Polar Geosci., **14**, 139–156, 2001

The crystal structure of scapolite in the Lützow-Holm Bay region, East Antarctica

Junji Yamakawa[1], Yumi Ando[2], Yasuhito Osanai[3] and Isao Kusachi[3]

[1]*Department of Earth Sciences, Faculty of Science, Okayama University, Tsushima-naka 3-1-1, Okayama 700-8530*
[2]*Graduate School of Social and Cultural Studies, Kyushu University, Ropponmatsu 4-2-1, Fukuoka 810-8560*
[3]*Department of Earth Sciences, Faculty of Education, Okayama University, Tsushima-naka 3-1-1, Okayama 700-8530*

Abstract: The crystal structure of scapolite from the Lützow-Holm Bay region, East Antarctica with cell formular

$(Na_{1.97}Ca_{1.48}K_{0.46}Mg_{0.03})_{3.94}(Al_{4.15}Si_{7.85}Fe_{0.01})_{12.01}O_{24.00}\,(Cl_{0.65}(CO_3)_{0.42})_{1.07}$, Me_{39},

was determined in tetragonal, $P4_2/n$, a=12.122(2); c=7.585(2) Å by the single crystal X-ray diffraction method. The structure is the same as that of meionite but with some difference in atomic coordinates and Al percentage in the tetrahedon. The CO_3 groups were mainly disordered on the xy plane and off-centred from the Anion site. The cation site was 8-coordinate rather than 6-coordinate.

key words: scapolite, meionite, marialite, crystal structure, East Antarctica

1. Introduction

Scapolite is referred to a family of framework aluminosilicates with tetragonal symmetry. The general formula is $M_4T_{12}O_{24}A$, where the major components are M=Na and Ca, T=Si and Al, A=Cl, CO_3 and SO_4. The natural scapolites form a solid-solution series beteween the idealized end-members, $Na_4Al_3Si_9O_{24}Cl$ (marialite) and meionite, $Ca_4Al_6Si_6O_{24}CO_3$ (meionite). The index of chemical composition, at the percentage of meionite composion, has been defined as

100 (Ca+Sr+Fe+Mn+Mg)/(Na+K+Ca+Sr+Fe+Mn+Mg).

During the mineralogical survey of the calc-silicate gneisses collected by the geologists of the 39th Japanese Antarctic Research Expedition (JARE) in the Skallen region, Lützow-Holm Bay region, East Antarctica, two types of zoned scapolite were found (Kusachi *et al.*, 1999). One type (A97122403A) varies from Me_{39} in the core to Me_{57} at the rim. The other (A97122705E) varies from Me_{75} in the core to Me_{63} at the rim.

One of the main topics of interest is scapolite solid solution that has had a relationship between composition and variation of space groups from $I4/m$ to $P4_2/n$. Previous works have plotted cell parameters against Me percentage but have not investigated how the resulting trends are related to the crystal structure (Teertstra and Sherriff, 1996). To determine the crystal structure, including the space group, the single

crystal method is the most reliable one. Until now, only Me_{20} (Lin and Burley, 1973a), Me_{33} (Levien and Papike, 1976), Me_{70} (Papike and Stephenson, 1966), Me_{77} (Peterson *et al.*, 1979) and Me_{93} (Lin and Burley, 1973b) have been analyzed by this method. The rest of the solid-solution members are still unresolved. This paper is an attempt to refine the crystal structure of a natural scapolite which has an intermediate solid-solution composition, Me_{39} (A97122403A).

2. Geological outline and petrology

The Skallen region is situated on the east coast of Lützow-Holm Bay, *c.* 60 km from Syowa Station, East Antarctica (Fig. 1). The area is underlain by various kinds of metamorphic rocks and later intrusions of granitic and pegmatitic rocks. The metamorphic rocks, which belong to the granulite-facies terrane in the Lützow-Holm Complex (Hiroi *et al.*, 1987), are composed mainly of garnet-bearing quartzo-feldspathic gneiss, garnet-hornblende gneiss, and two pyroxene-hornblende gneisses with subordinate thin intercalations of garnet-sillimanite gneiss, garnet-orthopyroxene gneiss, charnockite, impure marble and skarns.

Lenticular-shaped blocks or thin intercalations of impure marbles occur mainly in the northern and southeastern areas. These marbles are normally coexisting with various kinds of skarn-type metamorphic rocks between marbles and surrounding gneisses (Figs. 2 and 3). The critical evidence for the skarns discussed here (A97122403A) indicates well-layered structure with compositional banding.

A97122403A distributes along the E-W trending large shear zone cutting across the region in the northern area (Figs. 2 and 3). A97122403A is composed mainly of scapolite and diopside with subordinate amounts of K-feldspar, phlogopite, apatite, calcite, dolomite and quartz. Scapolite occurs as subhedral to anhedral crystals up to 4 cm in length. The mineral is gray to white in hand specimens, and colorless in thin sections.

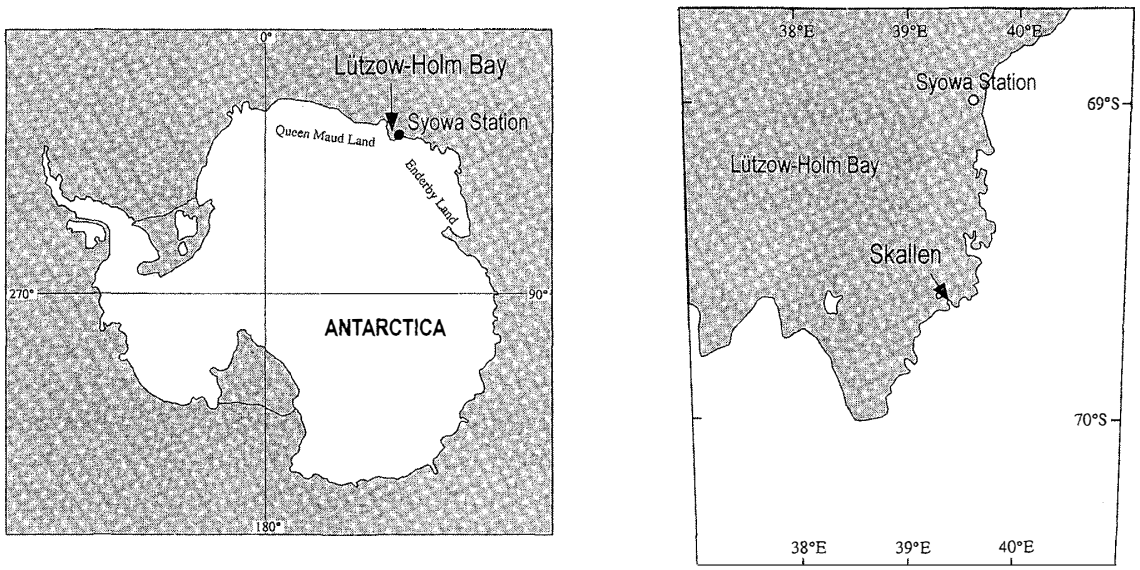

Fig. 1. Location map of Skallen region in Lützow-Holm Bay, East Antarctica.

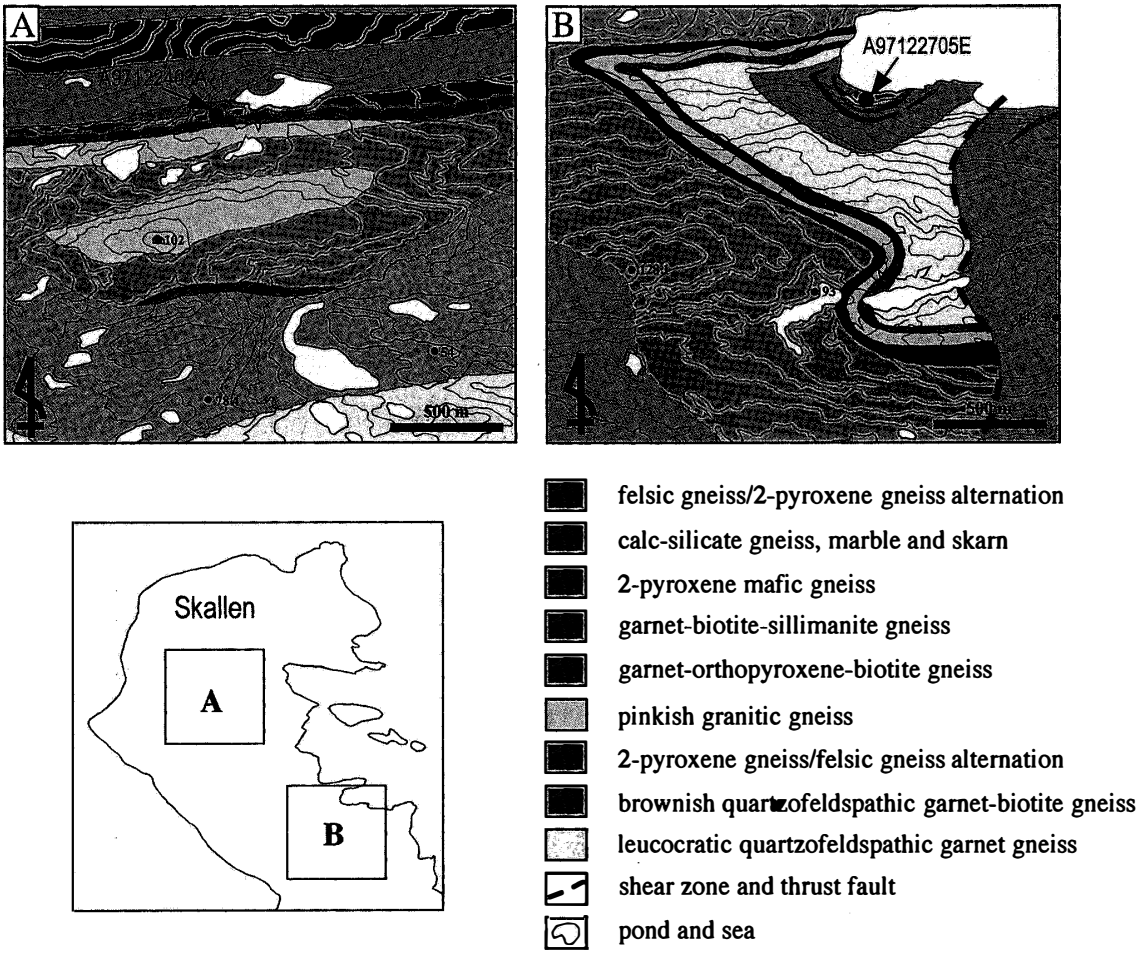

Fig. 2. Simplified geological map of the investigated area in Skallen. A: northern area, B: southeastern area.

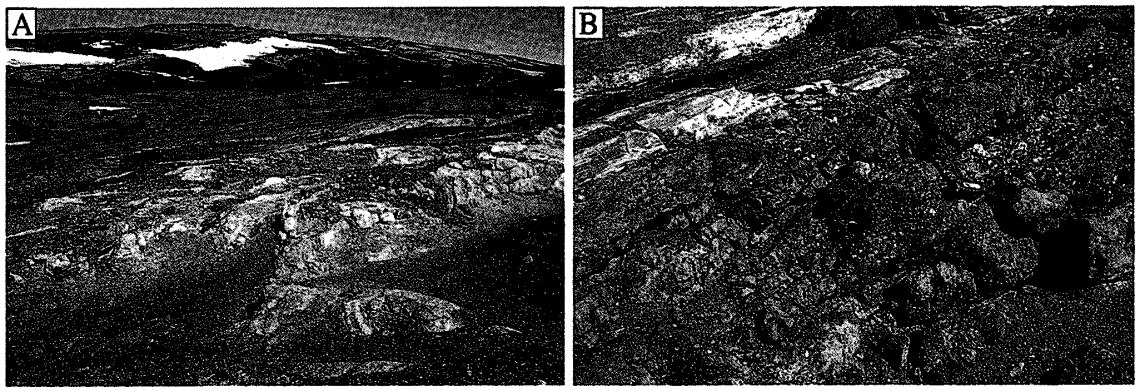

Fig. 3. Modes of occurrence of scapolite-bearing skarn-type metamorphic rocks (A97122403A) in Skallen. A: leucocratic marble and skarn layers along the shear zone. B: close up of skarn-type metamorphic rock.

Under crossed nicols, the mineral shows remarkable variation in birefringence from core to rim. The interference color varies from yellow in the core to blue at the rim. Diopside occurs at the boundary of scapolite grains. Phlogopite occurs as anhedral inclusions in scapolite and diopside crystals. Apatite occurs sporadically as euhedral to subhedral

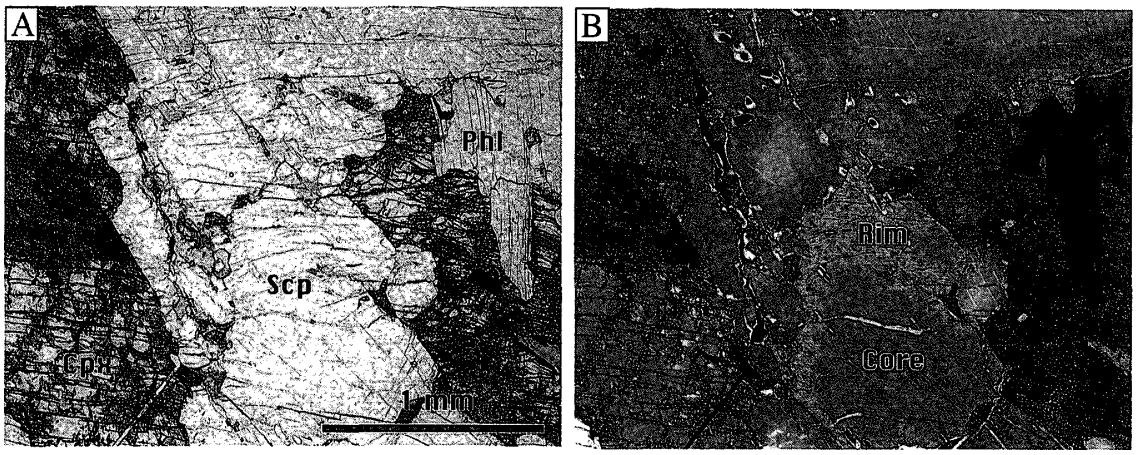

Fig. 4. Photomicrographs showing zoning of scapolite in A97122403A from Skallen. A: plane polarized light B: crossed polars. Abbreviations: Scp; scapolite, Cpx; diopside, Phl; phlogopite.

crystals. Small amounts of calcite and dolomite occur in boundaries of scapolite grains, and are also included in scapolite and diopside crystals. K-feldspar also occurs sporadically as anhedral grains in veins intruded into scapolite. Quartz is found locally as grains interlocking with K-feldspar.

The representative mode of occurrence of zoned scapolite under the microscope in A97122403A from Skallen is shown in Fig. 4.

3. Experiment

The chemical composition for the scapolite A97122403A was analyzed with energy dispersive instruments (JEOL JSM-5310S + JED-2400S) with natural mineral standards at Okayama University. The focused beam with diameter of 10 μm was used to probe the chemical composition of core and rim parts of the specimen. In each part, three points were analyzed and compared to check the analytical accuracy and partial homogeneity. Oxide ZAF correction was applied to analyses. The careful chemical analyses revealed the presensce of Cl in the sample. The CO_3 contents were analyzed by the Perkin-Elmer CHNS/O analyzer at Okayama University. A powderd specimen (1.56 mg) and whole specimen (2.00 mg) were analyzed by the instrument. The chemical composition for the core part of the specimen was determined as:

$$(Na_{1.97}Ca_{1.48}K_{0.46}Mg_{0.03})_{3.94}(Al_{4.15}Si_{7.85}Fe_{0.01})_{12.01}O_{24.00}(Cl_{0.65}(CO_3)_{0.42})_{1.07}.$$

The Me percentage has been defined as 100(Ca+Sr+Fe+Mn+Mg)/(Na+K+Ca+Sr+Fe+Mn+Mg). For the core part of this specimen, it was determined as 39.

The crystal structure of the sample was determined by the single crystal X-ray diffraction method. The transparent, right gray crystal was shaped as a sphere about 0.3 mm in diameter by a looped-file air-flow type grinder. The core parts have about 0.7 mm diameter on average, so the rim part of the specimen was removed with this process. The sphered specimen was mounted on the glass-fiber by epoxy resin binder. The glass fiber was mounted on a glass rod by the same binder, and the rod was mounted on the support pin by Chanel's nail color '*Rouge péché*'. This sample assembly was mounted on the

Table 1. h; k; l, F_{obs}, and σF_{obs}.

H	K	L	F_{obs}	σF_{obs}	H	K	L	F_{obs}	σF_{obs}
0	0	2	36.92	0.17	2	0	0	91.53	0.12
0	0	4	434.90	0.78	2	0	1	21.83	0.16
0	1	1	42.77	0.12	2	0	2	32.99	0.19
0	1	2	5.16	0.32	2	0	3	7.98	0.33
0	1	3	17.25	0.27	2	0	4	9.57	0.36
0	1	4	35.16	0.26	2	0	5	36.60	0.29
0	1	5	14.01	0.46	2	1	0	1.92	0.49
0	2	0	90.57	0.12	2	1	1	34.47	0.16
0	2	1	21.94	0.17	2	1	2	24.12	0.21
0	2	2	32.58	0.19	2	1	3	26.88	0.24
0	2	3	7.56	0.29	2	1	4	29.48	0.27
0	2	4	10.47	0.46	2	1	5	132.37	0.26
0	2	5	35.96	0.30	2	2	0	89.80	0.15
0	3	1	127.28	0.16	2	2	1	29.51	0.18
0	3	3	189.29	0.39	2	2	2	78.73	0.18
0	3	4	17.27	0.35	2	2	3	11.24	0.40
0	3	5	183.16	0.27	2	2	4	40.81	0.26
0	4	0	302.70	0.60	2	2	5	49.71	0.29
0	4	1	11.23	0.34	2	3	1	10.38	0.35
0	4	2	31.36	0.23	2	3	2	19.04	0.26
0	4	3	37.28	0.25	2	3	3	130.87	0.22
0	4	4	154.45	0.25	2	3	4	19.73	0.33
0	5	1	22.02	0.26	2	3	5	13.45	0.53
0	5	2	6.38	0.38	2	4	0	8.66	0.30
0	5	3	114.43	0.24	2	4	1	19.83	0.25
0	5	4	37.96	0.29	2	4	2	85.06	0.21
0	6	0	53.62	0.23	2	4	3	23.60	0.29
0	6	1	4.66	0.52	2	4	4	41.82	0.28
0	6	2	54.89	0.25	2	5	1	109.00	0.21
0	6	3	26.71	0.33	2	5	2	7.65	0.34
0	6	4	57.94	0.29	2	5	3	36.92	0.27
0	7	1	40.21	0.26	2	5	4	7.68	0.46
0	7	2	14.43	0.44	2	6	0	270.53	0.41
0	7	3	157.43	0.27	2	6	2	8.12	0.36
0	8	0	9.52	0.46	2	6	3	13.92	0.46
0	8	1	33.38	0.30	2	7	1	17.28	0.39
0	8	2	51.18	0.30	2	7	2	16.81	0.42
1	0	1	42.86	0.12	2	7	3	5.66	0.62
1	0	2	5.64	0.28	2	8	1	16.31	0.43
1	0	3	17.58	0.28	3	0	0	3.94	0.38
1	0	4	35.36	0.26	3	0	1	128.74	0.16
1	0	5	14.43	0.44	3	0	2	5.31	0.36
1	1	0	41.64	0.10	3	0	3	188.71	0.39
1	1	1	5.91	0.21	3	0	4	17.46	0.34
1	1	2	317.85	0.56	3	0	5	181.12	0.27
1	1	3	25.72	0.24	3	1	0	86.68	0.16
1	1	4	26.98	0.28	3	1	1	23.14	0.20
1	1	5	7.19	0.45	3	1	2	59.71	0.19
1	2	1	48.95	0.15	3	1	3	17.69	0.31
1	2	2	6.05	0.31	3	1	4	14.67	0.39
1	2	3	11.61	0.36	3	1	5	37.74	0.31
1	2	5	30.05	0.33	3	2	1	311.61	0.60
1	3	0	226.81	0.28	3	2	2	18.39	0.27
1	3	1	3.31	0.50	3	2	3	93.92	0.22
1	3	2	263.10	0.34	3	2	4	8.16	0.36
1	3	3	8.04	0.36	3	2	5	260.68	0.50
1	3	4	16.23	0.36	3	3	0	126.42	0.18
1	3	5	17.39	0.43	3	3	2	72.18	0.21
1	4	1	8.97	0.28	3	3	3	8.94	0.37
1	4	3	116.95	0.22	3	3	4	28.17	0.30
1	4	4	26.46	0.31	3	4	1	154.43	0.20
1	5	0	62.66	0.21	3	4	2	21.61	0.29
1	5	1	4.38	0.51	3	4	3	9.24	0.39
1	5	2	84.71	0.22	3	4	4	13.03	0.46
1	5	3	10.49	0.36	3	5	0	30.45	0.24
1	5	4	100.16	0.27	3	5	1	10.51	0.44
1	6	1	191.28	0.22	3	5	2	80.25	0.23
1	6	2	14.30	0.41	3	5	3	7.86	0.40
1	6	3	106.77	0.25	3	5	4	20.27	0.39
1	6	4	5.42	0.65	3	6	1	84.91	0.24
1	7	0	226.06	0.44	3	6	2	6.84	0.43
1	7	1	20.16	0.35	3	6	3	86.36	0.27
1	7	2	80.69	0.26	3	7	0	114.69	0.25
1	7	3	21.27	0.38	3	7	1	16.49	0.40
1	8	1	7.80	0.44	3	7	2	159.23	0.26

Table 1. (continued).

H	K	L	F_{obs}	σF_{obs}	H	K	L	F_{obs}	σF_{obs}
3	8	1	45.66	0.30	6	3	2	21.28	0.33
4	0	0	312.55	0.60	6	3	3	17.61	0.40
4	0	1	10.86	0.34	6	4	0	139.70	0.24
4	0	2	30.94	0.23	6	4	1	8.98	0.41
4	0	3	37.29	0.24	6	4	2	18.49	0.37
4	0	4	153.39	0.25	6	4	3	7.16	0.46
4	1	1	168.34	0.34	6	5	1	77.74	0.26
4	1	2	28.06	0.24	6	5	2	8.95	0.38
4	1	3	225.92	0.41	6	6	0	297.72	0.49
4	1	4	11.82	0.50	6	6	1	5.22	0.67
4	2	0	160.04	0.18	7	0	1	39.85	0.26
4	2	1	10.03	0.39	7	0	2	14.21	0.41
4	2	2	55.73	0.22	7	0	3	155.02	0.27
4	2	3	4.23	0.59	7	1	0	164.92	0.24
4	2	4	50.48	0.27	7	1	1	3.30	0.79
4	3	1	101.90	0.20	7	1	2	51.21	0.27
4	3	2	6.59	0.34	7	2	1	158.05	0.25
4	3	3	24.58	0.30	7	2	2	27.88	0.31
4	3	4	9.30	0.35	7	2	3	174.69	0.27
4	4	0	114.65	0.21	7	3	0	45.58	0.27
4	4	1	11.84	0.39	7	3	2	170.02	0.26
4	4	2	22.92	0.29	7	4	1	115.28	0.26
4	4	3	13.81	0.42	7	4	2	4.07	0.80
4	4	4	22.30	0.36	7	5	0	42.67	0.30
4	5	1	71.11	0.23	7	5	1	8.31	0.42
4	5	2	15.70	0.38	8	0	0	11.16	0.38
4	5	3	214.92	0.26	8	0	1	33.31	0.30
4	6	0	49.40	0.26	8	0	2	51.63	0.29
4	6	1	29.46	0.29	8	1	1	13.12	0.47
4	6	2	66.35	0.26	8	1	2	17.72	0.41
4	7	0	10.12	0.42	8	2	0	87.47	0.27
4	7	1	26.28	0.33	8	2	1	15.79	0.44
4	7	2	9.79	0.46	8	3	1	53.97	0.29
5	0	1	20.38	0.27	0	0	6	266.50	0.53
5	0	2	6.91	0.34	0	1	6	19.78	0.44
5	0	3	113.11	0.24	0	1	7	68.59	0.35
5	0	4	37.89	0.29	0	2	6	48.89	0.32
5	1	0	76.00	0.20	0	2	7	10.06	0.47
5	1	1	10.76	0.40	0	3	6	11.79	0.47
5	1	2	97.47	0.22	0	3	7	66.72	0.35
5	1	3	19.56	0.35	0	4	5	25.98	0.35
5	1	4	70.41	0.27	0	4	6	75.39	0.32
5	2	1	91.24	0.21	0	5	5	85.59	0.30
5	2	2	10.29	0.34	0	5	6	13.52	0.63
5	2	3	77.52	0.25	0	6	5	16.51	0.49
5	2	4	14.99	0.46	0	6	6	8.42	0.57
5	3	0	142.25	0.21	0	7	4	14.86	0.52
5	3	1	18.11	0.30	0	7	5	133.80	0.32
5	3	2	142.13	0.23	0	8	3	6.68	0.59
5	3	3	5.63	0.54	0	8	4	45.66	0.34
5	3	4	34.42	0.32	0	8	5	19.29	0.51
5	4	1	86.56	0.23	0	9	1	109.86	0.29
5	4	3	50.51	0.27	0	9	2	6.06	0.64
5	5	0	12.00	0.45	0	9	3	83.05	0.32
5	5	1	16.14	0.37	0	9	4	8.98	0.51
5	5	2	69.45	0.26	0	10	0	84.42	0.31
5	5	3	5.10	0.65	0	10	2	55.22	0.33
5	6	1	12.32	0.50	0	10	3	24.90	0.44
5	6	2	18.71	0.39	0	11	1	37.66	0.38
5	7	0	192.53	0.27	1	0	6	19.66	0.43
5	7	1	21.88	0.38	1	0	7	67.53	0.35
6	0	0	54.22	0.23	1	1	6	75.22	0.30
6	0	1	4.32	0.54	1	1	7	25.05	0.43
6	0	2	55.21	0.24	1	2	6	13.41	0.55
6	0	3	26.46	0.32	1	2	7	17.24	0.54
6	0	4	57.21	0.29	1	3	6	6.28	0.63
6	1	1	90.07	0.22	1	3	7	7.97	0.56
6	1	2	9.02	0.40	1	4	5	41.48	0.31
6	1	3	204.06	0.25	1	4	6	17.81	0.50
6	1	4	4.91	0.70	1	5	5	12.04	0.44
6	2	0	111.94	0.22	1	5	6	28.23	0.40
6	2	1	11.29	0.45	1	6	5	186.69	0.30
6	2	2	104.72	0.24	1	6	6	29.71	0.40
6	2	3	14.86	0.45	1	7	4	101.59	0.29
6	3	1	123.06	0.23	1	7	5	25.45	0.43

Table 1. (continued).

H	K	L	F_{obs}	σF_{obs}	H	K	L	F_{obs}	σF_{obs}
1	8	3	83.05	0.30	4	3	5	57.37	0.31
1	8	4	8.31	0.51	4	3	6	4.71	0.86
1	8	5	8.71	0.52	4	4	5	15.58	0.49
1	9	0	22.83	0.38	4	4	6	41.48	0.37
1	9	1	36.24	0.33	4	5	4	8.95	0.42
1	9	2	123.96	0.30	4	5	5	43.95	0.34
1	9	3	17.65	0.50	4	5	6	17.38	0.54
1	9	4	73.15	0.34	4	6	4	29.38	0.37
1	10	1	32.78	0.36	4	6	5	5.04	0.82
1	10	2	16.61	0.52	4	7	3	70.75	0.30
1	10	3	167.31	0.33	4	7	4	13.03	0.61
1	11	0	19.56	0.49	4	7	5	34.15	0.39
1	11	1	12.01	0.47	4	8	0	157.61	0.28
1	11	2	39.82	0.39	4	8	1	31.13	0.34
2	0	6	48.76	0.33	4	8	2	88.08	0.30
2	0	7	10.22	0.46	4	8	3	21.39	0.43
2	1	6	27.80	0.39	4	8	4	95.95	0.33
2	1	7	124.87	0.34	4	9	1	59.41	0.32
2	2	7	12.12	0.47	4	9	3	6.91	0.62
2	3	6	15.60	0.49	4	10	0	49.78	0.35
2	4	5	52.02	0.30	4	10	1	6.88	0.64
2	4	6	58.79	0.34	4	10	2	90.50	0.34
2	5	5	78.66	0.30	5	0	5	85.44	0.30
2	5	6	10.24	0.46	5	0	6	13.44	0.62
2	6	4	183.27	0.28	5	1	5	14.25	0.53
2	6	5	9.53	0.46	5	1	6	4.58	0.90
2	6	6	39.92	0.39	5	2	5	62.56	0.31
2	7	4	9.36	0.44	5	2	6	23.47	0.45
2	7	5	20.38	0.48	5	3	5	7.61	0.52
2	8	2	284.29	0.51	5	3	6	16.45	0.53
2	8	3	15.86	0.48	5	4	4	26.12	0.35
2	8	4	56.66	0.33	5	4	5	61.73	0.32
2	8	5	14.59	0.62	5	4	6	13.30	0.45
2	9	1	93.60	0.29	5	5	4	4.92	0.74
2	9	3	55.54	0.33	5	5	5	11.90	0.47
2	9	4	6.60	0.67	5	6	3	32.88	0.33
2	10	0	86.42	0.32	5	6	4	24.41	0.39
2	10	1	13.70	0.59	5	6	5	8.70	0.51
2	10	2	27.29	0.41	5	7	2	62.78	0.30
2	10	3	18.55	0.54	5	7	3	21.99	0.42
2	11	1	32.33	0.40	5	7	4	93.34	0.33
2	11	2	12.97	0.48	5	8	1	31.20	0.36
3	0	6	12.10	0.45	5	8	2	6.87	0.57
3	0	7	66.52	0.35	5	8	3	96.41	0.32
3	1	6	94.65	0.31	5	8	4	12.35	0.48
3	1	7	22.76	0.46	5	9	0	109.48	0.31
3	2	6	17.13	0.50	5	9	1	11.02	0.41
3	3	5	8.56	0.42	5	9	2	43.79	0.36
3	3	6	16.26	0.51	5	9	3	19.71	0.52
3	4	5	180.97	0.29	5	10	1	125.92	0.34
3	4	6	21.85	0.44	5	10	2	11.36	0.52
3	5	5	29.30	0.38	6	0	5	16.74	0.47
3	5	6	44.54	0.37	6	0	6	11.56	0.50
3	6	4	21.95	0.40	6	1	5	66.30	0.32
3	6	5	125.67	0.32	6	1	6	4.84	0.90
3	7	3	19.60	0.43	6	2	4	20.23	0.39
3	7	4	71.42	0.31	6	2	5	11.55	0.46
3	7	5	16.52	0.51	6	2	6	31.54	0.41
3	8	2	18.09	0.43	6	3	5	121.62	0.32
3	8	3	26.21	0.39	6	4	4	57.08	0.31
3	8	4	4.36	0.93	6	4	5	31.40	0.39
3	9	0	98.68	0.30	6	5	3	188.14	0.28
3	9	1	8.91	0.45	6	5	4	13.04	0.42
3	9	2	42.99	0.34	6	5	5	9.52	0.46
3	9	3	14.36	0.57	6	6	2	67.14	0.30
3	10	1	16.61	0.51	6	6	3	22.11	0.42
3	10	2	8.04	0.54	6	6	4	154.24	0.32
3	10	3	8.67	0.51	6	6	5	21.38	0.48
3	11	0	150.77	0.34	6	7	1	73.67	0.30
3	11	1	5.41	0.81	6	7	2	20.80	0.44
4	0	5	26.78	0.34	6	7	3	16.04	0.52
4	0	6	74.51	0.32	6	7	4	11.67	0.49
4	1	5	65.04	0.29	6	8	0	52.44	0.33
4	1	6	32.16	0.38	6	8	1	6.41	0.63
4	2	6	38.13	0.36	6	8	2	149.64	0.32

Table 1. (continued).

H	K	L	F_{obs}	σF_{obs}	H	K	L	F_{obs}	σF_{obs}
6	8	3	7.97	0.56	9	3	2	30.04	0.38
6	9	1	101.17	0.33	9	3	3	4.19	0.97
6	10	0	140.00	0.35	9	3	4	24.95	0.46
7	0	4	14.56	0.51	9	4	1	26.85	0.38
7	0	5	133.25	0.32	9	4	2	9.02	0.49
7	1	4	115.24	0.29	9	4	3	62.96	0.34
7	1	5	29.49	0.39	9	5	0	191.70	0.31
7	2	5	114.88	0.33	9	5	2	139.47	0.32
7	3	3	9.65	0.46	9	5	3	11.12	0.42
7	3	4	85.69	0.31	9	6	1	40.76	0.36
7	3	5	30.53	0.40	9	6	2	12.28	0.49
7	4	3	11.79	0.40	9	7	0	58.22	0.36
7	4	4	5.28	0.76	9	7	1	9.64	0.46
7	4	5	165.33	0.34	10	0	0	84.39	0.31
7	5	2	113.39	0.29	10	0	1	7.95	0.50
7	5	3	12.80	0.58	10	0	2	55.67	0.33
7	5	4	64.74	0.33	10	0	3	24.77	0.43
7	6	1	42.60	0.32	10	1	1	46.77	0.34
7	6	2	17.10	0.49	10	1	2	6.76	0.60
7	6	3	60.49	0.33	10	1	3	25.45	0.44
7	6	4	18.60	0.52	10	2	0	44.42	0.34
7	7	0	14.96	0.53	10	2	1	20.99	0.43
7	7	1	21.40	0.43	10	2	2	34.01	0.37
7	7	2	164.96	0.31	10	2	3	27.87	0.42
7	7	3	21.38	0.47	10	3	1	20.92	0.45
7	8	1	14.50	0.57	10	3	2	6.77	0.61
7	8	2	20.12	0.48	10	3	3	25.12	0.45
7	8	3	8.51	0.54	10	4	0	11.56	0.46
7	9	0	18.00	0.52	10	4	2	177.23	0.33
7	9	1	14.68	0.61	10	5	1	17.22	0.52
8	0	3	7.71	0.48	10	5	2	7.77	0.58
8	0	4	45.32	0.34	10	6	0	145.00	0.34
8	0	5	19.36	0.51	11	0	1	38.28	0.38
8	1	3	74.54	0.30	11	1	0	112.51	0.33
8	1	4	7.57	0.53	11	1	1	16.02	0.56
8	1	5	34.90	0.39	11	1	2	10.32	0.45
8	2	2	238.32	0.28	11	2	1	42.07	0.37
8	2	3	14.35	0.51	11	2	2	11.66	0.48
8	2	4	56.85	0.33	11	3	0	3.86	1.03
8	2	5	25.41	0.44	11	3	1	8.99	0.51
8	3	2	4.06	0.89	0	0	8	29.23	0.44
8	3	4	28.75	0.40	0	1	8	3.98	1.17
8	4	0	142.83	0.28	0	4	7	38.63	0.40
8	4	1	6.15	0.57	0	5	7	92.17	0.37
8	4	2	56.45	0.31	0	6	7	46.03	0.40
8	4	3	8.10	0.49	0	7	6	16.87	0.58
8	4	4	57.46	0.35	0	8	6	27.31	0.46
8	5	1	39.67	0.33	0	9	5	106.54	0.36
8	5	2	11.03	0.40	0	10	4	22.27	0.50
8	5	3	116.72	0.32	0	10	5	7.83	0.68
8	5	4	21.58	0.47	0	11	3	132.85	0.35
8	6	0	24.45	0.38	0	11	4	12.28	0.46
8	6	1	8.91	0.43	0	12	0	100.59	0.36
8	6	2	64.28	0.33	0	12	1	14.44	0.45
8	6	3	25.94	0.43	0	12	2	74.48	0.37
8	7	1	17.14	0.51	0	12	3	12.09	0.46
8	7	2	5.11	0.84	1	0	8	5.78	0.80
8	7	3	109.17	0.35	1	1	8	77.10	0.39
8	8	0	9.52	0.45	1	4	7	30.97	0.42
8	8	1	29.03	0.41	1	5	7	7.96	0.57
9	0	1	109.73	0.29	1	6	7	43.49	0.41
9	0	2	6.16	0.61	1	7	6	43.28	0.38
9	0	3	83.20	0.32	1	9	5	37.89	0.41
9	0	4	9.32	0.47	1	10	5	67.72	0.39
9	1	0	241.87	0.28	1	11	4	24.01	0.51
9	1	1	6.28	0.56	1	12	1	45.31	0.40
9	1	2	96.60	0.30	1	12	3	71.78	0.38
9	1	3	7.19	0.55	1	13	0	8.42	0.57
9	1	4	112.10	0.33	2	1	8	22.27	0.51
9	2	1	12.93	0.54	2	4	7	20.89	0.49
9	2	2	7.22	0.56	2	5	7	47.78	0.40
9	2	3	15.60	0.53	2	6	7	11.41	0.44
9	2	4	10.17	0.44	2	7	6	7.01	0.67
9	3	0	27.70	0.35	2	8	6	91.09	0.37
9	3	1	14.53	0.48	2	9	5	143.02	0.36

Table 1. (continued).

H	K	L	F_{obs}	σF_{obs}	H	K	L	F_{obs}	σF_{obs}
2	10	4	39.00	0.41	7	5	5	5.88	0.75
2	10	5	20.87	0.55	7	5	6	4.07	1.15
2	11	3	25.00	0.46	7	6	5	31.56	0.42
2	11	4	9.62	0.54	7	7	4	19.42	0.49
2	12	0	75.92	0.37	7	7	5	14.00	0.51
2	12	1	6.72	0.71	7	8	4	13.61	0.65
2	12	2	75.15	0.37	7	9	2	119.45	0.35
3	2	7	12.31	0.48	7	9	3	13.22	0.48
3	3	7	4.78	0.87	7	10	0	9.84	0.52
3	4	7	16.21	0.61	7	10	1	55.13	0.38
3	5	7	15.18	0.64	7	10	2	7.94	0.61
3	6	6	17.92	0.54	7	11	0	104.78	0.38
3	6	7	33.44	0.44	8	0	6	26.68	0.47
3	7	6	31.35	0.43	8	1	6	21.84	0.52
3	8	5	32.10	0.43	8	2	6	31.54	0.43
3	8	6	11.90	0.54	8	3	5	99.68	0.35
3	9	5	16.35	0.59	8	3	6	10.96	0.48
3	11	2	64.44	0.37	8	4	5	20.81	0.52
3	11	3	5.78	0.78	8	5	5	17.74	0.57
3	12	1	25.20	0.47	8	6	4	24.10	0.46
3	12	2	16.99	0.61	8	7	4	15.97	0.58
4	0	7	38.87	0.39	8	8	2	48.97	0.37
4	1	7	123.25	0.35	8	8	3	10.40	0.46
4	2	7	13.95	0.64	8	8	4	32.10	0.45
4	3	7	24.26	0.46	8	9	1	50.51	0.39
4	4	7	14.10	0.66	8	9	2	11.03	0.47
4	5	7	124.54	0.38	8	9	3	14.86	0.63
4	6	6	24.68	0.46	8	10	0	74.66	0.38
4	7	6	7.21	0.68	8	10	1	5.94	0.85
4	8	5	23.54	0.48	9	0	5	106.91	0.36
4	9	4	32.99	0.42	9	1	5	8.89	0.53
4	9	5	92.73	0.38	9	2	5	17.72	0.57
4	10	3	16.33	0.55	9	3	5	7.41	0.63
4	11	1	14.36	0.46	9	4	4	9.53	0.48
4	12	0	82.30	0.38	9	4	5	12.48	0.50
4	12	2	18.22	0.61	9	5	4	53.76	0.38
5	0	7	91.67	0.37	9	5	5	7.84	0.62
5	1	7	16.90	0.61	9	6	3	69.29	0.36
5	2	7	9.24	0.53	9	6	4	6.67	0.71
5	3	7	10.29	0.48	9	7	2	66.08	0.36
5	4	7	16.35	0.62	9	7	3	22.83	0.49
5	5	6	34.03	0.40	9	8	1	93.51	0.36
5	6	6	41.83	0.39	9	8	2	12.79	0.51
5	7	5	12.22	0.51	9	8	3	86.60	0.39
5	7	6	20.08	0.57	10	0	4	22.22	0.51
5	8	5	83.10	0.37	10	0	5	9.70	0.51
5	9	4	58.92	0.38	10	1	4	14.05	0.66
5	9	5	12.03	0.46	10	1	5	24.16	0.50
5	10	3	119.20	0.36	10	2	4	44.60	0.39
5	10	4	4.86	1.02	10	3	4	9.19	0.52
5	11	0	19.97	0.53	10	4	3	5.26	0.83
5	11	1	8.71	0.56	10	4	4	38.72	0.41
5	11	2	19.57	0.52	10	5	3	40.28	0.39
5	11	3	5.38	0.88	10	5	4	9.95	0.51
6	0	7	46.00	0.40	10	6	1	20.33	0.51
6	1	7	157.95	0.37	10	6	2	42.14	0.40
6	2	7	11.91	0.45	10	6	3	10.83	0.48
6	3	6	17.72	0.56	10	7	0	4.94	0.89
6	3	7	8.50	0.57	10	7	1	17.34	0.55
6	4	6	36.27	0.40	10	7	2	12.51	0.52
6	6	6	80.89	0.38	10	8	0	14.63	0.66
6	7	5	44.62	0.40	10	8	1	9.55	0.51
6	8	4	28.62	0.44	11	0	3	134.85	0.35
6	8	5	20.56	0.53	11	0	4	12.64	0.54
6	9	3	12.25	0.50	11	1	3	13.81	0.63
6	9	4	19.96	0.53	11	1	4	33.20	0.43
6	10	1	5.52	0.84	11	2	3	133.76	0.36
6	10	2	54.40	0.38	11	2	4	10.36	0.48
6	10	3	4.01	1.10	11	3	2	46.26	0.37
6	11	1	27.20	0.46	11	3	3	12.39	0.50
7	0	6	16.65	0.57	11	4	0	11.13	0.50
7	1	6	56.96	0.38	11	4	1	29.83	0.41
7	2	6	39.75	0.39	11	4	2	13.33	0.49
7	3	6	59.97	0.38	11	4	3	77.72	0.38
7	4	6	5.15	0.91	11	5	0	38.40	0.40

Table 1. (continued).

H	K	L	F_{obs}	σF_{obs}	H	K	L	F_{obs}	σF_{obs}
11	5	1	28.40	0.44	1	11	7	19.68	0.71
11	5	2	35.38	0.42	1	12	4	14.76	0.68
11	5	3	9.45	0.54	1	12	5	12.97	0.60
11	6	1	10.94	0.44	1	12	6	5.98	0.95
11	6	2	6.69	0.70	1	13	1	14.63	0.68
11	7	0	87.34	0.38	1	13	2	93.47	0.39
12	0	0	101.45	0.36	1	13	3	9.49	0.63
12	0	1	13.81	0.65	1	13	4	34.95	0.50
12	0	2	74.34	0.37	1	13	5	22.95	0.60
12	0	3	12.53	0.52	1	14	1	22.33	0.56
12	1	1	41.73	0.38	1	14	2	13.42	0.59
12	1	2	7.36	0.66	1	14	3	76.68	0.44
12	1	3	65.46	0.39	1	14	4	17.00	0.72
12	2	0	40.56	0.40	1	15	0	56.15	0.46
12	2	2	35.12	0.43	1	15	2	67.72	0.46
12	3	1	81.99	0.37	2	0	9	16.97	0.69
12	3	2	5.92	0.78	2	1	9	81.04	0.43
12	4	0	80.47	0.38	2	2	8	15.85	0.60
12	4	1	14.36	0.64	2	2	9	30.16	0.51
12	4	2	63.26	0.39	2	3	8	35.94	0.46
13	1	0	41.76	0.42	2	3	9	29.20	0.54
0	1	9	6.66	0.80	2	4	8	51.71	0.42
0	2	9	17.23	0.67	2	4	9	31.72	0.53
0	3	8	6.11	0.80	2	5	8	6.85	0.78
0	3	9	52.73	0.45	2	5	9	9.39	0.64
0	4	8	9.79	0.52	2	6	8	28.49	0.50
0	4	9	18.32	0.67	2	6	9	7.72	0.78
0	5	8	16.43	0.68	2	7	7	10.06	0.53
0	5	9	31.89	0.53	2	7	8	32.74	0.51
0	6	8	22.16	0.56	2	8	7	9.27	0.55
0	7	7	110.45	0.39	2	8	8	109.97	0.44
0	7	8	13.06	0.48	2	9	6	9.76	0.53
0	8	7	31.12	0.49	2	9	7	25.91	0.54
0	9	7	18.80	0.60	2	10	6	25.95	0.53
0	9	8	8.89	0.71	2	10	7	19.36	0.65
0	10	6	14.19	0.51	2	11	5	40.43	0.45
0	10	7	33.89	0.52	2	11	6	5.83	0.96
0	11	5	5.96	0.85	2	12	3	18.70	0.59
0	11	6	14.18	0.53	2	12	4	29.15	0.48
0	11	7	55.57	0.48	2	12	6	56.78	0.47
0	12	4	58.81	0.41	2	13	1	67.77	0.40
0	12	5	6.94	0.76	2	13	2	7.09	0.77
0	12	6	12.52	0.50	2	13	3	58.48	0.43
0	13	1	41.14	0.44	2	13	4	7.52	0.76
0	13	2	14.67	0.50	2	13	5	126.02	0.44
0	13	3	7.18	0.77	2	14	0	44.81	0.44
0	13	4	10.29	0.57	2	14	1	7.26	0.74
0	13	5	44.52	0.49	2	14	2	34.25	0.49
0	14	0	54.43	0.43	2	15	1	10.25	0.62
0	14	1	10.16	0.59	2	15	2	4.84	1.31
0	14	2	7.45	0.75	3	0	8	6.24	0.78
0	14	3	11.64	0.55	3	0	9	52.51	0.46
0	14	4	20.16	0.68	3	1	8	27.13	0.49
0	15	1	68.42	0.45	3	1	9	20.49	0.63
0	15	2	8.54	0.75	3	2	8	8.63	0.61
0	15	3	26.08	0.59	3	2	9	93.39	0.43
1	1	9	8.17	0.70	3	3	8	11.80	0.56
1	2	9	4.61	1.17	3	3	9	4.38	1.29
1	3	8	77.74	0.39	3	4	8	9.12	0.58
1	3	9	12.33	0.51	3	4	9	79.11	0.45
1	4	8	8.17	0.63	3	5	8	40.55	0.45
1	5	8	8.57	0.65	3	5	9	16.81	0.76
1	5	9	8.64	0.70	3	7	8	41.16	0.49
1	6	8	4.86	1.04	3	8	7	30.23	0.49
1	6	9	25.63	0.60	3	8	8	20.46	0.65
1	7	7	4.87	1.06	3	9	6	46.24	0.43
1	7	8	12.61	0.60	3	9	7	21.32	0.57
1	8	7	36.79	0.47	3	10	5	6.49	0.79
1	8	8	14.76	0.55	3	10	6	18.25	0.65
1	9	6	35.87	0.44	3	10	7	24.32	0.60
1	9	8	57.56	0.48	3	11	4	53.55	0.41
1	10	6	20.43	0.59	3	11	5	6.75	0.77
1	10	7	127.50	0.43	3	11	6	31.24	0.53
1	11	5	6.36	0.81	3	12	3	11.84	0.48
1	11	6	17.18	0.69	3	12	5	33.38	0.51

Table 1. (continued).

H	K	L	F_{obs}	σF_{obs}	H	K	L	F_{obs}	σF_{obs}
3	13	0	46.33	0.43	5	13	3	7.64	0.76
3	13	1	11.47	0.48	5	13	4	31.71	0.52
3	13	2	57.08	0.42	5	14	1	32.78	0.52
3	13	3	10.18	0.56	5	14	3	71.30	0.46
3	13	4	48.08	0.47	6	0	8	20.17	0.60
3	13	5	12.39	0.54	6	0	9	6.74	0.83
3	14	1	8.74	0.65	6	1	9	43.79	0.49
3	14	2	7.36	0.78	6	2	8	31.71	0.49
3	14	3	66.24	0.45	6	3	8	22.51	0.57
3	14	4	20.38	0.66	6	4	7	9.34	0.57
3	15	0	32.24	0.54	6	5	7	101.64	0.40
3	15	1	22.60	0.61	6	5	8	21.25	0.60
3	15	2	41.41	0.49	6	6	7	26.58	0.52
4	0	8	8.06	0.60	6	6	8	9.28	0.63
4	0	9	18.16	0.68	6	7	6	8.79	0.61
4	1	8	13.88	0.50	6	7	7	53.67	0.45
4	1	9	45.06	0.47	6	8	6	20.83	0.59
4	2	8	38.04	0.45	6	8	7	4.67	1.24
4	3	8	20.09	0.60	6	9	5	125.50	0.39
4	3	9	7.31	0.79	6	10	4	45.65	0.42
4	4	9	5.96	0.95	6	10	5	7.95	0.68
4	6	7	24.57	0.52	6	10	6	54.75	0.46
4	6	8	19.23	0.60	6	11	3	38.79	0.44
4	7	7	7.04	0.75	6	11	4	14.86	0.71
4	7	8	6.54	0.89	6	11	5	6.37	0.85
4	8	6	68.76	0.39	6	12	0	24.05	0.52
4	8	8	22.77	0.61	6	12	1	6.41	0.79
4	9	7	25.49	0.56	6	12	2	30.76	0.49
4	10	5	9.60	0.56	6	12	3	9.02	0.62
4	10	6	16.61	0.69	6	12	4	18.20	0.69
4	10	7	24.10	0.59	6	12	5	10.21	0.64
4	11	4	10.92	0.49	6	13	1	78.76	0.42
4	11	5	14.89	0.51	6	13	2	7.78	0.74
4	11	6	17.92	0.70	6	13	3	21.10	0.62
4	12	3	16.94	0.61	6	13	4	10.02	0.62
4	12	4	24.77	0.54	6	14	0	36.06	0.50
4	12	5	7.95	0.72	6	14	1	22.05	0.61
4	13	1	45.81	0.42	6	14	2	6.19	0.93
4	13	2	10.24	0.55	7	0	7	110.12	0.38
4	13	3	18.58	0.66	7	0	8	13.15	0.58
4	13	4	19.71	0.64	7	1	7	15.21	0.50
4	14	0	35.78	0.50	7	1	8	34.11	0.49
4	14	1	12.98	0.58	7	2	7	61.06	0.41
4	14	2	112.97	0.43	7	2	8	8.92	0.67
4	15	0	8.42	0.74	7	3	7	5.51	0.90
4	15	1	15.80	0.55	7	3	8	65.09	0.44
5	0	8	17.14	0.61	7	4	7	81.27	0.40
5	0	9	31.74	0.51	7	5	7	25.63	0.53
5	1	8	30.09	0.49	7	5	8	74.61	0.46
5	1	9	6.78	0.88	7	6	6	12.70	0.43
5	2	8	8.21	0.65	7	6	7	41.35	0.47
5	2	9	8.24	0.76	7	7	6	68.19	0.41
5	3	8	60.40	0.43	7	7	7	10.54	0.59
5	4	8	12.79	0.57	7	8	5	33.08	0.46
5	5	7	17.51	0.60	7	8	6	25.10	0.54
5	5	8	24.42	0.54	7	8	7	28.86	0.55
5	6	7	23.45	0.54	7	9	4	18.64	0.56
5	6	8	9.61	0.59	7	9	6	30.70	0.53
5	7	7	10.87	0.54	7	10	3	16.22	0.62
5	7	8	24.66	0.59	7	10	4	6.54	0.77
5	8	7	87.87	0.43	7	10	5	49.47	0.45
5	9	6	57.72	0.43	7	10	6	8.88	0.69
5	9	7	23.31	0.57	7	11	2	39.66	0.43
5	10	5	61.08	0.41	7	11	3	7.00	0.73
5	10	6	10.50	0.58	7	11	4	44.83	0.45
5	11	4	10.01	0.54	7	11	5	9.43	0.64
5	11	5	6.22	0.89	7	12	0	6.17	0.85
5	11	6	11.06	0.60	7	12	1	23.02	0.53
5	12	1	53.71	0.40	7	12	2	13.01	0.56
5	12	2	5.69	0.87	7	12	3	31.26	0.51
5	12	3	85.36	0.40	7	12	4	4.52	1.21
5	12	5	4.83	1.21	7	13	0	93.85	0.43
5	13	0	86.23	0.41	7	13	1	14.59	0.55
5	13	1	6.36	0.84	7	13	2	57.48	0.46

Table 1. (continued).

H	K	L	F_{obs}	σF_{obs}	H	K	L	F_{obs}	σF_{obs}
7	13	3	16.07	0.76	10	3	6	9.78	0.55
7	14	1	34.09	0.53	10	3	7	25.72	0.57
8	0	7	31.80	0.47	10	4	5	7.84	0.63
8	0	8	6.59	0.86	10	4	6	46.70	0.46
8	1	7	55.79	0.43	10	5	5	18.58	0.60
8	1	8	21.79	0.62	10	5	6	12.09	0.50
8	2	7	21.02	0.59	10	6	4	113.83	0.39
8	2	8	105.73	0.44	10	6	5	9.49	0.58
8	3	7	32.35	0.49	10	6	6	42.66	0.49
8	3	8	22.98	0.63	10	7	3	66.35	0.40
8	4	6	19.86	0.55	10	7	4	18.51	0.59
8	4	7	15.73	0.72	10	7	5	9.19	0.61
8	4	8	10.55	0.62	10	7	6	15.37	0.55
8	5	6	11.89	0.54	10	8	2	76.36	0.40
8	5	7	66.71	0.43	10	8	3	7.29	0.71
8	6	6	32.21	0.47	10	8	5	13.13	0.62
8	6	7	23.26	0.59	10	9	0	12.86	0.54
8	7	5	105.78	0.39	10	9	1	22.13	0.52
8	7	6	5.22	1.07	10	9	2	6.58	0.76
8	7	7	101.52	0.44	10	9	3	24.17	0.53
8	8	5	37.92	0.46	10	9	4	17.36	0.70
8	9	4	8.77	0.59	10	9	5	13.97	0.58
8	9	5	57.57	0.45	10	10	0	35.36	0.47
8	10	2	61.37	0.40	10	10	1	7.75	0.71
8	10	4	49.48	0.45	10	10	2	11.78	0.49
8	10	5	10.89	0.57	10	10	3	7.83	0.73
8	11	1	48.65	0.42	10	10	4	28.86	0.54
8	11	3	56.23	0.44	10	11	1	8.49	0.67
8	11	4	8.73	0.70	10	11	3	103.38	0.45
8	12	0	82.54	0.42	10	12	0	23.64	0.73
8	12	1	10.99	0.55	10	12	1	10.24	0.59
8	12	2	14.84	0.55	11	0	5	7.73	0.66
8	12	3	7.71	0.80	11	0	6	15.16	0.69
8	13	0	6.36	0.90	11	0	7	61.02	0.46
8	13	1	37.53	0.51	11	1	5	9.65	0.54
9	0	8	9.45	0.65	11	1	6	44.48	0.46
9	1	6	31.10	0.46	11	2	5	26.26	0.50
9	1	7	5.90	0.89	11	2	6	18.30	0.63
9	1	8	34.21	0.52	11	3	4	35.73	0.43
9	2	7	9.26	0.60	11	3	5	13.72	0.53
9	3	7	11.12	0.52	11	3	6	7.61	0.70
9	4	6	6.91	0.75	11	4	4	10.96	0.48
9	4	7	35.41	0.50	11	4	5	4.38	1.19
9	5	6	22.26	0.56	11	4	6	18.87	0.65
9	5	7	12.53	0.52	11	5	4	25.73	0.48
9	6	5	23.86	0.52	11	5	5	21.30	0.58
9	6	6	12.85	0.61	11	5	6	6.60	0.88
9	6	7	70.50	0.46	11	6	3	60.49	0.40
9	7	4	37.89	0.42	11	6	4	10.65	0.56
9	7	5	14.35	0.51	11	6	5	33.44	0.49
9	7	6	49.29	0.47	11	7	1	11.48	0.45
9	8	4	5.36	0.96	11	7	2	12.29	0.55
9	8	5	145.90	0.41	11	7	3	23.99	0.53
9	8	6	22.95	0.60	11	7	4	54.78	0.44
9	9	2	17.35	0.62	11	8	1	23.72	0.52
9	9	4	21.37	0.58	11	8	3	67.77	0.43
9	10	1	78.71	0.40	11	8	4	19.51	0.66
9	10	2	6.86	0.77	11	9	0	46.44	0.44
9	10	4	15.01	0.55	11	9	2	61.74	0.44
9	10	5	95.75	0.45	11	9	3	5.78	0.92
9	11	0	94.27	0.42	11	9	4	38.60	0.49
9	11	1	5.07	1.05	11	10	1	23.41	0.57
9	11	2	24.67	0.56	11	10	3	32.88	0.52
9	11	3	20.20	0.61	11	11	0	40.31	0.50
9	11	4	59.44	0.47	12	0	4	59.36	0.42
9	12	0	8.66	0.64	12	0	5	6.84	0.77
9	12	1	24.03	0.55	12	0	6	12.38	0.49
9	12	2	6.43	0.87	12	1	4	9.88	0.52
9	12	3	42.69	0.50	12	1	5	12.42	0.55
10	0	6	12.86	0.55	12	1	6	8.01	0.72
10	0	7	34.27	0.51	12	2	4	15.12	0.67
10	1	7	22.31	0.61	12	2	5	5.55	0.94
10	2	6	19.71	0.56	12	3	3	4.81	1.03
10	2	7	13.71	0.56	12	3	4	7.74	0.69
10	3	5	57.10	0.41	12	3	5	89.29	0.43

Table 1. (continued).

H	K	L	F_{obs}	σF_{obs}	H	K	L	F_{obs}	σF_{obs}
12	4	3	13.95	0.50	14	2	4	6.36	0.92
12	4	4	20.33	0.58	14	3	1	51.97	0.44
12	4	5	5.80	0.94	14	3	2	13.03	0.50
12	5	1	25.96	0.49	14	3	3	32.95	0.50
12	5	3	39.94	0.44	14	3	4	7.74	0.76
12	5	4	7.33	0.73	14	4	0	18.86	0.62
12	5	5	49.99	0.46	14	4	2	140.43	0.42
12	6	0	9.54	0.53	14	4	3	10.73	0.56
12	6	1	9.56	0.54	14	5	1	23.98	0.57
12	6	2	8.62	0.57	14	5	3	53.98	0.47
12	6	3	19.49	0.60	14	6	0	23.50	0.58
12	6	4	35.84	0.49	14	6	1	26.28	0.56
12	6	5	10.82	0.60	14	6	2	30.50	0.55
12	7	1	26.58	0.51	14	7	1	43.42	0.49
12	7	2	4.41	1.10	15	0	1	67.67	0.45
12	7	3	92.80	0.42	15	0	2	11.27	0.55
12	7	4	6.06	0.91	15	0	3	26.08	0.59
12	8	0	50.80	0.44	15	1	0	52.43	0.45
12	8	2	57.82	0.45	15	1	2	48.19	0.48
12	8	3	10.34	0.59	15	2	1	12.67	0.59
12	9	0	6.47	0.84	15	3	0	11.03	0.54
12	9	1	8.20	0.67	15	3	1	11.93	0.53
12	9	2	9.41	0.64	15	3	2	12.28	0.53
12	9	3	37.43	0.49	15	4	1	61.05	0.47
12	10	0	29.38	0.55					
12	10	1	6.18	0.92					
13	0	1	41.78	0.42					
13	0	2	15.53	0.63					
13	0	3	8.37	0.64					
13	0	4	10.62	0.55					
13	0	5	47.12	0.47					
13	1	1	6.43	0.76					
13	1	2	95.15	0.39					
13	1	4	25.20	0.54					
13	1	5	9.44	0.61					
13	2	1	5.48	0.90					
13	2	2	13.70	0.52					
13	2	3	7.48	0.71					
13	2	4	6.70	0.80					
13	2	5	18.34	0.70					
13	3	0	48.92	0.42					
13	3	1	12.27	0.55					
13	3	2	17.02	0.61					
13	3	3	12.74	0.56					
13	3	4	41.03	0.47					
13	4	1	15.52	0.64					
13	4	2	14.05	0.57					
13	4	3	42.98	0.46					
13	4	4	7.43	0.74					
13	5	0	84.12	0.41					
13	5	2	68.98	0.43					
13	5	3	5.51	0.97					
13	5	4	38.85	0.50					
13	6	1	13.23	0.57					
13	6	2	6.50	0.82					
13	6	3	49.18	0.47					
13	6	4	10.19	0.59					
13	7	0	49.92	0.45					
13	7	1	15.47	0.52					
13	7	2	28.28	0.54					
13	7	3	10.22	0.63					
13	8	1	93.97	0.45					
13	8	2	10.55	0.62					
14	0	0	54.88	0.42					
14	0	1	10.31	0.56					
14	0	3	12.65	0.59					
14	0	4	19.50	0.66					
14	1	1	6.16	0.81					
14	1	2	9.11	0.61					
14	1	3	109.07	0.43					
14	1	4	22.05	0.59					
14	2	0	14.77	0.50					
14	2	1	19.42	0.60					
14	2	2	35.93	0.47					
14	2	3	19.21	0.68					

Table 2. Atomic coordinates and isotoropic temperature factors of scapolite (39% Me, Lützow-Holm Bay region, East Antarctica). Standard deviations, σ are given in parentheses.

ATOM	x	y	z	B_{iso}
Na,Ca,K	0.2137(2)	0.1368(2)	1.0143(3)	1.91(4)
T(1)	0.4099(1)	0.3390(1)	0.0034(2)	0.61(3)
T(2)	0.3359(1)	0.9131(1)	0.2120(2)	0.61(3)
T(3)	0.0834(1)	0.3405(1)	0.2008(2)	0.68(3)
C,Cl	1/2	1/2	1/2	4.21(18)
O(1)	0.3078(3)	0.8771(3)	0.0128(6)	1.15(7)
O(2)	0.0593(4)	0.6493(4)	0.2058(6)	1.42(8)
O(3)	0.3476(4)	0.0451(4)	0.2187(6)	1.43(7)
O(4)	0.3693(4)	0.2699(4)	0.1722(6)	1.34(7)
O(5)	0.2712(4)	0.6280(4)	0.1719(6)	1.24(7)
O(6)	0.4578(3)	0.6486(3)	0.0032(6)	1.09(7)
O(7)	0.9910(36)	0.9196(26)	0.9973(52)	8.16(83)

Table 3. Interatomic distances in scapolite (39% Me, Lützow-Holm Bay region, East Antarctica).

(a) T–O distances and O–T–O angles of tetrahedra.

Atoms		Distance (Å)	Atoms	Angle (Å)
T(1)	– O(4)	1.608(3)	O(4)–T(1)–O(5)	107.49(16)
	– O(5)	1.629(3)	O(4)–T(1)–O(6)	110.76(4)
	– O(6)	1.610(3)	O(4)–T(1)–O(6′)	110.90(7)
	– O(6′)	1.606(2)	O(5)–T(1)–O(6)	109.12(4)
	Average	1.614(3)	O(5)–T(1)–O(6′)	107.59(8)
			O(6)–T(1)–O(6′)	110.85(7)
T(2)	– O(1)	1.609(4)	O(1)–T(2)–O(2)	113.89(7)
	– O(2)	1.605(2)	O(1)–T(2)–O(3)	108.53(4)
	– O(3)	1.608(3)	O(1)–T(2)–O(5)	104.68(12)
	– O(5)	1.646(2)	O(2)–T(2)–O(3)	112.75(6)
	Average	1.617(3)	O(2)–T(2)–O(5)	105.93(12)
			O(3)–T(2)–O(5)	110.74(3)
T(3)	– O(1)	1.735(4)	O(1)–T(3)–O(2)	108.16(4)
	– O(2)	1.735(3)	O(1)–T(3)–O(3)	112.32(6)
	– O(3)	1.730(2)	O(1)–T(3)–O(4)	104.44(13)
	– O(4)	1.746(2)	O(2)–T(3)–O(3)	114.65(6)
	Average	1.737(3)	O(2)–T(3)–O(4)	111.72(4)
			O(3)–T(3)–O(4)	105.10(13)

(b) M–O interatomic distances.

Atoms		Distance (Å)
NaCaK	– O(1)	2.357(3)
	– O(2)	2.535(3)
	– O(3)	2.504(3)
	– O(4)	2.755(3)
	– O(4′)	2.819(5)
	– O(5)	2.886(8)
	– O(7)	2.577(4)
	– O(7′)	2.396(3)
	Average	2.604(4)

arcless type goniometer-head, and set on the intensity measuring instrument. The X-ray diffraction intensity measurements were made on a Rigaku AFC-5R diffractometer with graphite monochromated Mo$K\alpha$ radiation (50 kV, 200 mA) at the X-ray Laboratory of Okayama University. 1511 reflections were collected, of which 1271 were of unique intensity. Lorentz and polarization corrections were applied. The absorption correction for the intensities based on the ψ-scan method was also applied.

The lattice constants were determined as a=12.122(2); c=7.585(2) Å by 20 peaks that have $2\theta > 50°$ and $F_{obs}>150$ with a tetragonal restricted least-square refinement program. The Laue symmetry was determined as $P4/m$ from the collected intensities. The reflection conditions were $hk0$ with $h+k=2n$ and $00l$ with $l=2n$. The probable space group is $P4_2/n$. The statistical test for centrosymmetry proposed by Wilson (1949) and Howells *et al.* (1950) was carried out using a computer program WILSON (Yamakawa and Kawahara, personal communication). Results of this statistical procedure correspond to a centric distribution. Therefore, the space group of the sample was determined as $P4_2/n$.

The initial trial structure model was derived from the intensities using the direct method program MULTAN (Main *et al.*, 1978). Diagonal least-square refinment with an isotropic temperature factor was used to refine the trial model using the program RSDLS3 (Sakurai, 1971). Difference Fourier syntheses were calculated for the trial model to determine the rest of the structure.

Full-matrix least square refinement with isotropic temperature factors and unit weighting scheme was performed by RSFLS4 (Sakurai, 1971) and gave a residual [$R = \Sigma||F_o|-|F_c||/\Sigma|F_o|$] of 0.079 (unweighted) based on $P4_2/n$.

A table of F_{obs} values is listed in Table 1. The refined parameters are listed in Table 2.

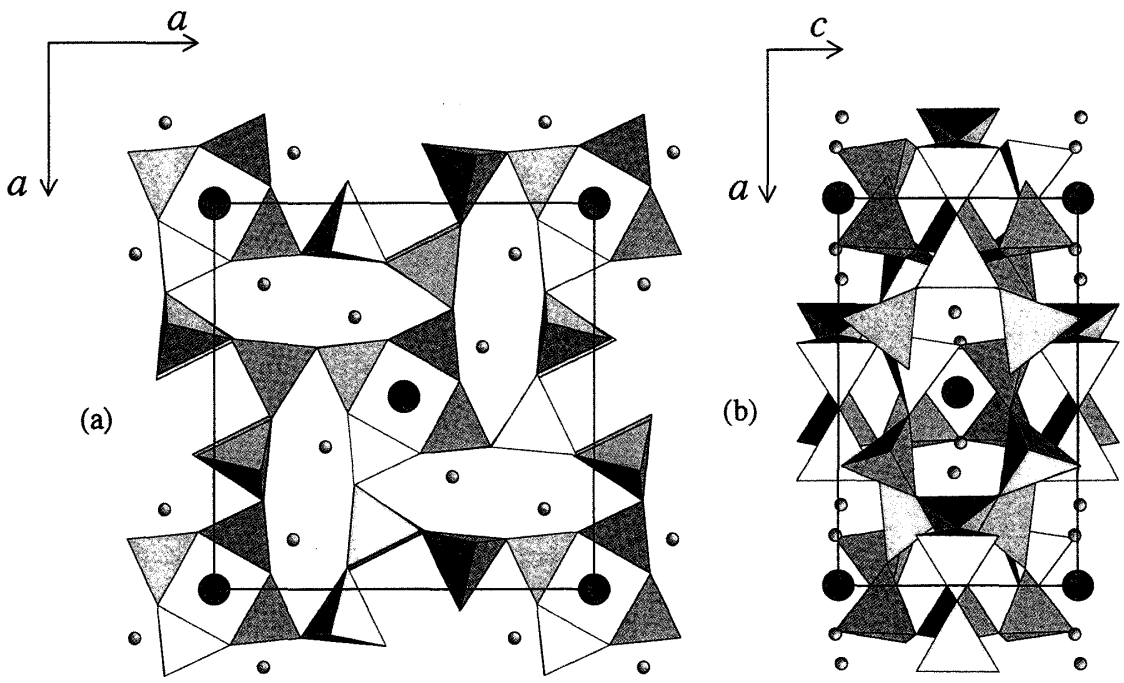

Fig. 5. The crystal structure of scapolite A97122403A. (a) along c-axis. (b) along a-axis. Large spheres represent Cl and CO_3 sites, small spheres represent Na, Ca, K sites and tetrahedra represent TO_4 units.

The bond lengths and angles are in Table 3. The crystal strucure is illustrated in Fig. 5a and b.

4. Discussion

The cell parameters a and c of Me_{39} agaisnt Si apfu are plotted with the trend of cell parameter reported by Teertstra and Sherriff (1996) in Fig. 6a and 6b respectively. The cell parameters of the sample agree approximately with those trend, but the c cell edge is slightly larger than the trend. The c cell edges of the trend are scatterd at intermediate Si apfu region. Therefor, the larger c cell edge of the sample is considered as statistically reasonable one

The space group of Me_{39} is determined as $P4_2/n$. This is the same as the result of Me_{33} (Levien and Papike, 1976). Therefore, the space group of natural scapolites that have intermediate compositions are $P4_2/n$ rather than $I4/m$. The space group of the sample against the Me percentage is showed in Fig. 7. with other single crystal X-ray structural studies. Figure 7 indicates the possibility of the fact that the space group of scapolites that have intermediate Me percentages are $P4_2/n$. But there is insufficient structural data

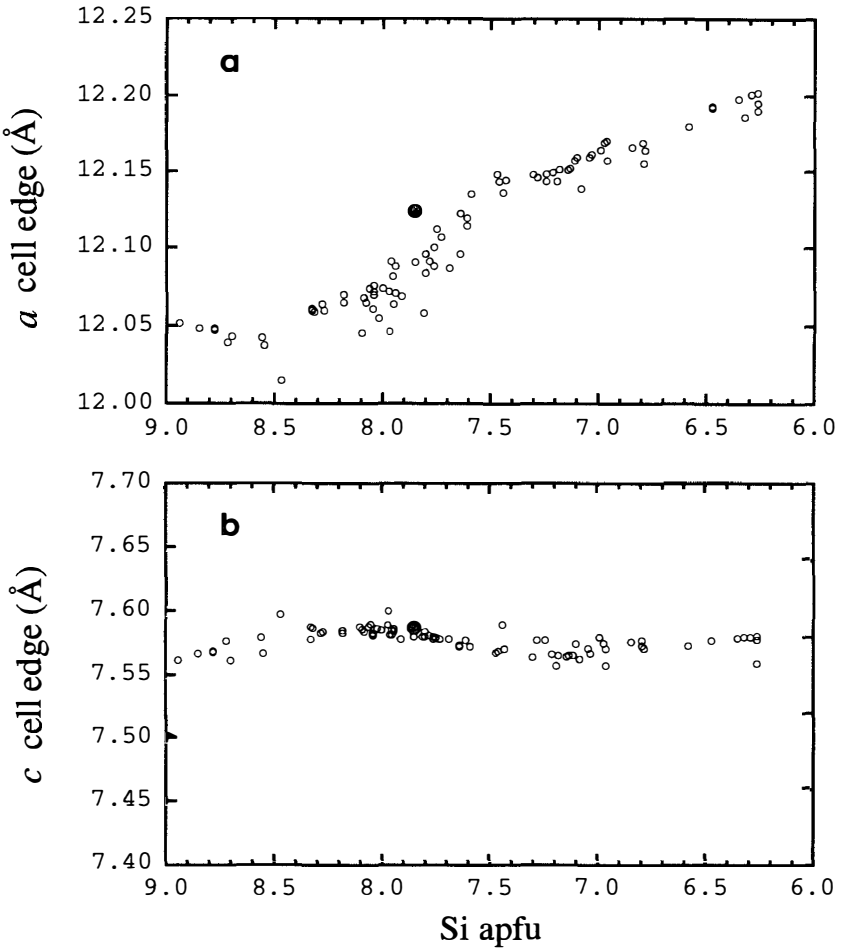

Fig. 6. Plots of (a) a cell edge and (b) c cell edge vs. Si apfu. The solid circle shows the cell parameter of this work. The open circles show the compiled data after Teertstra and Sherriff (1996).

to solve the problem.

The crystal structure of Me_{39} is similar to that of marialite (Lin and Burley, 1973a). Significant differences were not observed. The role of the CO_3 group in the sample is not conclusive because the intensity data collection maximum ($2\theta \leq 55°$, Mo$K\alpha$) is insufficient for the detailed argument. In spite of some limitation, the group seemes to be similar to that described as mizzonite (Papike and Stephenson, 1966). Positionally, the CO_3 group is mainly disorderd on the *xy* plane, though it could tilt slightly from this plane, as indicated by the very high thermal factors of Cl and O(7).

The important interatomic distances and angles are listed in Tables 2a and b. Using the average (Si,Al)-O bond length of the three types of tetrahedra (Table 2a) and the curve of Smith and Bailey (1963), the Al, Si occupancy of each tetrahedral site is estimated as follows: T(1) (4% Al, 96% Si); T(2) (6% Al, 94% Si); T(3) (92% Al, 8% Si). The Si content in the unit cell derived from the crystal structure analysis is found to be 7.92 apuf (atoms per unit formular). The other curve of Jones (1968) is also used, and the occupancies were estimated as: T(1) (6% Al, 94% Si); T(2) (9% Al, 91% Si); T(3) (85% Al, 15% Si). The Si content is found to be 7.99 apuf. These are consistent with the unit-cell content by EPMA analysis of 7.85.

The empirical bond valences (Brown and Shannon, 1973) were calculated with parameters of Brown and Wu (1976) for T- and M-site atoms. The valences for the T-site

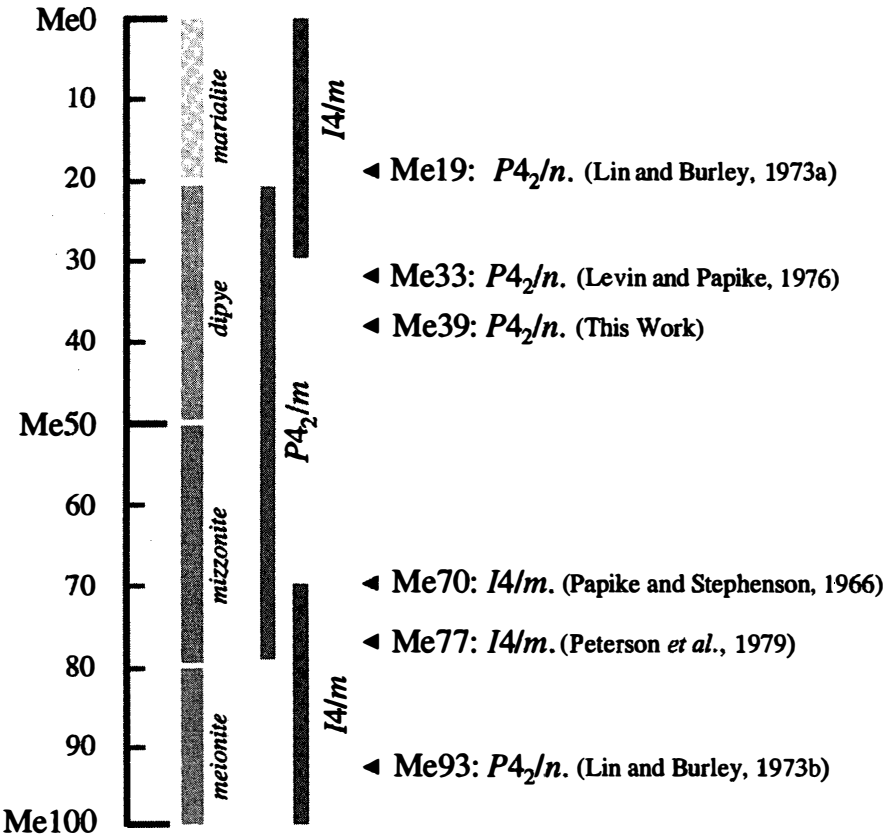

Fig. 7. Space group variation vs. meionite percentage for scapolite solid solution series. The Me percentages are calculated by 100×(Ca+Sr+Fe+Mn+Mg)/(N a+K+Ca+Sr+Fe+Mn+Mg).

were determined as follows: T(1) (4.095); T(2) (4.058); T(3) (2.986). These are also consistent with the site occupancy. For the M-site, the valence was determined as 1.109 with the 8-coordinates. It was also consistent with the site occupancy of chemical composition by EPMA analyses.

Peterson *et al.* (1979) refined the crystal structure of a Me_{77} scapolite and reported the *R* value of 0.029 (unweighted) with 2280 reflexions. They analyzed that the disorderd CO_3^{2-} and SO_2^{2-} in anion site. We also concern with the disorder of those anions in Me_{39} scapoilite from Antarctica. This is the subject for a future study.

Acknowledgments

We would like to sincerely thank all members of JARE-39. Thanks are also due to all crew members of icebreaker *Shirase* for their help during the helicopter operation. Profs. K. Shiraishi and H. Ishizuka and Dr. Y. Motoyoshi are much appreciated for their encouragement for the severe field work.

References

Brown, J.B. and Shannon, R.D. (1973): Empirical bond-strength-bond-length curves for oxides. Acta. Cryst., **A29**, 266–282.

Brown, I.D. and Wu, K.K. (1976): Empirical parameters for calculating cation-oxygen bond valences. Acta. Cryst., **B32**, 1957–1959.

Hiroi, Y., Shiraishi, K., Motoyoshi, Y. and Katsushima, T. (1987): Progressive metamorphism of calc-silicate rocks from the Prince Olav and Soya Coasts, East Antarctica. Proc. NIPR Symp. Antarct. Geosci., **1**, 73–97.

Howells, E.R., Philips, D.C. and Rodgers, D. (1950): The probability distribution of x-ray intensities. II. Experimental investigation and x-ray detection of centres of symmetry. Acta Cryst., **3**, 210–214.

Jones, J.B. (1968): Al-O and Si-O tetrahedral distances in aluminosilicate framework structures. Acta Cryst., **B24**, 355–358.

Kusachi, I., Osanai, Y., Toyoshima, T., Owada, M., Tsunogae, T., Hokada, T. andCrowe, W.A. (1999): Mineralogy of scapolite from Skallen in the Lützow-Holm Bay region, East Antarctica. Polar Geosci., **12**, 143–156.

Levien, L. and Papike, J.J. (1976): Scapolite crystal chemistry: aluminum-silicon distributions, carbonate group disorder, and thermal expansion. Am. Mineral., **61**, 864–877.

Lin, S.B. and Burley, B.J. (1973a): Crystal structure of a sodium and chlorine-rich scapolite. Acta Cryst., **B29**, 1272–1278.

Lin, S.B. and Burley, B.J. (1973b): The crystal structure of meionite. Acta Cryst., **B29**, 2024–2026.

Main, P., Woolfson, M.M. and Germain, G. (1978): MULTAN: A Computer Program for the Automatic Solution of Crystal Structures. University of York.

Papike, J.J. and Stephenson, N.C. (1966): The crystal structure of of mizzonite, a calcium- and carbonate-rich scapolite. Am. Mineral., **51**, 1014–1027.

Peterson, R.C., Donnay, G. and Lepage, Y. (1979): Sulfate disorder in scapolite. Canad. Mineral., **17**, 53–61.

Sakurai, T. (1971): UNICS: Universal Crystallographical Computation Program System. Tokyo, Crystallographical Society of Japan.

Smith, J.V. and Bailey, S.W. (1963): Second review of Al-O and Si-O Tetrahedral distances. Acta Cryst., **16**, 801–811.

Teertstra, D.K. and Sherriff, B.L. (1996): Scapolite cell-parameter trends along the solid-solution series. Am. Mineral., **81**,169–181.

Wilson, A.J.C. (1949): The probability distribution of X-ray intensities. Acta Cryst., **2**, 318–321.

(Received February 5, 2001; Revised manuscript accepted May 16, 2001)