	11	15.3	15.2	3	7	12	11.0	10.8	-5	7	13	8.6	7.5	1	1	15	18.6	19.1
-6	10	10	7.1	7.5	1	7	11	13.6	13.6	1	7	12	3.8	2.9	-1	7	13	8.2	8.4	3	1	15	7.5	7.7
-4	10	10	6.4	5.9	5	7	11	8.9	8.8	-1	7	12	8.8	8.9	1	7	13	13.4	13.5	0	2	15	20.7	21.7
-2	10	10	14.1	14.3	4	8	11	11.0	11.1	-3	7	12	14.2	14.2	2	8	13	6.5	6.3	-4	2	15	7.3	8.1
0	10	10	10.1	9.9	2	8	11	8.9	8.6	-5	7	12	8.8	9.5	-4	8	13	19.7	19.6	-5	3	15	33.0	33.7
2	10	10	11.7	11.9	0	8	11	20.9	21.1	-6	8	12	8.3	8.5	-5	9	13	16.4	16.4	-3	3	15	9.3	9.7
4	10	10	7.6	7.4	-2	8	11	14.1	13.9	-4	8	12	12.4	13.3	-1	9	13	35.0	35.2	1	3	15	5.5	5.4
3	11	10	7.8	7.9	-4	8	11	8.4	7.6	-2	8	12	12.4	12.9	1	9	13	32.8	33.3	2	4	15	11.4	12.0
1	11	10	11.2	11.4	-5	9	11	19.9	19.8	0	8	12	21.5	21.8	2	10	13	6.0	5.7	-2	4	15	11.0	10.9
-1	11	10	6.1	5.1	-3	9	11	20.7	20.1	2	8	12	7.0	7.2	0	10	13	11.2	10.4	-4	4	15	7.6	7.1
-3	11	10	5.3	3.6	1	9	11	22.7	22.6	3	9	12	19.4	20.0	-4	10	13	6.9	6.1	-6	4	15	12.2	11.9
-4	12	10	11.3	11.4	2	10	11	20.3	20.0	1	9	12	4.1	5.2	-1	11	13	7.5	6.7	-5	5	15	10.6	9.6
-2	12	10	19.8	20.0	0	10	11	12.0	12.1	-1	9	12	32.1	32.5	-4	0	14	58.5	58.4	-1	5	15	17.5	17.7
0	12	10	9.2	9.1	-2	10	11	6.3	7.2	-3	9	12	33.7	33.8	-2	0	14	45.8	46.4	1	5	15	16.3	16.7
1	13	10	7.8	7.0	-4	10	11	6.5	5.7	-5	9	12	5.5	5.2	0	0	14	5.4	5.9	3	5	15	7.3	7.6
-1	13	10	5.8	5.9	-3	11	11	8.9	8.8	-4	10	12	10.6	10.3	4	0	14	9.5	9.7	2	6	15	21.4	21.4
6	0	11	21.5	22.0	-1	11	11	9.3	9.6	-2	10	12	19.4	19.7	3	1	14	18.7	19.1	0	6	15	12.7	13.1
4	0	11	22.9	23.1	1	11	11	9.2	9.9	1	11	12	3.7	3.9	1	1	14	12.7	12.6	-2	6	15	24.8	25.2
2	0	11	47.2	47.1	0	12	11	22.0	21.9	-1	11	12	5.6	5.0	-1	1	14	8.0	8.3	-1	7	15	16.0	16.3
0	0	11	46.3	46.1	-2	12	11	4.1	5.0	-3	11	12	9.1	9.4	-3	1	14	14.2	13.4	1	7	15	15.5	15.4
-2	0	11	10.3	10.6	-1	13	11	9.1	9.2	-2	12	12	16.6	16.5	-5	1	14	1.5	2.1	-2	8	15	6.8	8.0
-4	0	11	10.1	9.3	-8	0	12	5.6	5.5	0	12	12	12.6	12.6	-7	1	14	3.5	5.5	-4	8	15	5.5	6.5
-6	0	11	12.2	11.3	-6	0	12	23.1	22.9	4	0	13	24.5	24.3	-6	2	14	16.4	17.1	-4	0	16	13.8	13.7
-5	1	11	2.4	1.8	-2	0	12	29.5	29.3	2	0	13	8.4	8.8	-4	2	14	10.0	9.7	-2	0	16	5.9	5.8
-3	1	11	16.8	17.2	0	0	12	29.5	29.6	0	0	13	49.1	49.4	-2	2	14	7.0	7.6	0	0	16	7.4	7.8
-1	1	11	23.1	23.1	2	0	12	52.4	52.3	-2	0	13	7.8	7.3	4	2	14	15.3	14.8	1	1	16	4.1	4.2
1	1	11	18.1	17.7	4	0	12	43.6	43.5	-4	0	13	21.9	21.8	3	3	14	13.8	13.2	-1	1	16	14.0	13.8
3	1	11	6.2	5.7	5	1	12	7.2	6.8	-6	0	13	31.6	31.3	1	3	14	16.5	17.1	-3	1	16	18.7	19.1
5	1	11	7.9	8.0	3	1	12	14.3	14.2	-7	1	13	9.2	9.2	-1	3	14	8.6	8.7	-5	1	16	8.3	8.7
2	2	11	31.8	32.0	-1	1	12	13.2	12.9	-5	1	13	12.3	12.0	-3	3	14	31.3	30.9	-4	2	16	15.7	16.1
0	2	11	20.7	20.2	-3	1	12	17.8	17.1	-3	1	13	4.9	5.6	-5	3	14	6.3	5.6	0	2	16	9.0	8.8
-2	2	11	13.1	13.9	-5	1	12	13.5	13.4	-1	1	13	9.9	9.8	-4	4	14	5.4	5.4	1	3	16	11.5	12.3
-4	2	11	10.7	10.8	-7	1	12	4.6	4.1	1	1	13	14.6	14.5	-2	4	14	13.1	13.7	-1	3	16	10.9	11.6
-6	2	11	21.0	20.3	-4	2	12	19.4	18.6	5	1	13	13.2	13.1	2	4	14	18.1	17.7	-3	3	16	13.6	13.4
-8	2	11	6.2	4.7	-2	2	12	32.8	32.8	4	2	13	11.2	10.8	3	5	14	17.2	17.2	-5	3	16	13.3	12.8
-7	3	11	26.9	26.6	0	2	12	6.6	6.9	2	2	13	8.8	8.6	1	5	14	10.5	11.2	-2	4	16	17.0	17.3
-5	3	11	32.1	31.3	2	2	12	7.8	7.7	0	2	13	15.7	15.4	-1	5	14	8.6	8.4	-1	5	16	11.6	12.2
-3	3	11	32.8	32.3	4	2	12	11.8	11.3	-2	2	13	17.9	18.1	-3	5	14	12.8	12.4	-3	5	16	17.8	17.2
1	3	11	29.6	29.0	5	3	12	5.0	4.7	-4	2	13	9.1	9.2	-6	6	14	13.8	13.0	-2	6	16	9.1	9.6
5	3	11	35.1	34.3	3	3	12	30.7	30.2	-6	2	13	16.7	16.8	-4	6	14	35.9	35.6	-1	7	16	10.4	10.5
6	4	11	9.2	9.4	1	3	12	8.1	7.1	-7	3	13	4.2	3.1	-2	6	14	43.9	44.0	-3	7	16	14.8	14.9
4	4	11	14.7	14.3	-1	3	12	47.6	47.3	-5	3	13	22.7	22.9	0	6	14	9.4	9.9	0	0	17	6.3	6.5
2	4	11	11.1	11.2	-3	3	12	46.0	45.7	-3	3	13	5.0	4.4	2	6	14	13.0	13.4	-2	0	17	11.8	12.3
0	4	11	28.9	28.6	-5	3	12	8.8	9.0	-1	3	13	52.9	53.1	3	7	14	14.2	14.8	-4	0	17	21.7	21.5
-2	4	11	19.9	20.5	-7	3	12	4.4	3.9	1	3	13	45.9	46.2	1	7	14	10.9	9.7	-3	1	17	6.1	7.3
-4	4	11	8.5	8.0	-6	4	12	10.8	11.2	3	3	13	10.0	10.1	-1	7	14	5.4	5.6	1	1	17	3.4	5.1
-8	4	11	12.6	12.9	-4	4	12	17.0	17.1	2	4	13	7.2	6.8	-3	7	14	12.1	11.9	-4	2	17	10.9	11.6
-7	5	11	3.5	3.5	-2	4	12	15.8	15.8	-2	4	13	2.3	2.6	-5	7	14	2.8	3.0	-1	3	17	6.0	5.3
-3	5	11	15.1	14.2	0	4	12	27.0	27.5	-4	4	13	23.9	24.6	-2	8	14	11.0	11.1	1	3	17	23.6	24.3
-1	5	11	20.4	20.7	2	4	12	9.2	9.0	-6	4	13	10.7	11.1	2	8	14	14.1	14.0	-3	5	17	5.3	6.4
1	5	11	15.8	15.3	4	4	12	7.2	7.0	-7	5	13	7.3	7.7	1	9	14	12.9	12.3	-1	5	17	0.6	1.7
3	5	11	4.8	4.6	5	5	12	5.8	6.1	-5	5	13	12.0	11.5	-1	9	14	4.1	4.4	-2	6	17	16.6	15.8
5	5	11	7.3	6.7	3	5	12	14.2	14.1	-3	5	13	4.3	4.4	-3	9	14	22.8	22.9	-2	0	18	24.0	24.6
4	6	11	5.9	4.8	-1	5	12	11.3	11.2	-1	5	13	9.7	9.3	4	0	15	15.9	15.6	0	0	18	40.8	41.8
2	6	11	21.5	21.7	-3	5	12	13.7	13.7	1	5	13	12.3	12.4	2	0	15	11.6	11.4	-1	1	18	7.0	8.2
0	6	11	45.6	45.4	-5	5	12	11.3	11.6	4	6	13	11.6	12.0	0	0	15	31.7	32.8					
-2	6	11	15.9	15.4	-6	6	12	8.9	9.2	2	6	13	6.6	6.3	-2	0	15	17.2	17.4					

Discussion

Figure 1 shows the projection of the structure upon (001) plane together with the numbering scheme of atoms. Table 4 gives selected interatomic distances and bond angles.

The interatomic distances between the Si and basal (bridging) oxygen atoms, O_b, are all equal within the experimental errors, while the distance from the Si to the apical oxygen atom, O_a, is distinctively shorter than these. The mean Si—O distance of 1.625 Å is the same as that in tetrasilicic potassium fluoromica (TORAYA *et al.*, 1976). The SiO_4 tetrahedra in the present crystal have a symmetry very close to $3m$ with the mean O_b—O_b distance of 2.617 Å and the mean O_a—O_b distance of 2.684 Å. The mean O_b—Si—O_b and mean O_a—Si—O_b angles

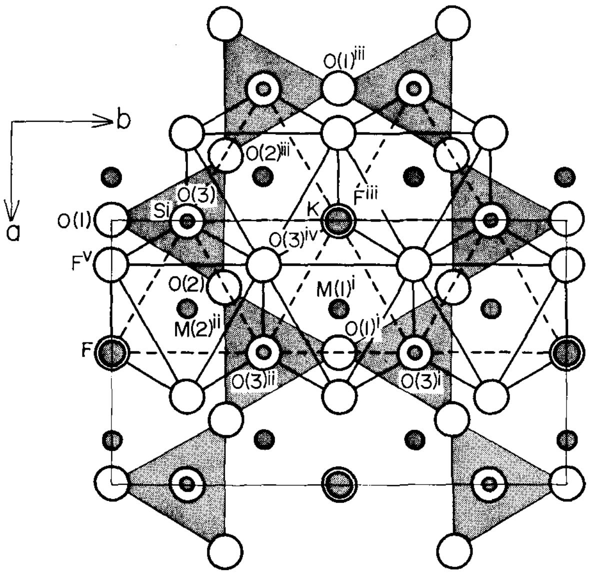

Fig. 1. A projection of the crystal structure onto the (001) plane, showing the octahedral and the lower tetrahedral layers

are 106.05° and 112.71°, respectively. The difference is larger than those in phlogopites by about 5° (Joswig, 1972; Hazen and Burnham, 1973).

Distortion of a (Si, Al) O_4 group in aluminosilicates can be expressed with the angle O_a—(Si, Al)—O_b and the ratio, d_a/d_b, where d_a is the (Si, Al)—O_a distance, and d_b the (Si, Al)—O_b distance, so long as the (Si, Al)O_4 group preserves the threefold rotational symmetry around the bond (Si, Al)—O_a. As far as the 1M-type micas are concerned, we can assume the point symmetry $3m$ for individual (Si, Al) O_4 tetrahedra as pointed out by Takéuchi (1975). In Tab. 5 the angle O_a—(Si, Al)—O_b and the ratio, d_a/d_b, are compared for some 1M-type micas. Clearly octahedral cations as well as Al^{3+} ions substituting Si^{4+} have influence upon the distortion. The SiO_4 tetrahedra in the present crystal have the same geometrical feature as in tetrasilicic potassium fluoromica (Toraya *et al.*, 1976), being elongated along the Si—O_a bonds.

The mean (Mg, Li)—O, F distance of the M(2) octahedron is slightly longer than that of the M(1) octahedron. In accordance with this fact, population analysis of the octahedral sites showed that Li^+ ions with a slightly larger ionic radius are more concentrated at the M(2) site than at M(1) by about 5%.

Twelve oxygen atoms around the K^+ ion form two octahedra penetrating with each other. The mean K—O distances are 3.117 Å and 3.068 Å for outer (larger) and inner (smaller) octahedra, respectively. The difference, Δ, of 0.049 Å is still smaller than the value of 0.063 Å in tetrasilicic potassium fluoromica. The small Δ value is a consequence of a small rotation of the SiO_4 tetrahedron, which again indicates a small dimensional misfit between the tetrahedral and octahedral layers. Actually the tetrahedral rotation angle, α, is only 1.08°, and the octahedral flattening angles, ψ, are 57.8° and 57.9° for M(1) and M(2) sites, respectively (DONNAY *et al.*, 1964). The basal oxygen atoms, O(1) and O(2), are at the same height forming a flat basal plane of the tetrahedral layer. Such tetrahedral layers without corrugation of basal planes as in the present crystal result from the nearly equal dimensions of the M(1) and M(2) octahedra.

Table 4. *Interatomic distances and bond angles*

Symmetry code

none	x	y	z
i	$\frac{1}{2}+x$	$\frac{1}{2}+y$	z
ii	$\frac{1}{2}+x$	$\frac{1}{2}-y$	z
iii	$-\frac{1}{2}+x$	$\frac{1}{2}-y$	z
iv	$\frac{1}{2}-x$	$\frac{1}{2}-y$	$1-z$
v	$1-x$	y	$1-z$

Tetrahedral site

Si—O(1)	1.638(1) Å	O(1)—Si—O(2)	106.04(6)°
Si—O(2)	1.638(1)	O(1)—Si—O(2)^{iii}	106.09(6)
Si—O(2)^{iii}	1.638(1)	O(2)—Si—O(2)^{iii}	106.02(5)
Si—O(3)	1.586(1)	O(1)—Si—O(3)	112.73(5)
		O(2)—Si—O(3)	112.70(5)
		O(2)^{iii}—Si—O(3)	112.69(5)
Mean Si—O	1.625 Å	Mean O—Si—O	109.38°
Mean Si—O$_b$	1.638	Mean O$_b$—Si—O$_b$	106.05
		Mean O$_a$—Si—O$_b$	112.71
O(1)—O(2)	2.617(1) Å	Si^{i}—O(1)^{i}—Si^{ii}	134.57(8)°
O(1)—O(2)^{iii}	2.618(1)	Si—O(2)—Si^{ii}	134.53(5) [2 ×]
O(2)—O(2)^{iii}	2.616(1)		
O(1)—O(3)	2.685(1)		
O(2)—O(3)	2.684(1)		
O(2)^{iii}—O(3)	2.684(1)		
Mean O—O	2.651 Å	Mean Si—O—Si	134.54°
Mean O$_b$—O$_b$	2.617		
Mean O$_a$—O$_b$	2.684		