

れ程大きなものではなかったと考えて問題はない。

寒霞溪火山岩類の活動が、中期中新世に起ったこと、土庄層群が、下部中新統最上部であることを考慮すると、坂手火山岩類は、中期中新世前期の活動であろう。これは、坂手火山岩類の古江流紋岩より分離したジルコンから得られた群色のデータ(宮地・唐木田, 1977及び私信)とも矛盾しない。

## 5. 謝 辞

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## STRUCTURE OF CaScAlSiO<sub>6</sub>-PYROXENE

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The crystal structure of CaScAlSiO<sub>6</sub>-pyroxene grown by the floating zone method has been refined by the least squares method using 680 reflections measured on an automatic single crystal diffractometer. The unweighted R factor is 0.020 for 587 unrejected reflections. The cell dimensions are:  $a_0=9.884\text{\AA}$ ,  $b_0=8.988\text{\AA}$ ,  $c_0=5.446\text{\AA}$ ,  $\beta=105.86^\circ$ , and  $V=465.43\text{\AA}^3$ ; space group C2/c. The average T-O, M1-0 and M2-0 distances are 1.695\AA, 2.102\AA and 2.513\AA, respectively. The structure is isomorphous with those of already reported Ca-Tschermak's pyroxenes, CaAl<sub>2</sub>SiO<sub>6</sub> and CaFeAlSiO<sub>6</sub>. The octahedral (M1) site is occupied by Sc. Within the tetrahedral (T) site, Si and Al ions are completely disordered.

## INTRODUCTION

From the viewpoint of crystal structure, Ca-bearing clinopyroxenes are grouped into two series (Ohashi, 1978b). One of them is Si-saturated type and the other is Tschermak's molecule type. The Tschermak's molecule type pyroxene has a M2 site coordinated by 8 oxygen atoms more evenly bonded to Ca<sup>2+</sup> than in Si-saturated type pyroxene. This characteristic structure may be found in CaScAlSiO<sub>6</sub>-pyroxene. It is generally possible for trivalent cations to occupy octahedral sites and tetrahedral sites in Tschermak's molecule type pyroxene. But, in the case of CaScAlSiO<sub>6</sub>-pyroxene, it is expected that the octahedral sites are occupied by Sc ions and the tetrahedral sites by Al and Si ions from the large differences in the ionic radius among them (Ohashi, 1978a).

## SYNTHESIS OF CaScAlSiO<sub>6</sub> SINGLE CRYSTALS

CaScAlSiO<sub>6</sub>-pyroxene melts incon-

gruently to Sc<sub>2</sub>O<sub>3</sub> and liquid at about 1534°C (Ohashi, 1978a). The single crystals were grown by the floating zone method using an apparatus of an infrared radiation convergence type with a 1.5 kw quartz halogen lamp as the radiation source (Ii and Ohashi, unpublished data). The maximum solubility of CaAl<sub>2</sub>SiO<sub>6</sub> in CaScAlSiO<sub>6</sub>-pyroxene at 1 atm is about 32 mol% at about 1400°C. The cell dimensions of the pyroxene solid solution are found to change linearly against the change of mol% along the join CaScAlSiO<sub>6</sub>-CaAl<sub>2</sub>SiO<sub>6</sub> (Ohashi, 1978b). The chemical composition of the crystal chosen for structure analysis was determined from the cell volume as Ca<sub>1.0</sub>Sc<sub>0.99</sub>Al<sub>1.01</sub>Si<sub>1.0</sub>O<sub>6</sub>. For the purposes of structure determination, however, we have assumed the ideal composition CaScAlSiO<sub>6</sub>.

## MEASUREMENT OF INTENSITY DATA AND REFINEMENT OF THE STRUCTURE

From x-ray Weissenberg photographs, the space group was determined to be C2/c. For the intensity measurements, which were

carried out at room temperature, several spherical specimens were prepared. A single crystal sphere of radius 0.07 mm showing the best crystallinity as judged by a transmission Laue photograph was mounted on a computer controlled single-crystal diffractometer (Philips PW 1100). The unit-cell dimensions were obtained by the least squares method based on  $\sin \theta$  measured on the diffractometer. The cell dimensions are; a 9.884 (2), b 8.988 (1), c 5.446 (1) Å,  $\beta$  105.86 (1); V 465.43 Å<sup>3</sup>; Z 4. The calculated density is 3.37 g/cm<sup>-3</sup>.

The intensities were collected on the same diffractometer, scan speed being 3°/min. In the range of  $2\theta \leq 60^\circ$ , 680 reflections were measured.

The observed intensities were corrected for Lorentz, polarization and monochromator polarization factors. No absorption corrections were made. Judging from the size ( $r=0.07$  mm) and its spherical form of the specimen crystal the effect was considered to be small enough for negligence. The least squares refinement was based on

592 Fo values above  $2\sigma(\text{Fo})$ , where  $\sigma(\text{Fo})$  was the standard deviation. The structure refinement was made on a HITAC 8800/8700 computer, employing the MINEPAC system (Miyamoto, Takeda and Takano, 1974). Initial positional parameters, with isotropic temperature factors, were taken from those of CaAl<sub>2</sub>SiO<sub>6</sub> (Okamura, Ghose and Ohashi, 1974). The atomic scattering factors were those given by Cromer and Mann (1968) for ionized cations and 0<sup>-1</sup>. Anomalous dispersion corrections were made by using the coefficients of Cromer and Liberman (1970). The chemical composition has been constrained to CaScAlSiO<sub>6</sub>. At the earlier stage of the refinement, isotropic temperature factors were used, while the site occupancies were varied. After convergence was reached in the refinement with isotropic temperature factors, three cycles of refinement using anisotropic temperature factors were employed. At this stage reflections  $\text{Fo} < 30$  and  $\frac{\Delta F}{\sigma F} > 5.0$  were rejected from the refinement. The unweigh-

Table 1. Atomic parameters of CaScAlSiO<sub>6</sub>

	X	Y	Z	B eq	$\beta_{11}$	$\beta_{22}$
M1 (Sc)	0	.90431 (4)	1/4	.446 (10)	.00134 (5)	.00129 (5)
M2 (Ca)	0	.31236 (5)	1/4	.729 (10)	.00266 (5)	.00176 (5)
T (Al+Si)	.29057 (5)	.09199 (4)	.23218 (8)	.378 (10)	.00104 (5)	.00123 (5)
O1	.11283 (12)	.08975 (11)	.13842 (21)	.634 (18)	.00210 (12)	.00187 (12)
O2	.36548 (12)	.25503 (13)	.33043 (22)	.756 (18)	.00241 (12)	.00213 (12)
O3	.35306 (11)	.02108 (13)	.99366 (20)	.753 (20)	.00181 (12)	.00262 (14)

Table 1. (Continued)

$\beta_{33}$	$\beta_{12}$	$\beta_{13}$	$\beta_{23}$
.00372 (15)	0	.00035 (6)	0
.00463 (15)	0	-.00025 (6)	0
.00308 (15)	-.00009 (3)	.00028 (6)	-.00011 (6)
.00483 (37)	.00015 (9)	.00081 (17)	.00024 (15)
.00660 (35)	-.00023 (9)	.00121 (16)	.00049 (17)
.00703 (43)	.00001 (9)	.00111 (17)	-.00079 (16)

Table 2. Bond lengths and bond angles of CaScAlSiO<sub>6</sub>

Bond Length		Bond Angle	
Atom	Value (Å)	Atom	Value (°)
Octahedron (M1)			
M1-O1A1, B1	2.182 (1)	O-M1-O angles	
-O1A2, B2	2.105 (1)	O1A2, O1B2	177.09 (6)
-O2C1, D1	2.019 (1)	(2)O1A1, O2D1	169.99 (5)
mean of 6	2.102	O1A1, O1B1	80.39 (6)
		O2C1, O2D1	96.73 (7)
O1A1-O1B1	2.817 (2)	(2)O1A1, O2C1	91.73 (4)
O2C1-O2D1	3.019 (2)	(2)O1A1, O1A2	95.15 (4)
(2)O1A1-O2C1	3.018 (2)	(2)O1A1, O1B2	82.62 (5)
(2)O1A1-O1A2	3.165 (1)	(2)O1A2, O2C1	92.03 (5)
(2)O1A2-O2C1	2.968 (2)	(2)O1A2, O2D1	89.90 (4)
(2)O1A2-O2D1	2.915 (2)	T-O1A1-M1	121.65 (6)
(2)O1A1-O1B2	2.831 (2)	T-O1A2-M1	119.54 (6)
mean of 12	2.969	T-O2C1-M1	141.02 (7)
M1-M1	3.221 (1)		
M1-TA1	3.355 (1)		
M1-TA2	3.320 (1)		

Table 2. (Continued)

Bond Length		Bond Angle	
Atom	Value (Å)	Atom	Value (°)
Polyhedron (M2)			
M2-O1A1, O1B1	2.447 (1)	O1A1, O1B1	70.28 (5)
-O2C2, O2D2	2.387 (1)	O2C2, O2D2	150.59 (6)
-O3C1, O3D1	2.543 (1)	O3C1, O3D1	84.95 (5)
-O3C2, O3D2	2.677 (1)	O3C2, O3D2	111.98 (5)
mean of 6	2.459	(2)O1A1, O2C2	81.82 (4)
mean of 8	2.513	(2)O1A1, O3C1	120.58 (4)
		(2)O1A1, O3C2	89.33 (4)
O1A1-O1B1	2.817 (2)	(2)O2C2, O3C1	64.95 (4)
O3C1-O3D1	3.435 (2)	(2)O2C2, O3C2	112.38 (4)
(2)O1A1-O2D2	2.915 (2)	(2)O3C1, O3C2	63.50 (2)
(2)O1A1-O2C2	3.166 (2)	(2)O1A1, O2D2	74.16 (4)
(2)O1A1-O3C2	3.605 (2)	(2)O1A1, O3D1	134.22 (4)
(2)O2C2-O3C1	2.771 (2)	(2)O1A1, O3D2	157.88 (4)
(2)O2C2-O3D2	3.409 (2)	(2)O2C2, O3D2	84.44 (4)
(2)O3C1-O3C2	2.749 (1)	(2)O3C1, O3D2	67.74 (4)
(2)O3C1-O3D2	2.911 (2)	(2)O2C2, O3D1	142.93 (4)
Tetrahedron (Si, Al)			
T-O1	1.690 (1)	O1-T-O2	116.25 (6)
T-O2	1.663 (1)	O1-T-O3A1	109.15 (6)
mean, non-brg.	1.677	O1-T-O3A2	110.57 (6)
T-O3A1	1.707 (1)	O2-T-O3A1	110.61 (6)
T-O3A2	1.721 (1)	O2-T-O3A2	103.10 (6)
mean, brg.	1.714	O3A1-T-O3A2	106.65 (4)
mean of 4	1.695	mean of 6	109.39
O1-O2	2.848 (2)	T-O3-TA2	136.68 (7)
O1-O3A1	2.768 (2)	O3A2-O3A1-O3A2	164.16 (10)
O1-O3A2	2.804 (2)		
O2-O3A1	2.771 (2)		
O2-O3A2	2.650 (2)		
O3A1-O3A2	2.749 (1)		
mean of 6	2.765		
T-TA2	3.186 (1)		

Table 3. Thermal ellipsoids of CaScAlSiO<sub>6</sub>

Atom	Axis	rms amplitude, Å	Angle (°) with a	Angle (°) with b	Angle (°) with c
M1	1	0.071	71 (5)	90	35 (5)
	2	0.073	90	180	90
	3	0.082	161 (5)	90	55 (5)
M2	1	0.076	73 (1)	90	32 (1)
	2	0.085	90	180	90
	3	0.122	163 (1)	90	58 (1)
T	1	0.063	64 (6)	71 (7)	47 (7)
	2	0.071	69 (21)	38 (20)	125 (14)
	3	0.073	35 (16)	121 (22)	117 (16)
O1	1	0.080	90 (8)	115 (16)	30 (16)
	2	0.088	74 (10)	150 (15)	118 (16)
	3	0.099	16 (10)	76 (10)	99 (8)
O2	1	0.085	112 (6)	139 (6)	51 (7)
	2	0.100	104 (14)	119 (10)	137 (9)
	3	0.107	26 (10)	116 (9)	104 (12)
O3	1	0.088	142 (25)	65 (13)	50 (17)
	2	0.093	127 (26)	116 (14)	118 (19)
	3	0.111	95 (5)	142 (6)	53 (6)

(weighted  $R=0.027$ ) for 587 unrejected reflections. The final parameters with standard deviations are listed in Table 1. Bond lengths and angles as well as ellipsoids of thermal vibration with standard deviations are listed in Tables 2 and 3, respectively.

## DESCRIPTION OF THE STRUCTURE

The structure of CaScAlSiO<sub>6</sub>-pyroxene is isomorphous with other Tschermak's molecule type pyroxenes. The variation of the

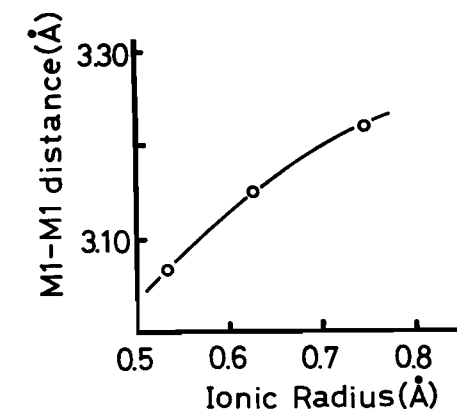


Fig. 1. Variation of the nearest M1-M1 distance (Å) with the radius (Å) of the cation occupying the M1 site for the refined Tschermak's molecule type pyroxenes (CaAl<sub>2</sub>SiO<sub>6</sub>, CaFeAlSiO<sub>6</sub> and CaScAlSiO<sub>6</sub>).

ted R-factor is 0.023 and the weighted R-factor is 0.037 for 592 reflections and 0.020

nearest M1-M1 distance with the radius of the cation occupying the M1 site for the refined Tschermak's molecule type pyroxene structures (CaAl<sub>2</sub>SiO<sub>6</sub>-pyroxene: Okamura, Ghose and Ohashi, 1974; CaFeAlSiO<sub>6</sub>-pyroxene: Okamura, Ghose and Ohashi, unpublished data) is shown in Fig. 1. A smooth curve can be drawn through those points representing the Al, 0.82Fe+0.18Al and Sc members. In the Tschermak's molecule type pyroxene, the M2-site is coordinated by 8 oxygen atoms more evenly bonded to Ca<sup>2+</sup> than in Si-saturated type pyroxene. The variation of mean 8(M2-0) and 6(M2-0) with mean 6(M1-0) for the Tschermak's molecule type pyroxene structures is shown in Fig. 2.

As shown by the results of the refinements (Table 1), the tetrahedral sites are occupied by Al and Si in the CaScAlSiO<sub>6</sub>-pyroxene. As expected from ionic radius (Ohashi, 1978a), there is no evidence for the presence of Sc in the tetrahedral site. Al-Si are completely disordered in the tetrahedral site. The T-O distances and the O<sub>3</sub>-O'<sub>3</sub>-O''<sub>3</sub> angles in three Tschermak's molecule type pyroxenes are shown in Table 4.

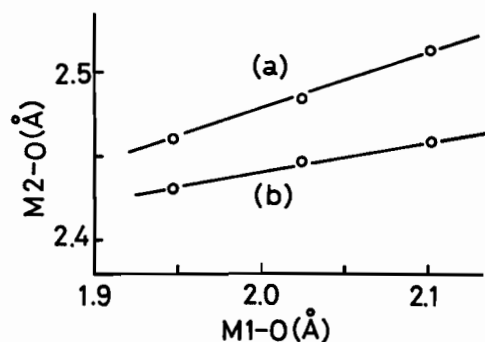


Fig. 2. (a) Mean 8(M2-0) and (b) mean 6(M2-0) distances plotted against mean 6(M1-0) distances in Tschermak's molecule type pyroxenes (CaAl<sub>2</sub>SiO<sub>6</sub>, CaFeAlSiO<sub>6</sub> and CaScAlSiO<sub>6</sub>). (Ohashi 1978b)

Table 4. The T-O distances (Å) and the O<sub>3</sub>-O'<sub>3</sub>-O''<sub>3</sub> angles (°) in three Tschermak's molecule type pyroxenes

	CaAl <sub>2</sub> SiO <sub>6</sub>	CaFeAlSiO <sub>6</sub>	CaScAlSiO <sub>6</sub>
T-O1	1.693(1)	1.695(1)	1.690(1)
T-O2	1.665(1)	1.671(1)	1.663(1)
mean, non-brg.	1.679	1.683	1.677
T-O3A1	1.683(1)	1.703(1)	1.707(1)
T-O3A2	1.701(1)	1.722(1)	1.721(1)
mean, brg.	1.692	1.713	1.714
mean of 4	1.686	1.698	1.695
O3A2-O3A1-O3A2	165.93(6)	164.35(5)	164.16(10)

CaScAlSiO<sub>6</sub>-pyroxene has a shortest non bridging T-O, a longest bridging T-O and a smallest O<sub>3</sub>-O'<sub>3</sub>-O''<sub>3</sub> angle among them. However, the non bridging T-O is nearly equal to that of CaAl<sub>2</sub>SiO<sub>6</sub>-pyroxene and supports the results that the non bridging T-O distances is a linear function of Al/(Al+Si) ratio in tetrahedral site in several C2/c pyroxenes and sillimanite (Takeda, 1972; Okamura, Ghose and Ohashi, 1974).

## DISCUSSION

The maximum solubility of CaAl<sub>2</sub>SiO<sub>6</sub> in CaScAlSiO<sub>6</sub>-pyroxene at 1 atm is about 32 mol% at about 1400°C. It is pointed out that this large solubility can be attributed to the similarity of the structure between CaScAlSiO<sub>6</sub> and CaAl<sub>2</sub>SiO<sub>6</sub> (Ohashi, 1978b). The Tschermak's molecule type pyroxene has a M2 site coordinated by 8

Table 5. The maximum solubilities of CaAl<sub>2</sub>SiO<sub>6</sub> and the ratios of mean 6(M2-0) and mean 8(M2-0) in some clinopyroxenes

	The max. sol. (mol%)	mean of 6(M2-0)	mean of 8(M2-0)	The ratio of 6/8
NaFeSi <sub>2</sub> O <sub>6</sub>	6	2.414	2.518	0.959
CaMgSi <sub>2</sub> O <sub>6</sub>	12	2.425	2.498	0.971
CaScAlSiO <sub>6</sub>	32	2.459	2.513	0.979
CaFeAlSiO <sub>6</sub>		2.447	2.484	0.985
CaAl <sub>2</sub> SiO <sub>6</sub>		2.431	2.461	0.988

(Ref. Ohashi, 1978b)

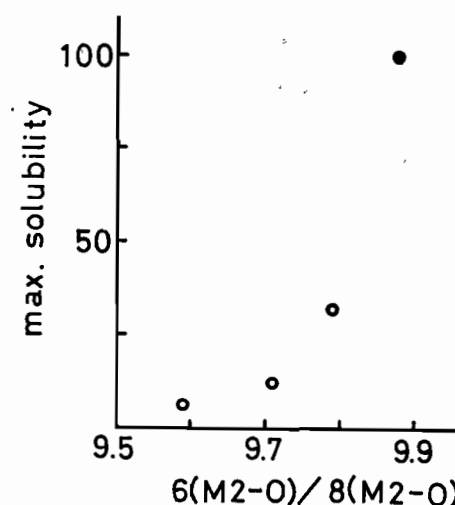


Fig. 3. Variation of the maximum solubility of CaAl<sub>2</sub>SiO<sub>6</sub> in some pyroxenes (NaFeSi<sub>2</sub>O<sub>6</sub>, CaMgSi<sub>2</sub>O<sub>6</sub> and CaScAlSiO<sub>6</sub>) and the ratio of mean 6(M2-0) and mean 8(M2-0) of the host pyroxenes.

oxygen atoms more evenly bonded to Ca<sup>2+</sup> than in Si-saturated type pyroxene. The maximum solubilities of CaAl<sub>2</sub>SiO<sub>6</sub> in some pyroxenes are listed in Table 5. The variation of the maximum solubility of CaAl<sub>2</sub>SiO<sub>6</sub> with the ratio of the mean 6(M2-0) and the mean 8(M2-0) of the host pyroxene is shown in Fig. 3. The maximum solubility of CaAl<sub>2</sub>SiO<sub>6</sub> is high in the host pyroxene having CaAl<sub>2</sub>SiO<sub>6</sub>-pyroxene like M2-O<sub>8</sub> polyhedron.

It is known that the maximum solubilities of CaAl<sub>2</sub>SiO<sub>6</sub> in some pyroxenes increase with increasing pressure (Clark, Schairer and Neufville, 1962; Yoshikawa, 1975). Now, from these facts, although details can not be discussed until a series of experimental studies on CaMgSi<sub>2</sub>O<sub>6</sub> or other Si-saturated pyroxenes using high pressure X-ray single crystal diffractometer, it is possible to consider that the geometrical feature of M2-O<sub>8</sub> polyhedron in the Si-saturated C2/c-pyroxenes becomes similar

to that of the Tschermak's molecule type pyroxenes at high pressure. There are two structure data supporting this consideration. The crystal structures of two pyroxenes having the chemical compositions between Si-saturated type and Tschermak's molecule type have been reported (Oka-pyroxene: Peacor, 1967; Allende-pyroxene: Dowty and Clark, 1973). Their chemical compositions, averaged radii of ions occupying the M1-sites, mean 6(M1-0), 6(M2-0) and 8(M2-0) distances are listed in Table 6. The variation of the mean 6(M1-0) distances with the averaged ionic radii of ions occupying the M1-sites is shown in Fig. 4. The variation of the mean 6(M2-0) and 8(M2-0) distances with 6(M1-0) distances

Table 6.

Oka Al-pyroxene (Peacor 1967)				
Number of ions per six oxygen atoms	Ionic radius (Å)			
Si	1.51 (T)			
Al	0.49	2.00	(standard)	(weighted)
Al	0.17		0.535	0.091
Ti	0.07		0.605	0.042 (averaged)
Fe <sup>+3</sup>	0.16 (M1)		0.645	0.103 0.673
Fe <sup>+2</sup>	0.06	1.03	0.780	0.047
Mg	0.57		0.720	0.410
Mn	0.01		(total) 0.693	
Ca	0.98 (M2)			
Na	0.01	1.00		
Average bond distances (Å)				
6(M1-0) 2.069; 6(M2-0) 2.440; 8(M2-0) 2.504;				

Table 6. (Continued)

Allende pyroxene (Dowty and Clark 1973)				
Number of ions per six oxygen atoms	Molecular composition		Ionic radius (Å)	
Si	1.26	CaMgSi <sub>2</sub> O <sub>6</sub>	0.39	(standard) (Weighted)
Al	0.74	CaAl <sub>2</sub> SiO <sub>6</sub>	0.13	Mg 0.720 0.281
Al	0.13	CaTiAlSiO <sub>6</sub>	0.35	Al 0.535 0.070
Ti <sup>+3</sup>	0.35	CaTiAl <sub>2</sub> O <sub>6</sub>	0.13	Ti <sup>+3</sup> 0.670 0.235
Ti <sup>+4</sup>	0.13			Ti <sup>+4</sup> 0.605 0.079
Mg	0.39			(averaged)
Ca	1.00			0.665
Average bond distances (Å)				
6(M1-0) 2.059; 6(M2-0) 2.448; 8(M2-0) 2.500;				

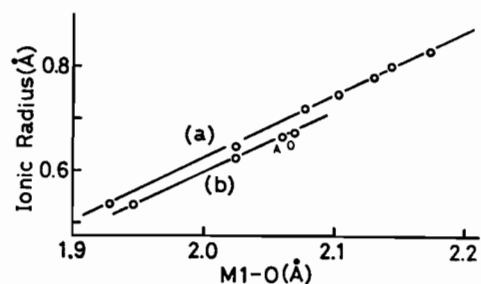


Fig. 4. Variation of the ionic radii and mean (M1-O) distances in some pyroxenes. (a): Si-saturated type, (b): Tschermak's molecule type. A: Allende, O: Oka. (Ohashi, 1978b)

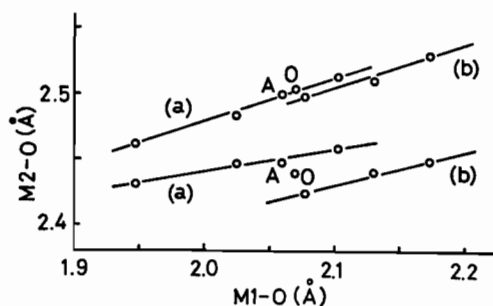


Fig. 5. Mean 8(M2-O) and mean 6(M2-O) distances plotted against mean 6(M1-O) distances in calcium pyroxenes. (a): Tschermak's molecule type, (b): Si-saturated type. A: Allende, O: Oka. (Ohashi, 1978b)

is shown in Fig. 5. The mean 6(M1-O) and 8(M2-O) distances of the two pyroxenes are plotted on a line belonging to Tschermak's molecule type pyroxene structure and the mean 6(M2-O) distances are plotted in an intermediate region between the Si-saturated type and Tschermak's molecule type. From these facts it is concluded that the structure of the calcium pyroxene solid solution with high tetrahedral Al content is like to that of Tschermak's molecule type pyroxene.

From the view point of thermochemistry,  $\text{CaAl}_2\text{SiO}_6$ - $\text{CaMgSi}_2\text{O}_6$  pyroxene solid solution are grouped into two classes (New-

ton, Charlu and Kleppa, 1977). One of them is  $\text{CaAl}_2\text{SiO}_6$  rich solid solution. The other is  $\text{CaMgSi}_2\text{O}_6$  rich solid solution. Newton et. al. (1977) assumed a local charge balance type ( $\text{CaAl}_2\text{SiO}_6$  rich type) and a complete disorder type ( $\text{CaMgSi}_2\text{O}_6$  rich type) in the  $\text{CaAl}_2\text{SiO}_6$ - $\text{CaMgSi}_2\text{O}_6$  pyroxene solid solution. However, the existence of a complete disorder type is doubtful. Because, it is considered that the reason why  $\text{CaAl}_2\text{SiO}_6$ -bearing solid solution are stable at 1 atm depends on the  $\text{Al}^{\text{IV}}\text{-O-Al}^{\text{VI}}$  coupling (Ohashi, 1978b). It is possible to consider that the existence of two types in  $\text{CaAl}_2\text{SiO}_6$ - $\text{CaMgSi}_2\text{O}_6$  pyroxene solid solution depends on the structural differences. That is, the  $\text{CaAl}_2\text{SiO}_6$  rich type can have the mean 6(M1-O) and 8(M2-O) distances belonging to Tschermak's molecule type structure and the  $\text{CaMgSi}_2\text{O}_6$  rich type can have the intermediate distances belonging to the structure between the Tschermak's molecule type and Si-saturated type.

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#### $\text{CaScAlSiO}_6$ 輝石の構造

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帯域融法によってつくった  $\text{CaScAlSiO}_6$  輝石の結晶造をリファインした。格子常数は  $a_0=9.884\text{Å}$ ,  $b_0=8.988\text{Å}$ ,  $c_0=5.446\text{Å}$ ,  $\beta=105.86^\circ$ ,  $V=465.43\text{Å}^3$  で、空間群は  $C2/c$  である。

T-O, M1-O 及び M2-O の平均距離は、それぞれ  $1.695\text{Å}$ ,  $2.102\text{Å}$  及び  $2.513\text{Å}$  である。 $\text{CaScAlSiO}_6$  輝石の構造は、 $\text{CaAl}_2\text{SiO}_6$  や  $\text{CaFeAlSiO}_6$  などの Ca-チェルマックス輝石と同型である。M1 サイトは Sc イオンに占められている。T サイトには Si イオンと Al イオンとが完全に無秩序に分布している。