The Structure of Partially Disordered, Synthetic Strontium Feldspar

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Abstract

The crystal structure of $SrAl_2Si_2O_8$ with a celsian-type framework structure has been refined to R=0.047 by full-matrix least-squares methods using 1058 'a'-type (h+k even, l even) and 258 much weaker 'b'-type reflections (h+k odd, l odd). The cell parameters are a=8.388 (3), b=12.974 (4), c=14.263 (6) Å, $\beta=115.2$ (1)°; the space group is I2/c.

This compound was synthesized in a Verneuil furnace from a stoichiometric mixture of $SrCO_3$, SiO_2 , and Al_2O_3 and shows a partially disordered Al/Si distribution. The mean T-O distances, $T_1O = 1.626$, $T_2Z = 1.630$, $T_1Z = 1.732$, and $T_2O = 1.735$ Å, when compared with the grand mean Si-O bond length of 1.614 Å and Al-O bond length of 1.747 Å in ordered primitive anorthite, indicate approximately 10 percent Al in the Si-rich and 10 percent Si in the Al-rich sites of this compound.

The Sr atom can be considered to be 7-coordinated, $\langle Sr-O \rangle = 2.691$ Å, or 9-coordinated, $\langle Sr-O \rangle = 2.786$ Å. These values are both 0.03 Å shorter than those reported by Grundy and Ito (1974) for a highly disordered, synthetic $(Sr_{0.84}Na_{0.03} \square_{0.13})Al_{1.7}Si_{2.3}O_8$ (space group C2/m).

Using the 7-coordinated model, there is a positive correlation of mean T-O distances to 2-, 3-, and 4-coordinated oxygen atoms and the parameter, $\sum [1/(Sr-O)^2]$, which is the sum of the inverse squares of the Sr-O distances to these oxygens:

C.N.(0)	$\frac{\text{Mean}}{\sum [1/(\text{Sr-O})^2]}$	Mean Si-O	Mean Al-O
2	0	1.610 Å	1.724 Å
3	0.137	1.632 Å	1.734 Å
4	0.287	1.644 Å	1.755 Å

Introduction

Although refinements have been published of the rubidium analog of sanidine, RbAlSi₃O₈ (Gasparin, 1971), and of the rubidium-iron analog of microcline, RbFeSi₃O₈ (Brunton, Harris, and Kopp, 1972), the crystal structures of synthetic analogs of feldspars have been largely neglected until recently. Bruno, Calleri, and Chiari (1973) reported a preliminary refinement of a partially disordered SrAl₂Si₂O₈, the strontium analog of celsian, which is the subject of this paper. This material was crystallized in a Verneuil furnace from a stoichiometric mixture of SrCO₃, SiO₂, and Al₂O₃ (Bruno and Gazzoni, 1970). Its space group is I2/c: only 'a'

(h + k even, l even) and 'b' (h + k odd, l odd) reflections were observed in X-ray photographs exposed for 72 hours.

Grundy and Ito (1974) have refined the structure of a highly disordered, synthetic feldspar, $(Sr_{0.84}Na_{0.03} \square_{0.13})Al_{1.7}Si_{2.3}O_8$, with C2/m symmetry; and Kroll and Phillips (personal communication) are presently engaged in an investigation of a synthetic $SrAl_2Si_2O_8$ which they have found to show 'a', 'b', 'c' (h + k even, l odd), and 'd' (h + k odd, l even) reflections, indicating a primitive space group and quite possibly a more highly ordered Al/Si arrangement than that observed in our $I2/c SrAl_2Si_2O_8$.

Kroll and Phillips in Münster and Calleri and Gazzoni in Torino are studying independently the crystal structures of feldspar and paracelsian analogs in the systems (Ca,Sr,Ba)[Al₂Si₂O₈]-(Ca,Sr,Ba) $[Ga_2Si_2O_8]$ and $(Ca,Sr,Ba)[Al_2Ge_2O_8]-(Ca,Sr,Ba)$ [Ga₂Ge₂O₈]. A clear picture of the crystal chemistry of $M^{2+}T_2^{2+,3+}T_2^{4+,5+}O_8$ framework structures should emerge, when the results of these analyses are combined with those from recent and present investigations of anorthite (Wainwright and Starkey, 1971), paracelsian—BaAl₂Si₂O₈ (Craig, Louisnathan, and Gibbs, 1973), its Sr analog—slawsonite (Griffen, personal communication), danburite—CaB₂Si₂O₈ (Phillips, Gibbs, and Ribbe, 1974), hurlbutite— CaBe₂P₂O₈ (Lindbloom, Gibbs, and Ribbe, 1974), celsian—BaAl₂Si₂O₈ (Griffen, personal communication), and C2/m and I2/c modifications of PbAl₂Si₂O₈ (Chiari et al, in preparation). For an analysis of the feldspar structural data accumulated through 1972, see Ribbe, Phillips, and Gibbs (1974) and the more recent review by Bruno and Facchinelli (1974).

Experimental Methods

The single crystal of $SrAl_2Si_2O_8$ used in this structural investigation was first studied by Bruno and Gazzoni (1970) who determined the lattice parameters by calibrated Weissenberg methods (Table 1). Bruno, Calleri, and Chiari (1973) reported the results of a preliminary crystal structure refinement using intensity data collected on a General Electric 3-circle diffractometer (CuK_{α} radiation) at Torino. The 768 strong 'a' and 197 weak 'b' reflections were measured at different scan rates to take into account

TABLE 1. Comparison of Unit Cell Parameters and Chemical Composition of Two Synthetic Strontium Feldspars

	Grundy	& Ito (1974)	This Paper
CELL PARAMETER			
a (Å) b (Å) c (Å)	:	8.328 12.980 7.136	8.388 12.974 2×7.132
β		115.6°	115.2°
Volume ($Å^3$)		695.7	2×702.2
Z		4	8
Space group		C2/m	12/c
COMPOSITION			
Formula	Sr ₈₄ Na ₀₃ [$^{]}.13^{\mathrm{A1}}$ 1.69 $^{\mathrm{Si}}$ 2.29 $^{\mathrm{O}}$ 8	$\mathrm{SrAl}_{2}\mathrm{Si}_{2}^{0}8$
Al/Si		0.738	1.000
A1/(A1+Si)		0.425	0.500
Calc. densit	У	2.98 g/cc	3.08 g/cc

the large difference in their average intensity, and for that reason separate scale factors had to be applied to these data. Although an isotropic refinement of the "average" structure in space group C2/m converged to R=0.10 and a partial anisotropic refinement in space group I2/c converged to R=0.058, yielding mean T-O distances of 1.626 Å for Si-rich and 1.739 Å for the Al-rich tetrahedra, the correlation matrix indicated strong interactions, especially between the scale factor of the 'b' reflections and the y coordinate of the Sr atom. As a result the thermal ellipsoids of several oxygens became non-positive definite.

For these reasons a new set of intensity data were collected at Pavia University from the same crystal on a Philips 4-circle diffractometer using graphite-monochromatized Mo radiation and a θ -2 θ step-scan procedure. Both 'a' and 'b' reflections were kept on the same scale, but the weak 'b' reflections were scanned eight times and then averaged to give improved precision. There were 1058 'a' and 258 'b' reflections whose intensities exceeded 3σ . These data were reduced in the conventional manner, although no absorption correction was applied. The crystal dimensions are $0.2 \times 0.04 \times 0.1$ mm normal to $\{100\}$, $\{010\}$, and $\{001\}$ respectively; $\mu = 86.3$ cm⁻¹.

Structure Refinement

Assuming C2/m symmetry ($c \simeq 7 \, \text{Å}$; Fig. 1a) and using the atomic coordinates of celsian (Newnham and Megaw, 1960, Table 5), we initially refined the 8-atom average structure of $SrAl_2Si_2O_8$ to R=0.089 with only the 'a' reflections. We continued the refinement in the true I2/c space group ($c \simeq 14 \, \text{Å}$; Fig. 1b) by including the 'b' reflections and introducing atomic coordinate shifts equivalent to those of I2/c celsian (Newnham and Megaw, 1960, Table 8). The Sr, $O_A(1)$, and $O_A(2)$ atoms were thus moved from special to general positions, and the three other oxygens and two tetrahedral atoms were "split" to account for the doubling of the c axis and change in space group.

Routine refinements of isotropic and anisotropic models were carried out to R=0.058 using the full-matrix least-squares program ORFLS (Busing, Martin, and Levy, 1962). On the assumption that the more intense reflections were affected by secondary extinction, several additional cycles of anisotropic refinement were run, omitting those reflections with $|F_{\rm obs}|>100$. The significant im-

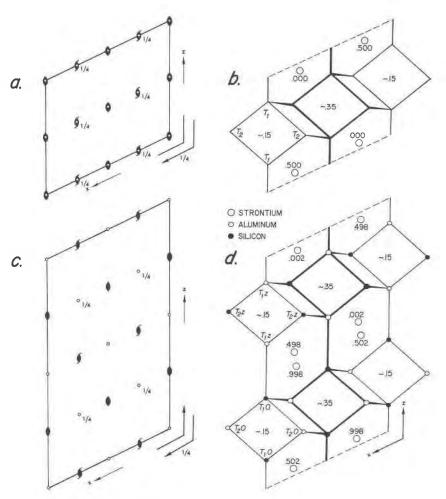


Fig. 1. (a) Symmetry elements of space group C2/m projected on (010). (b) Linkage of T atoms in a C2/m feldspar structure The approximate y coordinates are shown at the center of each four-fold tetrahedral ring whose T atoms are nearly co-planar Oxygen atoms have been omitted for clarity. The y coordinates of the Sr atoms (large open circles) are also indicated. (Modified after Megaw, 1974). (c) Symmetry elements of space group I2/c projected on (010). (d) Linkage of T atoms in an ordered I2/c feldspar, showing doubling of the c cell edge due to perfect alternation of Al and Si atoms in the framework. The T sites are labeled, and other conventions are as indicated in (b).

provement in R as well as in the standard errors led us to correct for extinction, using a program written by G. Chiari and the formula reported by Stout and Jensen (1968, p. 409). The correlation matrix indicated only modest parameter interactions, and giving the 'b' reflections three times the weight of the extinction-corrected 'a' reflections led to no further parameter shifts. The final residual is 0.047.

Observed and calculated structure factors are in Table 2.

The atomic coordinates of the final I2/c structure and the parameter shifts from the positions of the "average" atoms in the C2/m structure are listed in Table 3. Table 4 contains the isotropic and an-

was carried out, starting from the coordinates of the initial model. It converged to within one standard deviation of the expected atomic coordinates and thermal parameters. This result does not prove that our refinement is correct (our data may contain systematic errors), but it does indicate that the presence of 'b' reflections, together with small changes in the intensities of 'a' reflections, can give rise to significant positional differences from the average C2/m structure. (G.C.)

¹ Even though the refinement had converged, it was uncertain whether the relatively few, weak 'b' reflections produced physically significant shifts of atomic coordinates from the average C2/m structure. To check this a program was written to introduce random errors ranging from ± 0.1 to ± 10 percent on the $F_{\rm cal}$'s from our final model. Using these as " $[F_{\rm obs}]$ ", a complete anisotropic refinement

TABLE 2. Observed and Calculated Structure Factors for SrAl₂Si₂O₈

h	*	Fobs	Fcalc	ħ		Fobs	Fcalc	h	k	Fobs	Fcalc	ħ	A	Fobs	Fcalc	h	k	Fobs	Fcalc	h	R	Fobs	Fcalc	h k	Fobs	Fcalc	h	*	Fobs	Fcalc
2 6 8 10	0 0 0	9 8 95 0 33 8 12 9 27 4	39 1 89 5 33 3 11 5 25 5	7 9 5 2 2 10 11 2 5	1 1 2 2 2 3 3 7 2	62:1 34:0 28:8 37:4 17:3 13:3 13:3 48:7 41:0	48,4 32,1 30,4 35,9 12,9 13.0 93.4 40.0 19.1	· · · · · · · · · · · · · · · · · · ·		62-8 30.0 10.9 16.5 21.6 7.1 27.8 51.8 21.1 26.0	47-5 331-7 121-7 16-9 11-9 7-2 12-1 98-3 21-8	3 7 U 2 4 6 U 1 L	9 9 10 10 10 10	42 3 3 1 14 6 18 0 8 3 24 9 14 2 16 4	41 7 3 0 14 .6 19 .1 8 .6 23 .9 14 .2 15 .9 39 .2	-7 -2 -4 -6 -1 -3	15 16 16 16 17 17	4 1 13 6 13 0 20 7 10 9 27 9	3 9 12 7 11 6 18 3 10 3 25 1 9 1	中华女子中的 中中文	34444 555	9.5 13.8 2.7 21.9 17.7 7.0 12.6 58.7 51.1	10.0 16.7 2.3 23.9 19.1 7.9 13.0 56.2 33.3	1 0 6 8 1 0 3 9 5 10 2 10 2 10	0.8 24.8 9.9 11.8 53.7 9.1 22.3 29.6 10.9	0.6 23-5 9,8 10-9 33-4 9,5 22-7 28-8 20-7	12777	15 15 15 16 16 17 17	7 9 10 8 9 2 29 5 10 6 2 7 3 0	7 8 10 5 7 7 28 5 10 1 2 6 2 7
reador 357902 aguas olisaro dalamente lerres aceltas recentas recentas aguas de la composición del composición de la com	00 U U D D I I I I I I I I I I I I I I I I	39,88 39,89 31,99 31,99 31,90 31	80151 12152 12	6 3 HR 1937 7 M 1939 4 6 HR 1937 BOTKEL 357 MOR 4 HK 1957 BOTKER BEFORE 4 4 1958 BE WEST BOTKER 1980 1 7 1980 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1	2 222277 124444 445522 546542 1777788 588898 9000001 11111111111 11111111 4441444 47770 5000011 1211111	37.4 13.5 13.5 39.7 48.7	35.19 1.15.19	多了,他们还是在我们们们可以对,我们都将我们的,不知知的时候,我们都可以明显,我们们可以说,我们还有一个人的。" 医克里氏虫虫 医多子虫虫虫 医毒素蛋白 医白色素白色 医克里耳曼	55 SECOND 677777 REFERENCE MINUS 111111111111111111111111111111111111	16.5 17.1	16:9 7:2 32:1 38:3	17日日 《《日日日日》 日本土工工》 日本工工》 《日本工工》 《日本工工》 《日本工工》 《日本工工》 《日本工工》 《日本工工》 《日本工工》 《日本工工》 《日本工工》 · 18日本	10	14,6 8,3 8,3 8,3 8,4 8,4 8,4 8,4 8,4 8,4 8,4 8,4 8,4 8,4	14.6. 5.6. 14.2. 13.9. 14.2. 13.9. 14.2. 14.2. 15.9. 16.6. 16.6. 16.7. 16.8. 16.		18	27_9	25.1	计可称作序段 化性电影电话 医生物中毒 化铁铁镍矿矿 化电影性电影 经过的证券的 医皮肤性皮肤 医阴影性皮肤	40.4.4.5 555555 5886667 777778 8888890 88800 88800 111111111 111111111 11111111	217, 219, 27, 29, 219, 219, 219, 219, 219, 219, 219,	197.19 11.02 11.03 11.11.11 11.12 11.12 11.12 11.12 11.13 11		11.6 33.7 .8.1 22.3 29.6	10.9 33.4 9.5 22.7 28.8		17 17	29.5 10.6 2.7 3.0	
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isotropic temperature factors, and Table 5 the important interatomic distances and angles.

Discussion

The structure of this synthetic strontium feldspar (symbol: Srf) is most nearly analogous to that of celsian whose structure was determined in 1960 by Newnham and Megaw using visually estimated intensities from Weissenberg photographs taken about five zone axes. Because celsian is currently being refined by modern methods (Griffen, personal

communication), we will not belabor a comparison of our results with theirs. However, a recently published refinement of the structure of a defect strontium feldspar, synthetic $Sr_{0.84}Na_{0.03} _{0.13}Al_{1.69}Si_{2.29}O_8$ (symbol: dSrf) by Grundy and Ito (1974) is a useful reference point for discussion. The crystal data of both Srf and dSrf are listed in Table 1. Of fundamental difference is the symmetry (Fig. 1): dSrf has a highly disordered Al/Si distribution, shows no 'b' reflections, and thus has the unit cell of sanidine $(C2/m, c \simeq 7 \text{ Å})$; whereas Srf, because

Table 2, Continued

	A	R	Fobs	Fcalc	h		Fobs	Fcolc		*	Fobs	Fcalc	*	*	Fobs	Feale	h	4	Fobs	Fcalc	h	k	Fobs	Fealc	h	*	Fobs	Fcalc	ħ	k	Fobs	$F_{\rm calc}$
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•	-11 -2 -4	8	10 4	7 2 11 5 9 1	-5 -7 -9	1	43 5 22 4 8 9	42.0 21.5 7.2	9		17.2	19.1 3.1 19.0	2	No.	12_6 19_9 4_5	12 5 22 1 3 9	-4 -4 -1	44.44	13.3 18.2 28.7 29.2	16;7 30;9 20;8	-4 -1 -3 -2 -1	9 10 10 11 12	1.4 1.5 6.7 4.1 1.1	2.6	0 0 0	7 7 7	4.8 2.0 7.6 1.9	4.9 1.5 7.7 1.2	1254	**	7.A 2.Q 7.1	0.3 0.3 4.2 0.6
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	-3 -5	9	18 3 16 3	17.6 16.2	-1 -2 -3	1	11 8 15 5	11 7 15 4	7	0 0	13.5	15.9	0	4	9_5 11_6 12_6	9_0 11_2 12_4	14.4	6667	24.1 3.4 27.6 7.2	28.6 27.6 7.1	2 4	1	6 6	5 . 5 4 . 8	1111	1111	5.4 1.5 6.3 3.0	4,3 2,3 6,3 3,3	2	12	5 ₁ 3 4 ₄ 6	5, 9 5, 2
	-4 -6 -8	10 10 10 10	12,4 6.9 17,4 13,6 15,9	12.1 5.9 17.4 14.3 17.0	-7 -9 -11 -6 -8	7776	16.4 23.6 15.8 7.6 2.8	15 9 22 9 15 6 8 1 2 7	7 7 7 7 10 7	0 0 0 1	37.9 31.0 21.3 10.0	30-1 3-1 19-9 31-8	+2 +4 +6 -10 -10	0000	39 9 17 1 20 0 5 0 23 1	41_5 16_2 20_0 4_7	+0 +6 -5		1957 155 250	8.4 10.6	3	1 2 1	3,3 2,2 1,4 4,9	3 3 2 0 1 7 4 1	中ではなる	1	7.5 1.6 1.1 1.9	7,2 1,5 1,5 1,9	20	3	2,1 2,1 1,7 8,6	1 4 2 4 1 9 8 6
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	-6 1 -5 1	12 12 12 13	21 .3 26 .3 8 .1 27 .2 16 .5	20,9 26,7 7,9 27,0	-11 -2 -4 -6		16;3 12;9 15;9 12;8	16 0 13 2 15 7 12 6	-0 -10 -1 -1 -2 -5	2 2 3	16.8 12.5 3.6 12.2 15.7	16.2 12.6 3.7 32.1 13.6	-6 -11 -11 -1 -3 -5	1	24 0 10 9 12 4 14 9	24 .0 10 .1 12 .0 15 .1	-8	1 2	7-3	11.2	5 0	1000	5.7 3.2 4.0 4.4 2.8	5.7 3.2 4.3 4.6 2.6	-5	4 4 4	3-1 6-1 5-0	4-1 3-6 6-2	77777	1	4 1 13 4 3 8 2.9 1 1	3 Z 12 9 3 1 3 2 1 4
	-5 1	.3	12.8	18 0 12 6	-10 -1	7	10 i6 31 i3 38 i4	9 7 31 0 37 2	-7	3	45.7	44,2 29.3		4	4 .9 3 .6 16 .7	4.8 3.8 16.7	777	A.	5.7 8.1	5.0	1	T	1.4	1.3	-7 -4 -2 -2 -2 -2 -2	6	5.0 6.0 7.6	5 2 5 3 6 4 7 3	-1 -1 -7	A	4.1	4.4
-	2 1 4 1 6 1 1 1	4	8 6 24 8 11 7 12 2 7 8	7 5 25 2 11 5 12 1 7 4	1221111	7 7 8	30 8 16 7 8 2 8 6 4 1	29 8 15 6 9 6 8 2 4 1	-11 -7 -8	4	19.9 30.5 32.3 16.9 13.3	19.7 33.1 16.3 13.1	14 0 H O		13.0 15.3 9.3 16.2 17.3	13 1 15 4 8 7 15 2	0	1	0.9	1 = 2 0 = 4	1 3	10 10	2 9 3 9 2 5 3 6	3,5 3,6 2,2 3,8	7477	7 1 8	5=7 3=2 1=2 1=6	6 - 4 2 - 5 0 - 8 2 - 0	-14	5	8 0 1 4 8 6 5 4	7.7 1.0 8.4 5.5
-	2 I 4 I	6	5_5 4_8	4 9 3 8	-F		32 7 9 2 24 5	32,5 9,5 23,9	-10 -1 -1 -3 -7 -9	9 9 9	13.8 19.3 9,€ 42.6	14.9 19.2 9.1 W1.6	-3	9.00	4 .9 4 .5 8 .8	19 4 4 5 4 9 8 7	6 1 0 2	-	4 2 4 4 4 0 1 5	4 1 4 8 5 0 1 5		11	3 7 4 3 3 8 3 8	2 9 4 1 3 8 2 4	-5		2=1 1=9 3=6	2 - 3 1 - 4 3 - 6	-1 -3 -3 -4 -4	8 5 7	3 5 3 1 3 9 7 7	2 2 3 2 3 6 8 1
	6	1 -	2.0	2_9	-10 -4 -3 -1	*	21 .7 52 .0 26 .2	21 2 51 4 25 2		5	28.5 34.6	27.3 13.8	+2 +4 -4	4 4	8 5 19 7 10 8	8 ,6 20 ,3 10 ,5	8	74	1 0 2 1	0 B 2 0	4	1 2	5_4 5_6	5 = 4 7 = 0 1 = 7	7777	10 10 11	2.1 3.1 4.4	2-1 3-3 3-9	-5	*	8_1 8_5 4_3	7.7 8.3 4.6
Section 2	4	0	32.3 9.6 21.5 9.6 3.2	33 3 9 7 22 2 10 0 3 1	7777977	10 10 10 10	20 4 10 6 15 3 11 7 17 4 18 6	19,4 10,1 15,1 11,0 17,1 18,2	-11 -2 -4 -5 -10	***	7.4 39.1 2.4 73.1 15.0	5.7 33.3 2.4 22.6 14.4	+ff -10 +1 +1 +5 -7	6777	12 6 11 5 16 9 2 7 4 8	12 4 10 9 17 9 2 4 4 6	2000	****	1 1 2 8 2 1 4 2	1 1 2 7 2 5 4 0	241244	1	2 0 2 7 5 5 3 1 3 1 1 6	2 4 5 5 2 7 3 4 2 6	II 2	1	2 7	3-3 5-0	-1	1.	6.3	6.6
			19 0 24 9 28 0	19 9 26 4 28 0		31	7_9 17_2		-7		3,8 20.3 16.7 12.7	20.1 17.1		7	20,5 15,2 20,0 20,9	20 6 13 6 20 7	1 0	1	5.7 2.0 0.4 5.4	6 1 1 6 0 3 5 1	五七日本	A .	1.4 3.1 1.7	1 2 2 9 1 5	3 7 7 0	2 2 2	3 0 4 4 2 9 2 1	3,0 4,4 3,1 1,3	14000	3 3 1	2.0 1.2 7.8 3.5 3.2	1.8 0.9 3.1 3.7 3.1
3		1	27.9	29 3 27 4 8 2	コマテヤフィ	11 11 11 12 12	6_4 14_8 5_2 7_8	7.5 17.2 5.7 14.9 3.8 7.7	-1 -5 -7 -4 -1	777.8	12.7 11.9 14.0 16.6	12.6 11.0 13.4 15.7	中子子中中	3 3	20,9 19,9 11,0 17,1	20 7 19 9 10 1 16 9	1	8 8	8 4 2 3	8 5 2 4	-11	4	1 0 3 6 3 7	1 - 9 4 - 0 3 - 1	1	2	2 6 3 4 4 1	2 9 3 0 4 6 1 9	-6	+	2.1	ALS.
	4 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2		10 3 19 0 39 0 21 0	10 8 19 7 39 0 22 0			3.7 5.8 4.8 5.2 6.4	3,6 5,3 3,9 5,5 6,4	448444	# #	20.8 22.7 6.1	10.8 17.4 1.0	-3 -3 -3	9 9	9.9 9.4 23.1	10,2 9,8 22,9	3 4 3	9 9 9	4 4 1 7 2 8 5 1	4 9 2 4 3 4 5 9	子子でする	6 6 7 1	2 0 3 6 4 4 6 0 3 6	2 · 8 3 · 5 5 · 4 6 · 6 3 · 7	1	5	2,1 2,2 3,8	3 0	77475	3 4	2 7 4 1 5 6 1 7	2 J 1 7 3 6 4 8 1 0
	2 6		12 1 13 9	11 5 13 7		17 13 13 11 14 14	5.2 6.4 5.6	5_5 6_4 4_5			35.3 13.0	7.0 34.4 12.2	-6	10 10 10	13 5 24 3 14 5	13.4 23.9 13.7	0 1	11 11 12	4.9 1.8 1.0	4 6 1 7 0 7	\rightarrow I	R.	3 0	2+9	de.		2 2 4 3 5 3 5 2	1 6 3 6 4 9 4 6	77 4	3	30	3 2 5 2 2 3 2 3
	1 7 7 8 8 8		16 9 13 0 27 5 27 5	17.0 13.5 28.3 27.5	-6 1	14	5+8 20-7	5_1 20_2	797477	10	16.4 2.4 7.7 17.0 1.3	16.2 2.2 7.3 11.5 1.9		11 £ -	5 6 18 29 7	5_4	+1 +6 +1	1 1 1	1 2 1 8 3 0	1 0 1 2 3 9	22222	0 0 10	7 8 7 7 8 0 4 3 4 7	8 0 7 6 8 4 3 0 5 3	-4	1	7 . 7 3 . 7 5 . 7 1 . 9	7 5 3 3 5 6 1 3	4477774	0.07	5 2 2 5 2 2 3 1 5 1 5 0	2 3 2 8 5 6 5 0
	5 9 10		24 .7 5 .9 5 .0	24 .3 4 .7 4 .2	2 4	ii n	9.4 21.3 14.1	7.7 22.3 14.3		11	19,3	2.6	40	0 0	10 6 26 1 16 9	31.8 11.1 26.7 17.7	-1	17779	3 0 3 6 3 5 2 0	4 1 3 6 3 9 2 1		1 -	4-7	5 2	世界でなけ	1	4 0 2 2 3 1 6 4	4 1 2 2 2 6 5 7		1.	17	
	2 10 1 11 1 11 1 12		15 3 7 6 24 1 8 8	15 9 7 1 23 9 8 0	1 6	1 1 1	15.1 15.8 30.9	15 6 16 6 32 4	784534	11 11 11 11 11	24.1 7.0 27.2 10.6 11.1	23.5 7.2 27.2 9.7 13.3	1	1	23 0 14 6 7.2	23_1 15_6 6_9	+0 +0	-	2 9 3 2 2 8	3=9 4=0 2=0	0 7 4	1	4.0	316	7	3	4.6 2.7	4.3	77	1 1	11	7,1
70	1 12		3 .7 11 .8	4 6 11 1	1	100	11 2 21 5 7 7	11 7 23 0 7 2		13	19,1	18,5	マヤヤマナ	1	7.2 12.3 20.3 5.5	7_3 11.9 22.1 4.5	7776	5	1 8 5 4 3 7 2 1	2 - 3 5 - B 4 - 1 2 - 3	1	11111	A.6 6.5 1.2 1.1 A.8	9.1 1.0 0.6 4.8	*77777	4 5	1.6	2.9 1.3 2.3 5.7	777777	2 2 2 2	9.8 3/5 6/7 3/6	9.3 3.2 6.5 3.8

of its highly ordered Al/Si arrangement, has a doubled cell ($c \simeq 14 \,\text{Å}$, similar to anorthite) and an unconventional monoclinic space group, I2/c. In dSrf, as in the 'average' structure of Srf (see Fig. 1a,b and "Structure Refinement"), Sr and O_A1 atoms are on the mirror, OA2 is on a diad, whereas in Srf all atoms are shifted slightly into general positions. Atomic pairs O_BO-O_Bm , O_CO-O_Cm , $O_DO - O_Dm$, $T_1O - T_1z$, and $T_2O - T_2z$, which were symmetrically equivalent in the disordered C2/m structure, are distinct in the ordered I2/c unit cell; oxygens are pseudo-mirror-related and tetrahedral atoms are related by pseudo-translation in the z direction (Fig. 1c,d). The topologies of the tetrahedral frameworks of the two structures are very similar. The Al/Si alteration in Srf is nearly perfect (Fig. 1d). However, the mean T-O distances $(\langle T_1O-O\rangle = 1.627, \langle T_1z-O\rangle = 1.732, \langle T_2O-O\rangle =$

1.736, $\langle T_2 z - O \rangle = 1.630$ Å), when compared with $\langle \text{Si-O} \rangle = 1.613$ Å and $\langle \text{Al-O} \rangle = 1.747$ Å in anorthite (Wainwright and Starkey, 1971) indicate about 10 percent Al in Si-rich sites and 10 percent Si in Al-rich sites.

The 1.69 Al atoms in dSrf are highly disordered $(\langle T_1 - O \rangle = 1.670, \langle T_2 - O \rangle = 1.657 \text{ Å})$ with Al contents of T_1 and T_2 variously estimated from $t_1 = 0.43$ to 0.49 and $t_2 = 0.34$ to 0.39 (Grundy and Ito, 1974, Table 6). Linear equations relating mean T-O distances to Al content (Jones, 1968; Ribbe and Gibbs, 1969) yield the lower values for both sites, adding up to an estimated 1.54 Al atoms in this compound. The reason for this is evident in Figure 2 which shows that when compared to all other relevant feldspar structural data, the grand mean T-O distance in dSrf is discrepant with the value expected for an Al/(Al + Si) ratio of 0.435.

Table 3. Final Atomic Coordinates of I2/c SrAl₂Si₂O₈ and a Listing of Parameter Shifts from the Positions of the Atoms in the "Average" C2/m Structure*

Atom	X	\boldsymbol{y}	z
	At	omic Coordin	ates
Sr	0.2690(1)	-0.0020(1)	0.0656(1)
$T_1(0)$.0066(2)	.1746(1)	.1083(1)
$T_1(z)$.0032(2)	.1775(1)	.6164(1)
$T_{0}^{\perp}(0)$.6934(2)	.1200(1)	.1706(1)
$T_2^2(z)$.6845(2)	.1137(1)	.6716(1)
O _A (1) O _A (2) O _B (0)	.0045(4)	.1289(4)	.0003(2)
$0^{11}_{\Lambda}(2)$.5911(7)	.0002(3)	.1427(4)
$0_{\rm R}^{\rm G}(0)$.8267(6)	.1266(4)	.1054(3)
$0_{B}^{B}(z)$.8104(6)	.1263(4)	.6113(3)
O _C (0) O _C (z) O _D (0)	.0132(6)	.2984(4)	.1186(3)
$O_{C}(z)$.0188(6)	.3090(4)	.6304(3)
$O_{C}^{D}(0)$.1876(6)	.1245(4)	.1955(3)
$O_{\rm D}^{\rm D}(z)$.1960(6)	.1190(4)	.7027(3)
	Pa	rameter Shi	fts
Sr		-0.0020(1)	
T_{m1}	+0.0017(2)	0014(1)	-0.0040(1)
T_2^1	+.0044(2)	+.0031(1)	0005(1)
0.1	+.0045(4)		+.0003(2)
0 ^A 2		+.0002(3)	
O _R	+.0081(6)	+.0003(4)	0029(3)
02	0028(6)	0053(4)	0059(3)
o _D C	0042(6)	+.0027(4)	0036(3

^{*}Estimated standard errors are in parentheses and refer to the last decimal place.

It is uncertain whether or not the partially vacant alkaline earth site in dSrf is the cause of this discrepancy. While it is true that the lower effective charge at this site causes Sr-O distances to increase by ~ 0.03 Å over those in stoichiometric SrAl₂Si₂O₈, and the T-O distances are 0.005 Å shorter than expected, a cause-and-effect relationship is by no means established because the unit cell volumes and configurations of Srf and dSrf are not in any way constrained (see discussion below).

The other estimates by Grundy and Ito of the Al content of T_1 and T_2 are based on Brown and Shannon (1973) bond-strength calculations ($t_1 = 0.47$; $t_2 = 0.35$) and least-squares site-population refinement ($t_1 = 0.48$; $t_2 = 0.39$). Only the former is free of bias, because the latter was chemically constrained ($t_2 = 1.69 - t_1$, silicon contents being determined for T_1 and T_2 by difference from 1.0). But Brown and Shannon bond strengths are by no means precise enough for this sort of determinative use as evinced by calculations on K-feld-spars by Grundy and Ito (1974, Table 5).

Although the actual Al/Si distribution is somewhat uncertain, it is clear that the shorter a dimension in dSrf (and thus its smaller unit cell volume-Table 1) is due primarily to the fact that dSrf has a lower Al/Si ratio (0.74) than stoichiometric Srf (Al/Si = 1.00). The statement that "The shortening of the a dimension is further enhanced due to the presence of vacancies on the alkali cation site . . ." (Grundy and Ito, 1974, p. 1321) is incorrect because the mean Sr-O distance in dSrf is 0.03 Å longer than that in Srf, regardless of whether the Sr site is considered to be 7- or 9-coordinated. The longer Sr-O distances are expected because of the lower positive charge at the partially vacant Sr site, but the usual effect in feldspars of enlarging the alkali or alkaline earth site, if the Al/Si ratio remains constant, is an increase in a and in volume (Wright and Stewart, 1968). The smaller values of these parameters observed in dSrf can only be explained by the substitution of Si (~0.13 Å smaller than Al) for Al.

The steric details of the $SrAl_2Si_2O_8$ structure, when analyzed in the manner of Megaw, Kempster, and Radoslovich (1962), are well within the range of known aluminosilicate feldspars. Although I2/c Srf ($\langle Sr-O \rangle = 2.691 \,\text{Å}$) and celsian ($\langle Ba,K-O \rangle = 2.863 \,\text{Å}$; Newnham and Megaw, 1960) are monoclinic, and $P\bar{1}$ anorthite with its smaller M cation ($\langle Ca^{VII}-O \rangle = 2.517 \,\text{Å}$; Wainwright and Starkey, 1971) is triclinic, the tetrahedra in Srf are more like those of anorthite and are significantly more distorted than in celsian. In fact, using a distortion parameter σ^2_{tet} defined by Robinson, Gibbs, and

Table 4. Isotropic and Anisotropic Thermal Parameters for SrAl₂Si₂O₈*

	.00.	-	otropic		ture facto		
Atom	B(Å ²)	β11	β ₂₂	B33	B12	B13	B23
Sr	1.07(2)	21(1)	27(1)	13(1)	1(1)	2(1)	-2(0)
$T_1(0)$	0.64(4)	23(3)	15(1)	6(1)	-5(1)	3(1)	-1(1)
$T^{\perp}(z)$	0.69(5)	36(3)	16(1)	4(1)	-2(2)	6(1)	0(1)
$T_{1}^{1}(z)$ $T_{2}^{1}(0)$	0.64(5)	19(3)	16(1)	4(1)	-2(1)	1(1)	-1(1)
$T_2^2(z)$	0.67(4)	35(3)	12(1)	6(2)	1(1)	5(1)	1(1)
0.(1)	0.9(1)	39(7)	23(3)	6(3)	9(3)	8(3)	-2(2)
oA(2)	0.9(1)	30(8)	17(3)	13(2)	8(3)	`3(4)	4(2)
$o_{n}^{A}(0)$	1.2(1)	57(8)	28(3)	12(2)	-2(4)	17(4)	-2(2)
O _A (1) O _A (2) O _B (0) O _B (z)	1.2(1)	36(8)	31(3)	17(3)	-13(4)	16(4)	0(2)
	1.1(1)	43(7)	26(3)	7(3)	-11(4)	0(3)	-4(2)
O _C (0) O _C (z) O _D (0) O _D (z)	1.2(1)	43(8)	21(3)	18(3)	-5(4)	13(4)	-2(2)
0 (0)	1.3(1)	58(8)	29(3)	10(3)	3(4)	6(4)	2(2)
$O^{D}(z)$	1.2(1)	36(8)	31(3)	6(2)	4(4)	-3(4)	-1(2)

^{*}Estimated standard errors are in brackets and refer to the last decimal place.

Table 5. Interatomic Distances (Å) and Angles (Degrees) for Partially Disordered I2/c SrAl₂Si₂O₈*

	T-0		0-0	0-T-0
	distances		distance	s angle
$T_1(0)$ tetrah	edron			
$r_1^{(0)} - o_A^{(1)} - o_B^{(0)} - o_C^{(0)} - o_D^{(0)}$	1.644	O _A (1)-O _B (0) -O _C (0) -O _C (0) O _B (0)-O _C (0)	2.525	101.5
$-0_n^{\mathbf{A}}(0)$	1.617	$A = -0^{B}(0)$	2.754	115.5
$-0^{B}(0)$	1.612	-0°(0)	2.544	101.9
-0°(0)	1.633	0 (0)-0 ^D (0)	2.683	112.4
D(0)	1.055	BCCCO	2.739	114.9
		0 (0) -0 ^D (0)		110.0
	1 (07	o _B (0)-o _D (0) -o _C (0)	2.658	109.4
Mean	1.627		2.651	109.4
$\frac{T_1(z)}{z}$ tetrah	nedron			
$T_1(z) - 0_A(1)$ $-0_B(z)$ $-0_C(z)$ $-0_D(z)$	1.755	$0_{A}(1) - 0_{B}(z)$	2.655	99.6
$-0_{\rm p}^{\rm A}(z)$	1.721	$-0^{\mathrm{D}}(z)$	2.943	115.9
$-0^{B}_{a}(z)$	1.716	-0-(z)	2.661	99.4
$-0^{C}(z)$	1.735	0(z) - 0(z)	2.888	114.3
D (-)		B -0 (z)	2.929	115.9
		$ \begin{array}{ccc} A & -O_{C}^{B}(z) \\ & -O_{D}(z) \\ O_{B}(z) - O_{C}(z) \\ & -O_{D}(z) \\ O_{C}(z) - O_{D}(z) \end{array} $	2.836	110.5
Mean	1.732	C D	2.819	109.3
m (0) totrol	nodron			
$T_2(0)$ tetral		0 (2) 0 (0)	2. 700	106.8
¹ 2(0)-0 _A (2)	1.738	A(2)-0B(0)	2.788	
-0 _B (0)	1.734	-0 _C (0)	2.680	101.1
-0 _C (0)	1.732	-0 _D (0)	2.779	106.1
$T_{2}^{(0)}$ $-0_{A}^{(2)}$ $-0_{B}^{(0)}$ $-0_{C}^{(0)}$ $-0_{D}^{(0)}$	1.739	$0_{R}(0)-0_{C}(0)$	2.884	112.6
2		$-0_{n}^{0}(0)$	2.893	112.8
	-	$\begin{array}{c} o_{A}(2) - o_{B}(0) \\ - o_{C}(0) \\ - o_{D}(0) \\ o_{B}(0) - o_{C}(0) \\ - o_{C}(0) \\ o_{C}(0) - o_{D}^{D}(0) \end{array}$	2.944	116.0
Mean	1.736		2.828	109.2
$T_2(z)$ tetral	nedron			
$T_2(z) - O_A(2)$ $-O_B(z)$ $-O_C(z)$ $-O_D(z)$	1.641	0.(2)-0_(z)	2.642	107.8
-0 ^A (z)	1.629	A -0B(z)	2.542	102.9
-0 ^B (z)	1.609	-0°(2)	2.663	108.5
-0 ^C (2)	1.641	0 (2)-00(2)	2.707	113.4
-0 _D (2)	1.041	B(2)-0C(2)	2.678	109.9
		$0_A(2)-0_B(z)$ $-0_C(z)$ $-0_C(z)$ $0_B(z)-0_C(z)$ $0_C(z)-0_C(z)$	2.723	113.8
Mean	1.630	$0_{\underline{C}}(z) - 0_{\underline{D}}^{\underline{D}}(z)$	2.659	109.4
nean	1.030		2.037	107.4
	Sr-O			T-0-T
	distances			angles
Sr-0 _A (1)	2.630	$T_1(0) - 0_{\Delta}(1)$	-T ₁ (z)	137.8
$-0_{\Lambda}^{*}(1)$	2.650	$T_2^+(0) - 0_A^{(1)}(2)$	$-T_{2}(z)$	127.7
$-0^{A}(2)$	2.445	$T_1^{L}(0) - 0_n^{R}(0)$	$-T_{2}^{2}(0)$	144.4
$Sr-O_A(1)$ $-O_A(1)$ $-O_A(2)$ $-O_B(0)$	2.746	$T_1(0) - 0_A(1) - T_2(0) - 0_A(2) - T_1(0) - 0_B(0) - T_1(z) - 0_B(z) - T_1(z) - T$	$-T_2^2(z)$	145.6
-0.(z)	2.855	$T_{1}(0)-0_{C}(0)-T_{1}(z)-0_{C}(z)-T_{1}(0)-0_{D}(z)-T_{1}(z)-0_{D}(z)-T_{1}(z)-0_{D}(z)-T_{1}(z)-T_{D}(z)-T$	$-T_{2}(0)$	129.6
$-0^{\rm B}_{\rm b}(0)$	2.769	$T_{1}^{1}(z) - 0_{2}^{0}(z)$	$-T_0^2(z)$	132.3
$-0^{D}(z)$	2.743	$T_{+}^{\perp}(0) - 0_{-}^{C}(0)$	$-T_{0}^{2}(0)$	139.7
-0 ^D (0)	3.229	$T^{1}(z) - 0^{D}(z)$	$-T_{-}^{2}(z)$	138.1
-0B(0) -0D(z) -0C(0) -0C(z)	3.010	-1'-' D'D'		
C'2/	3.010		Mean	136.9

*Estimated standard error for all T-0 and Sr-0 bond lengths is 0.005 Å, for 0-0 distances 0.007 Å, and for 0-T-0 and T-0-T angles 0.3°.

Ribbe (1971), and relating it to the total number of polyhedral elements (edges plus corners) shared between a tetrahedron and the M-polyhedron, it is obvious from Figure 3 that the O-T-O bond angle strains in anorthite and Srf are very similar indeed.

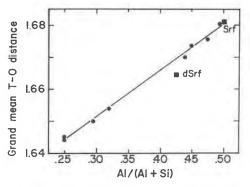


Fig. 2. Grand mean T–O distances versus Al/(Al + Si) for a variety of feldspars. In order of increasing $\langle\langle T$ – $O\rangle\rangle$, they are high and low albite, An₁₀, An₂₀, dSrf, An₇₀, An₃₀, celsian $P\bar{1}$ anorthite, and Srf. See Ribbe et al (1974) for references.

Phillips, Kroll, Pentinghaus, and Ribbe (1975) have found that the parameter $\langle M\text{-}O\rangle/\langle\langle T\text{-}O\rangle\rangle$ is linearly related to the mean T-O-T angle in paracelsian-type structures with the general formula $M^{2*}T_2^{3*,2*}T_2^{4*,5*}O_8$. The same relationship holds for feldspars of the type $M^{2*}\text{Al}_2\text{Si}_2\text{O}_8$ (Fig. 4), except that the slope of the feldspar line is only one-fourth as great as that of the paracelsian line, and $\langle T\text{-}O\text{-}T\rangle$ in feldspars is 10° greater than in paracelsians. It is thought that these may be indications of the greater flexibility of the feldspar tetrahedral framework whose T-O-T angles show substantial ranges within individual structures. The T-O-T angles within individual paracelsians are generally more

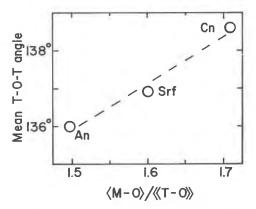
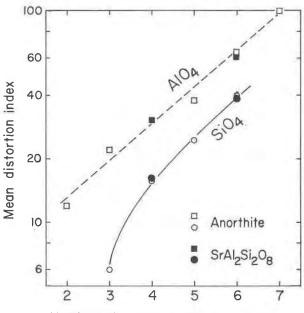


Fig. 3. Mean T-O-T angle versus the mean M-O distance (assuming 7-coordination) divided by the grand mean T-O distance for three feldspar structures: An (anorthite, Wainwright and Starkey, 1971), Srf (SrAl₂Si₂O₈, this paper), Cn (celsian, Newnham and Megaw, 1960).



Number of shared polyhedral elements

Fig. 4. Mean distortion index $\sigma_{\rm tet}^2$, as defined by Robinson *et al* (1970), plotted against the number of shared polyhedral elements (edges plus corners) for AlO₄ and SiO₄ tetrahedra in anorthite (open symbols) and Srf (dark symbols). *Cf* Fig. 8, p. 41, in Ribbe *et al* (1974).

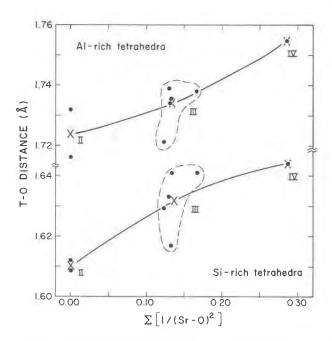


Fig. 5. Individual T-O distances in Srf plotted against the parameter $\Sigma[1/(Sr-O)^2]$ and grouped according to whether the oxygen atom involved in the T-O bond is 2-, 3-, or 4-coordinated (Roman numerals). Large X's indicate mean values for each coordination number.

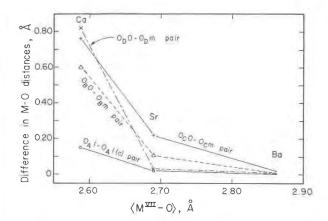


Fig. 6. Differences in interatomic distances for the pseudo-symmetrically related pairs of M-O bonds plotted against mean M-O distances for the seven-coordinated polyhedra in anorthite (Ca; values represent the means for 4 M atoms), in Srf, and in celsian (Ba).

restricted, but the mean T-O-T values for this group are much more sensitive to changes in the size of the large cation relative to the mean size of the cation occupying tetrahedral sites in the framework.

Inasmuch as there are 2-, 3-, and 4-coordinated oxygen atoms in Srf (as in anorthite-Megaw et al, 1962), it is expected that in general, T-O bonds to oxygens with the higher coordination numbers will be the longer. This is borne out in Figure 5 which is a plot of T-O distance against the sum of the inverse squares of the Sr-O distances to the oxygen involved. The value of the latter parameter is, of course, 0.0 for the 2-coordinated Q_cO and $O_c m$ atoms. It is ~0.28 for the 4-coordinated $O_A 1$ atom and 0.12 to 0.16 for the 3-coordinated $O_A 2$, O_B , and O_D atoms. Using this parameter, individual T-O distances in Srf cannot be as well predicted as in anorthite (Phillips, Ribbe, and Gibbs, 1973), but the principles influencing them are clearly comparable.

In the solid-solution series $(Ca,Sr)Al_2Si_2O_8$, synthesized by Bruno and Gazzoni (1968) and Nager, Hoffmann, and Nissen (1969), the triclinic- $(P\bar{1})$ -monoclinic (I2/c) transition occurs at approximately $An_{10}Srf_{90}$. Thus it is apparent that the radius of Sr is just large enough to prevent collapse of the tetrahedral framework in this partially disordered Srf. An examination of the M-O distances in anorthite, Srf, and celsian shows that as the cation radius increases, the M-coordination polyhedron becomes more regular in shape, *i.e.*, it approaches

C_s symmetry. This is graphically illustrated in Figure 6 where the differences in interatomic distances for the pseudo-symmetrically related pairs of M-O bonds are plotted against the mean M-O distance for the seven-coordinated polyhedra. (Because there are four non-equivalent Ca atoms in anorthite, the values for the Ca polyhedron are average ones). Note that the pseudo-center-related pair (O₄1) differ the least, even in anorthite, whereas the pseudo-mirror-related pairs (O_B, O_C, O_D) differ by 0.6-0.8 Å on the average in anorthite, by 0-0.2 Å in Srf, and less than 0.02 Å in celsian. Because of the ordered Al/Si distribution in these feldspars, the M-polyhedron is unlikely to attain C_s symmetry regardless of cation size, for even if the M atom were on a special position, it would be on a c-glide and not a mirror plane in these structures with $c \simeq$ 14 Å. By contrast, the Sr polyhedron in dSrf does have C_s symmetry, but dSrf is highly disordered with Al/Si < 1 and space group C2/m ($c \simeq 7 \text{ Å}$). A refinement of the structure of celsian (Griffen, in preparation) will provide more precise reference points for further comparisons of feldspar-like compounds. Additional discussion of $M^{2+}T_2^{3+}T_2^{4+}O_8$ structures may be found in Bruno and Facchinelli (1974).

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