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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, $\sum [1/(\text{Sr–O})^2]$, which is the sum of the inverse squares of the Sr–O distances to these oxygens:

C.N.(O)	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, $RbAlSi_3O_8$ (Gasparin, 1971), and of the rubidium-iron analog of microcline, $RbFeSi_3O_8$ (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 $SrAl_2Si_2O_8$, 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 $SrCO_3$, SiO_2, and Al_2O_3 (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)[$Al_2Si_2O_8$]–(Ca,Sr,Ba)[$Ga_2Si_2O_8$] and (Ca,Sr,Ba)[$Al_2Ge_2O_8$]–(Ca,Sr,Ba)[$Ga_2Ge_2O_8$]. 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—$BaAl_2Si_2O_8$ (Craig, Louisnathan, and Gibbs, 1973), its Sr analog—slawsonite (Griffen, personal communication), danburite—$CaB_2Si_2O_8$ (Phillips, Gibbs, and Ribbe, 1974), hurlbutite—$CaBe_2P_2O_8$ (Lindbloom, Gibbs, and Ribbe, 1974), celsian—$BaAl_2Si_2O_8$ (Griffen, personal communication), and $C2/m$ and $I2/c$ modifications of $PbAl_2Si_2O_8$ (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 ($CuK\alpha$ radiation) at Torino. The 768 strong '*a*' and 197 weak '*b*' reflections were measured at different scan rates to take into account 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-2θ 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}.

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

	Grundy & Ito (1974)	This Paper
CELL PARAMETER		
a (Å)	8.328	8.388
b (Å)	12.980	12.974
c (Å)	7.136	2×7.132
β	115.6°	115.2°
Volume (Å^3)	695.7	2×702.2
Z	4	8
Space group	$C2/m$	$I2/c$
COMPOSITION		
Formula	$Sr_{.84}Na_{.03}[\ ]_{.13}Al_{1.69}Si_{2.29}O_8$	$SrAl_2Si_2O_8$
Al/Si	0.738	1.000
Al/(Al+Si)	0.425	0.500
Calc. density	2.98 g/cc	3.08 g/cc

Structure Refinement

Assuming $C2/m$ symmetry ($c \simeq 7$ 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 ($c \simeq 14$ 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 $|F_{obs}| > 100$. The significant im-

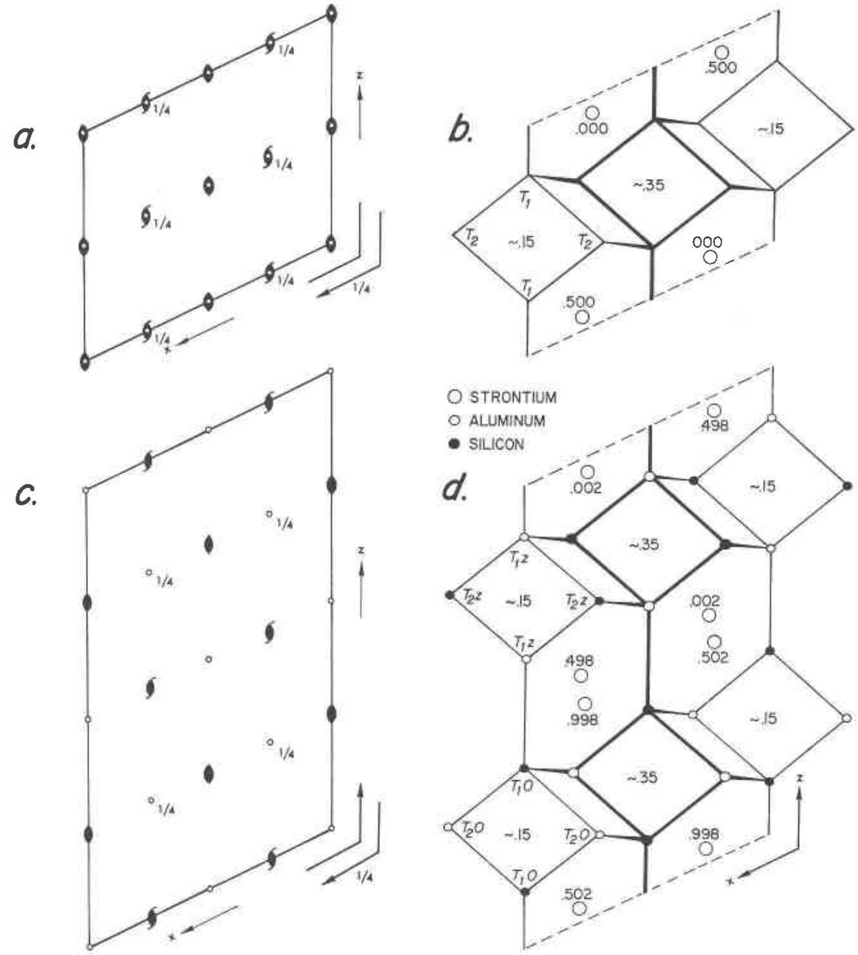

FIG. 1. (a) Symmetry elements of space group $C2/m$ projected on (010). (b) Linkage of T atoms in a $C2/m$ feldspar structure The approximate y coordinates are shown at the center of each four-fold tetrahedral ring whose T atoms are nearly co-planar Oxygen atoms have been omitted for clarity. The y coordinates 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.[1] 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-

[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_{calc}'s from our final model. Using these as "$|F_{obs}|$", a complete anisotropic refinement 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.)

TABLE 2. Observed and Calculated Structure Factors for $SrAl_2Si_2O_8$

h	k	F_{obs}	F_{calc}
	ℓ = 0		
2	0	39.8	39.1
4	0	95.0	89.5
6	0	33.8	33.3
8	0	12.0	11.5
10	0	27.4	25.5
1	1	3.8	4.1
3	1	31.9	32.6
5	1	8.0	7.2
7	1	40.1	38.9
9	1	15.5	14.9
0	2	26.4	33.9
2	2	101.3	94.8
4	2	6.9	5.6
6	2	50.6	49.5
10	2	13.9	13.8
1	3	45.3	49.8
3	3	37.5	36.6
7	3	7.3	6.3
9	3	37.4	35.1
0	4	30.6	33.0
2	4	8.1	9.1
4	4	19.4	19.8
6	4	64.7	64.6
8	4	35.9	34.4
10	4	24.7	24.1
1	5	15.6	14.8
3	5	14.9	15.3
5	5	1.9	2.3
7	5	26.4	25.5
9	5	17.7	16.5
0	6	74.7	82.9
2	6	4.5	4.0
4	6	56.5	57.7
6	6	9.0	9.1
8	6	35.6	34.3
10	6	4.0	3.7
1	7	10.9	11.0
3	7	22.6	24.7
7	7	29.3	28.5
9	7	15.5	14.4
0	8	61.3	65.7
2	8	82.7	90.0
4	8	3.5	3.3
6	8	20.6	19.9
8	8	22.1	20.7
1	9	28.3	31.1
3	9	1.9	1.6
5	9	33.1	34.3
7	9	10.7	10.4
9	9	24.0	23.2
0	10	51.9	56.0
2	10	24.7	26.1
4	10	25.0	26.3
6	10	8.8	8.7
8	10	8.0	6.6
1	11	2.0	2.7
3	11	22.9	24.1
5	11	1.6	1.9
7	11	23.2	23.2
0	12	7.6	7.3
2	12	5.9	5.0
4	12	22.0	22.7
6	12	22.5	22.4
8	12	27.3	26.7
1	13	8.2	8.1
0	14	4.4	4.0
2	14	22.9	22.3
4	14	28.8	28.6
1	15	13.1	12.3
3	15	8.8	7.9
5	15	10.1	9.9
0	16	44.7	39.4
2	16	14.6	13.4
4	16	19.7	17.6
1	17	8.4	7.1
3	17	23.3	21.4
0	18	25.4	22.1
2	18	15.3	13.1
	ℓ = 2		
0	0	20.0	20.5
2	0	14.8	16.4
4	0	26.6	26.6
6	0	23.7	24.1
8	0	10.0	10.3
10	0	3.8	3.4
1	1	4.5	4.0
3	1	51.0	48.5
5	1	36.5	35.1
7	1	42.1	40.6
9	1	34.0	32.1
0	2	28.8	30.4
2	2	37.4	35.9
4	2	13.3	12.9
10	2	13.5	13.0
1	3	39.7	35.9
3	3	48.7	48.0
5	3	41.0	40.2
7	3	12.3	11.1
9	3	18.4	18.1
0	4	52.4	53.6
2	4	53.9	50.6
4	4	15.6	15.9
6	4	19.5	18.8
8	4	20.1	19.1
10	4	10.9	10.0
1	5	39.0	39.8
3	5	59.8	59.1
5	5	28.8	28.6
7	5	14.8	13.8
9	5	10.3	10.3
0	6	39.1	41.3
2	6	22.7	22.9
4	6	6.2	6.2
8	6	8.5	7.5
1	7	7.2	7.4
3	7	32.9	33.2
5	7	31.1	30.8
7	7	27.4	26.2
9	7	27.5	26.3
0	8	5.5	5.8
2	8	11.6	13.2
4	8	22.3	23.2
6	8	11.3	10.2
8	8	16.8	14.9
3	9	18.3	19.7
5	9	23.5	22.8
7	9	30.9	30.1
9	9	24.7	23.5
0	10	10.0	10.2
2	10	20.5	21.8
4	10	10.6	10.5
6	10	11.2	10.3
1	11	23.0	24.7
3	11	25.8	27.0
5	11	19.5	19.5
7	11	11.1	10.6
0	12	25.2	25.6
2	12	17.0	17.0
4	12	5.3	5.4
6	12	11.0	10.4
1	13	31.8	32.0
3	13	26.3	26.9
5	13	18.8	19.1
0	14	17.8	17.0
2	14	10.2	9.8
4	14	4.8	5.2
6	14	8.5	9.2
1	15	9.0	8.2
3	15	18.9	18.3
5	15	9.9	10.6
0	16	6.1	5.3
2	16	5.3	5.4
4	16	8.6	7.5
1	17	3.9	3.5
3	17	7.8	6.5
2	18	9.1	7.9
-2	0	34.1	30.4
-4	0	57.3	55.1
-6	0	15.5	14.8
-8	0	53.9	51.8
-10	0	25.2	23.5
-1	1	19.1	19.9
-3	1	17.7	21.9
-5	1	27.0	26.9
-7	1	7.8	7.9
-9	1	8.6	7.9
-11	1	13.8	13.1
-2	2	38.5	42.7
-4	2	33.9	37.3
-6	2	45.9	46.0
-8	2	18.8	17.9
-10	2	32.2	30.8
-1	3	39.7	41.5
-3	3	38.8	46.5
-5	3	12.0	13.2
-7	3	9.0	9.2
-9	3	15.7	14.8
-11	3	6.4	5.5
-2	4	70.9	80.7
-4	4	51.8	58.9
-6	4	41.7	43.2
-8	4	11.1	9.8
-10	4	13.1	12.8
-1	5	42.8	47.5
-3	5	30.0	33.7
-5	5	10.9	12.7
-7	5	16.5	16.9
-9	5	11.6	11.9
-11	5	7.1	7.2
-2	6	27.8	32.5
-4	6	51.8	58.5
-6	6	21.3	23.3
-8	6	26.0	27.0
-10	6	9.5	9.1
-1	7	18.2	18.7
-3	7	10.1	11.6
-5	7	17.4	19.8
-7	7	1.7	1.1
-9	7	7.6	7.4
-4	8	14.2	14.9
-6	8	26.4	29.2
-8	8	19.9	20.9
-10	8	32.2	31.5
-3	9	20.5	22.1
-5	9	12.2	12.9
-7	9	15.6	16.4
-2	10	6.9	6.8
-4	10	18.6	19.9
-6	10	17.8	18.3
-8	10	20.8	21.6
-1	11	20.4	21.3
-3	11	16.0	16.1
-7	11	7.0	6.7
-9	11	3.0	3.2
-2	12	31.3	31.7
-4	12	32.9	32.2
-6	12	20.1	19.9
-8	12	9.9	9.0
-1	13	22.3	21.6
-3	13	11.7	11.3
-5	13	7.4	6.8
-7	13	12.9	12.8
-2	14	27.1	26.1
-4	14	25.5	23.8
-6	14	20.5	19.4
-1	15	8.4	7.1
-3	15	10.2	9.4
-4	16	13.4	11.4
-6	16	8.3	7.4
-1	17	3.3	3.2
-3	17	4.1	3.9
-5	17	13.6	11.8
	ℓ = 4		
0	0	104.0	92.7
2	0	29.8	28.9
4	0	86.2	82.9
6	0	14.8	14.2
8	0	31.0	30.7
1	1	50.2	50.5
3	1	32.4	32.2
5	1	30.0	29.8
7	1	4.2	3.5
9	1	3.9	5.2
0	2	22.9	22.3
2	2	50.5	47.9
4	2	5.9	5.2
6	2	42.3	41.6
8	2	10.7	9.5
1	3	35.1	33.0
3	3	43.8	43.4
5	3	22.2	21.7
7	3	32.2	31.1
0	4	6.7	7.6
2	4	35.6	34.6
4	4	20.2	19.6
6	4	13.6	13.2
8	4	25.5	25.6
1	5	42.7	42.3
3	5	19.9	19.1
5	5	48.1	46.5
7	5	15.3	14.5
9	5	19.0	18.3
0	6	39.7	39.0
2	6	23.7	23.6
4	6	29.3	28.9
6	6	34.1	33.0
1	7	39.2	39.3
3	7	23.3	22.9
5	7	27.8	27.2
7	7	8.6	8.0
0	8	10.9	11.4
2	8	73.9	73.0
4	8	10.9	10.2
6	8	46.9	45.9
8	8	2.8	2.6
1	9	13.4	13.1
3	9	42.3	41.7
5	9	3.1	3.0
7	9	14.6	14.6
0	10	18.0	19.1
2	10	8.3	8.6
4	10	24.8	23.9
6	10	14.2	14.2
8	10	16.4	15.9
1	11	37.7	39.2
5	11	29.7	29.3
0	12	6.8	7.9
2	12	24.8	24.7
4	12	2.4	2.2
1	13	12.8	12.4
3	13	13.1	13.1
5	13	22.6	22.0
0	14	14.0	13.7
2	14	9.7	10.3
4	14	15.2	14.0
1	15	24.7	24.2
3	15	3.2	3.8
0	16	13.5	12.7
2	16	10.0	10.0
4	16	16.8	16.6
1	17	26.7	25.2
0	18	8.4	7.2
-2	0	101.4	90.6
-4	0	42.5	39.8
-6	0	78.7	83.2
-8	0	22.0	21.1
-10	0	28.2	24.6
-1	1	77.1	71.8
-3	1	49.3	49.5
-5	1	27.2	30.5
-7	1	27.3	28.3
-9	1	6.0	6.3
-11	1	3.0	3.1
-2	2	17.4	16.8
-4	2	50.0	51.6
-8	2	37.3	38.1
-10	2	13.3	12.6
-1	3	75.2	72.0
-3	3	37.9	37.4
-5	3	32.4	38.6
-7	3	17.6	19.6
-9	3	24.2	24.3
-4	4	28.6	31.0
-6	4	16.9	20.1
-8	4	9.7	10.6
-10	4	26.5	26.9
-1	5	37.7	35.9
-3	5	39.9	42.4
-5	5	12.4	14.9
-7	5	34.1	38.9
-9	5	11.2	11.3
-11	5	13.9	13.9
-2	6	36.1	37.5
-4	6	15.6	18.3
-6	6	24.4	27.8
-8	6	5.1	4.9
-10	6	30.2	31.2
-1	7	35.4	36.9
-3	7	33.3	35.6
-5	7	18.2	20.1
-7	7	22.1	23.6
-9	7	9.4	9.9
-2	8	10.3	10.8
-4	8	69.0	75.2
-6	8	15.2	16.3
-8	8	41.6	44.7
-1	9	68.3	71.3
-3	9	14.5	15.5
-5	9	36.8	39.1
-9	9	12.2	13.0
-2	10	21.1	23.5
-4	10	12.1	13.1
-6	10	23.3	24.4
-8	10	13.0	13.4
-10	10	14.8	14.9
-1	11	14.5	15.1
-3	11	37.9	40.2
-5	11	4.1	3.3
-7	11	25.1	25.6
-2	12	10.6	10.5
-4	12	21.3	21.5
-1	13	10.4	9.8
-3	13	12.7	11.7
-5	13	10.9	10.2
-7	13	18.9	17.6
-2	14	14.1	14.1
-4	14	10.8	10.5
-6	14	13.2	11.5
-8	14	18.3	17.2
-1	15	27.9	27.1
-5	15	22.3	20.2
-7	15	4.1	3.9
-2	16	13.6	12.7
-4	16	13.0	11.6
-6	16	20.7	18.3
-1	17	10.9	10.3
-3	17	27.9	25.1
-2	18	9.8	9.1
	ℓ = 6		
0	0	10.1	10.2
2	0	3.8	3.6
4	0	12.8	11.4
6	0	26.8	26.6
8	0	33.0	33.1
1	1	58.5	56.4
3	1	29.0	29.3
5	1	15.0	14.2
0	2	19.4	19.0
2	2	46.5	45.4
4	2	29.0	29.2
6	2	25.9	25.8
8	2	25.9	24.8
3	3	4.5	4.2
5	3	14.7	14.7
7	3	4.1	3.5
0	4	58.7	58.1
2	4	73.7	71.9
4	4	52.0	50.9
6	4	22.1	21.2
8	4	12.1	11.5
1	5	19.3	19.1
3	5	27.0	27.3
5	5	3.9	3.0
7	5	10.3	9.4
0	6	45.6	44.8
2	6	34.7	35.1
4	6	34.4	34.0
6	6	15.9	15.5
8	6	17.5	17.5
1	7	33.4	32.5
3	7	22.2	22.1
7	7	2.3	1.8
0	8	11.5	11.5
2	8	16.0	15.7
4	8	2.9	2.7
6	8	22.9	22.9
1	9	22.3	22.0
3	9	32.0	30.9
5	9	7.8	7.0
7	9	4.9	4.2
0	10	9.5	8.6
2	10	16.2	15.9
4	10	17.7	17.4
6	10	19.8	19.8
1	11	18.2	18.1
3	11	10.3	10.3
5	11	5.2	5.2
0	12	34.1	35.2
2	12	28.7	28.2
4	12	32.9	32.0
6	12	9.5	9.5
1	13	3.6	2.7
3	13	8.3	8.2
5	13	9.7	10.2
0	14	14.1	14.2
2	14	29.8	29.9
4	14	11.3	10.7
1	15	8.7	8.1
3	15	7.4	7.8
2	16	5.6	4.4
1	17	18.1	16.2
-2	0	23.2	21.2
-4	0	75.5	70.5
-6	0	18.5	17.7
-8	0	25.1	27.7
-10	0	11.2	11.5
-12	0	5.3	4.8
-1	1	44.2	44.6
-3	1	14.8	14.5
-5	1	18.7	18.2
-7	1	21.5	21.7
-9	1	19.1	21.8
-11	1	29.4	28.7
-2	2	37.1	36.2
-4	2	12.2	11.9
-6	2	20.1	20.2
-8	2	10.7	13.5
-10	2	5.9	5.7
-1	3	30.0	31.1
-3	3	39.0	38.7
-5	3	63.4	68.1
-7	3	34.1	38.3
-9	3	23.2	27.0
-11	3	9.5	10.0
-2	4	13.8	14.7
-4	4	2.7	2.3
-6	4	21.9	23.5
-8	4	17.7	19.1
-10	4	7.0	7.9
-1	5	12.6	13.0
-3	5	58.7	58.2
-5	5	51.1	53.3
-7	5	42.1	46.4
-9	5	11.9	13.2
-11	5	12.3	13.7
-2	6	12.0	12.0
-4	6	31.3	32.1
-6	6	14.3	15.5
-8	6	3.1	3.3
-10	6	13.3	13.2
-1	7	31.9	31.7
-3	7	16.4	16.7
-5	7	17.2	18.1
-7	7	18.2	20.0
-9	7	13.1	14.4
-11	7	19.9	21.6
-2	8	33.5	34.0
-4	8	14.3	14.9
-6	8	35.6	38.7
-8	8	4.5	4.7
-10	8	10.8	11.2
-1	9	30.8	30.9
-3	9	10.4	10.1
-5	9	19.4	21.0
-9	9	26.2	27.3
-2	10	6.5	5.6
-4	10	18.4	19.6
-6	10	5.3	6.2
-8	10	7.6	6.9
-10	10	2.8	2.9
-3	11	28.4	30.6
-5	11	18.4	18.7
-7	11	33.2	32.8
-9	11	9.6	7.8
-11	11	3.5	3.5
-2	12	10.1	10.4
-4	12	17.0	17.3
-6	12	3.9	4.0
-1	13	14.8	15.8
-3	13	26.9	27.2
-5	13	30.8	30.4
-7	13	24.8	21.6
-2	14	21.2	21.6
-4	14	15.6	14.3
-1	15	20.7	19.8
-3	15	2.7	3.2
-5	15	22.3	20.3
-2	16	6.2	5.8
-4	16	14.5	12.5
-6	16	7.5	6.7
-1	17	5.4	4.6
	ℓ = 8		
0	0	14.8	15.3
2	0	66.5	66.9
4	0	14.8	14.2
6	0	20.6	20.6
8	0	17.3	16.8
1	1	38.7	37.8
3	1	19.0	18.2
5	1	33.6	33.6
7	1	7.2	8.1
0	2	62.7	61.5
2	2	11.2	10.6
4	2	41.2	42.1
8	2	14.2	14.5
1	3	20.8	19.8
3	3	15.0	15.2
5	3	3.3	3.1
7	3	31.9	32.0
0	4	23.6	22.5
2	4	20.1	19.8
4	4	45.6	45.8
6	4	21.2	22.0
1	5	8.8	8.6
3	5	9.3	8.7
5	5	18.1	18.1
7	5	18.0	18.5
2	6	44.5	44.6
4	6	10.1	9.5
6	6	30.0	29.8
1	7	25.4	25.4
3	7	8.6	7.8
5	7	27.0	26.8
7	7	9.1	8.6
0	8	57.4	56.9
2	8	6.8	6.6
4	8	24.8	23.5
6	8	9.9	9.8
1	9	11.6	10.9
3	9	33.7	33.4
5	9	9.5	9.5
0	10	23.3	22.7
2	10	25.6	24.8
4	10	10.9	10.7
6	10	7.2	7.0
1	11	9.2	10.2
3	11	3.0	2.8
5	11	16.8	16.9
0	12	3.9	3.7
2	12	20.0	19.3
4	12	18.1	17.6
1	13	8.8	8.6
3	13	4.4	3.1
0	14	15.7	15.4
1	15	4.8	4.5
3	15	10.1	10.3
0	16	8.9	8.6
-2	0	142.8	130.8
-4	0	24.0	24.2
-6	0	58.2	56.7
-8	0	13.4	12.3
-10	0	7.2	7.2
-12	0	13.1	13.0
-1	1	6.5	3.9
-3	1	8.2	8.2
-5	1	41.5	40.1
-7	1	21.3	20.0
-9	1	32.3	31.3
-11	1	13.0	14.6
-2	2	28.1	27.4
-4	2	61.2	58.7
-6	2	9.6	8.4
-8	2	31.7	31.2
-10	2	2.8	3.1
-12	2	3.9	6.3
-1	3	19.0	18.8
-3	3	23.6	23.0
-5	3	7.1	5.8
-7	3	17.2	17.6
-9	3	9.0	8.7
-11	3	21.9	26.2
-2	4	3.0	2.9
-4	4	20.5	18.9
-6	4	14.9	13.3
-8	4	38.5	40.1
-10	4	30.5	23.1
-1	5	4.2	3.1
-3	5	3.7	8.0
-5	5	3.1	2.5
-9	5	14.5	15.8
-11	5	15.4	17.8
-2	6	34.7	34.3
-4	6	6.5	5.0
-6	6	36.4	37.8
-8	6	11.8	11.7
-10	6	20.2	22.0
-1	7	4.1	4.2
-5	7	28.3	28.3
-7	7	10.6	10.3
-9	7	20.5	22.9
-11	7	13.1	13.2
-2	8	39.9	39.9
-4	8	38.0	37.9
-6	8	8.3	8.1
-8	8	14.0	14.7
-10	8	9.6	9.3
-1	9	25.8	25.5
-3	9	23.6	23.5
-5	9	14.8	15.6
-7	9	27.1	28.7
-9	9	15.1	15.5
-2	10	38.2	41.3
-4	10	20.5	21.1
-6	10	17.2	18.5
-8	10	4.9	5.6
-10	10	5.1	4.4
-1	11	3.0	3.0
-5	11	12.8	13.2
-7	11	4.6	3.8
-9	11	15.9	15.1
-2	12	11.3	10.8
-4	12	3.7	2.9
-6	12	12.6	13.0
-8	12	17.3	17.0
-1	13	3.6	3.5
-3	13	2.2	2.1
-5	13	2.2	2.2
-4	14	16.7	16.4
-6	14	3.2	3.5
-1	15	7.9	7.8
-3	15	10.8	10.5
-7	15	9.2	7.7
-2	16	29.5	28.5
-4	16	10.6	10.1
-1	17	2.7	2.6
-3	17	3.0	2.7
	ℓ = 10		
0	0	12.0	12.8
2	0	36.4	36.6
4	0	10.0	10.1
6	0	21.7	22.8
1	1	36.8	37.9
3	1	23.3	24.0
5	1	38.7	39.8
7	1	23.8	24.9
0	2	34.7	34.8
4	2	9.8	9.1
1	3	16.4	16.6
3	3	34.6	34.7
0	4	40.8	42.4
2	4	11.8	11.7
4	4	10.2	10.8
6	4	17.8	18.4
1	5	45.9	46.5
3	5	11.4	10.3
5	5	13.9	13.8
0	6	4.1	3.8
2	6	13.1	13.4
4	6	11.5	11.5
6	6	5.2	4.1
1	7	29.8	29.8
3	7	23.4	23.5
5	7	26.0	25.7
0	8	17.4	17.2
2	8	8.4	8.0
4	8	20.1	20.2
1	9	5.7	5.0
3	9	28.6	28.4
5	9	19.8	20.2
0	10	15.5	15.5
2	10	10.4	9.8
4	10	9.5	8.1
1	11	25.0	24.7
3	11	4.5	4.8
0	12	12.9	11.6
2	12	2.9	2.7
4	12	12.4	12.5
1	13	19.5	19.2
3	13	12.7	13.2
0	14	16.1	15.3
2	14	9.9	8.5
1	15	12.3	11.8
-2	0	23.1	22.5
-4	0	35.2	34.3
-6	0	50.9	50.4
-8	0	11.3	9.8
-10	0	53.0	50.8
-12	0	13.1	12.8
-1	1	10.1	8.9
-3	1	6.3	5.4
-5	1	5.1	5.2
-7	1	18.4	17.5
-11	1	11.9	10.7
-2	2	11.6	11.1
-4	2	39.0	38.3
-6	2	17.1	16.5
-8	2	40.7	39.5
-10	2	9.9	8.5
-12	2	24.0	24.8
-1	3	59.8	60.3
-3	3	16.6	16.9
-5	3	46.8	45.9
-7	3	16.2	15.1
-9	3	2.1	2.1
-11	3	21.1	21.3
-2	4	43.4	44.0
-4	4	62.0	60.6
-6	4	34.3	33.2
-8	4	28.0	26.4
-1	5	35.4	35.1
-3	5	46.2	45.3
-5	5	18.7	18.6
-9	5	21.2	21.1
-11	5	10.0	11.6
-2	6	43.5	43.1
-4	6	11.1	9.9
-6	6	49.0	48.8
-8	6	9.9	8.9
-10	6	24.7	25.3
-1	7	3.0	2.9
-3	7	8.5	8.1

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 $Sr_{0.84}Na_{0.03}\square_{0.13}Al_{1.69}Si_{2.29}O_8$ (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 ($C2/m$, $c \simeq 7$ Å); whereas Srf, because

TABLE 2, Continued

h	k	F_{obs}	F_{calc}
-5	7	3.1	3.2
-7	7	9.9	10.1
-9	7	4.2	4.2
-11	7	7.2	7.2
-2	8	11.9	11.5
-4	8	10.4	9.1
-6	8	5.5	4.7
-8	8	34.3	34.6
-10	8	14.3	15.1
-1	9	8.1	7.5
-3	9	18.3	17.6
-5	9	16.3	16.2
-9	9	17.3	17.1
-2	10	12.4	12.1
-4	10	6.9	5.9
-6	10	17.4	17.4
-8	10	13.6	14.3
-10	10	15.9	17.0
-1	11	9.4	8.6
-3	11	24.7	24.6
-5	11	7.4	7.4
-7	11	9.2	9.6
-9	11	9.4	10.4
-2	12	31.0	31.4
-4	12	21.3	20.9
-6	12	26.3	26.7
-8	12	8.1	7.9
-1	13	27.2	27.0
-3	13	18.5	18.0
-5	13	12.8	12.6
-7	13	5.5	5.2
-2	14	8.6	7.5
-4	14	24.8	25.2
-6	14	11.7	11.5
-1	15	12.2	12.1
-5	15	7.8	7.4
-2	16	5.5	4.9
-4	16	4.8	3.8
	ℓ = 12		
0	0	3.9	2.9
2	0	32.3	33.3
4	0	9.6	9.7
1	1	21.5	22.2
3	1	9.6	10.0
5	1	3.2	3.1
0	2	19.0	19.9
4	2	24.9	26.4
1	3	28.0	28.0
3	3	27.9	29.3
5	3	26.9	27.4
0	4	7.6	8.2
4	4	10.3	10.8
1	5	19.0	19.7
3	5	39.0	39.0
5	5	21.0	22.0
0	6	12.1	11.5
2	6	13.9	13.7
4	6	2.7	3.3
1	7	16.9	17.0
3	7	13.0	13.5
0	8	27.5	28.3
4	8	27.5	27.5
1	9	24.7	24.3
3	9	5.9	4.7
0	10	5.0	4.2
2	10	15.3	15.9
1	11	7.6	7.1
3	11	24.1	23.9
0	12	8.8	8.0
2	12	3.7	4.6
1	13	11.8	11.1

h	k	F_{obs}	F_{calc}
-2	0	24.4	24.9
-4	0	27.7	27.3
-6	0	18.7	18.3
-8	0	33.3	31.8
-10	0	20.6	19.5
-1	1	40.7	41.5
-3	1	59.2	59.0
-5	1	43.5	42.0
-7	1	22.4	21.5
-9	1	8.9	7.2
-2	2	8.0	8.1
-6	2	25.8	25.5
-8	2	8.5	8.0
-10	2	22.6	21.1
-1	3	11.8	11.7
-3	3	15.5	15.4
-5	3	13.4	13.2
-7	3	16.4	15.9
-9	3	23.6	22.9
-11	3	15.8	15.6
-6	4	7.6	8.1
-8	4	2.8	2.7
-10	4	9.0	8.6
-1	5	14.2	13.1
-3	5	5.3	3.6
-5	5	11.5	10.8
-7	5	11.5	11.4
-9	5	26.5	25.8
-11	5	16.3	16.0
-2	6	12.9	13.2
-4	6	15.9	15.7
-6	6	12.8	12.6
-10	6	10.6	9.7
-1	7	31.3	31.0
-3	7	38.4	37.2
-5	7	30.8	29.8
-7	7	16.7	15.6
-9	7	8.2	8.6
-2	8	8.6	8.2
-4	8	4.1	4.1
-6	8	32.7	32.5
-8	8	9.2	9.5
-10	8	24.5	23.9
-1	9	21.7	21.2
-3	9	52.0	51.4
-5	9	26.2	25.2
-7	9	20.4	19.4
-2	10	10.6	10.1
-4	10	15.3	15.1
-6	10	11.7	11.0
-8	10	17.4	17.1
-1	11	18.6	18.2
-3	11	7.9	7.5
-5	11	17.2	17.2
-7	11	6.4	5.7
-9	11	14.8	14.9
-2	12	5.2	3.8
-4	12	7.8	7.7
-6	12	3.7	3.6
-1	13	5.8	5.3
-3	13	4.8	3.9
-5	13	5.2	5.5
-2	14	6.4	6.4
-4	14	5.6	4.5
-6	14	5.8	5.1
-3	15	20.7	20.2
	ℓ = 14		
0	0	9.4	7.7
2	0	21.3	22.3
4	0	14.1	14.3
1	1	15.1	15.6
3	1	15.8	16.6
0	2	30.9	32.4
2	2	11.2	11.7
4	2	21.5	23.0
1	3	7.7	7.2

h	k	F_{obs}	F_{calc}
3	3	13.8	14.7
0	4	39.2	41.0
2	4	22.6	24.7
4	4	17.1	12.8
1	5	19.4	20.0
0	6	11.6	11.5
2	6	26.8	27.9
1	7	12.4	12.1
3	7	5.4	5.3
0	8	17.7	17.0
1	9	28.0	28.2
0	10	9.6	9.8
2	10	11.9	13.0
1	11	9.0	9.8
0	12	13.3	13.7
-2	0	13.5	13.9
-4	0	10.9	10.2
-6	0	37.9	38.1
-8	0	3.0	5.3
-10	0	21.3	19.9
-1	1	30.0	31.8
-3	1	13.7	14.3
-5	1	12.4	11.6
-7	1	6.9	6.4
-9	1	16.3	15.3
-11	1	13.2	11.8
-2	2 *	4.6	3.8
-6	2	22.8	23.3
-8	2	14.9	16.2
-10	2	12.5	12.6
-1	3	5.6	3.7
-3	3	32.2	32.1
-5	3	15.7	15.6
-7	3	43.7	44.2
-9	3	19.9	19.3
-11	3	30.5	29.7
-2	4	33.1	33.1
-4	4	16.9	16.3
-8	4	13.3	13.3
-10	4	13.8	14.9
-1	5	19.3	19.2
-3	5	9.6	9.1
-5	5	42.6	41.6
-7	5	28.5	27.3
-9	5	34.6	33.8
-11	5	7.4	6.7
-2	6	33.1	33.5
-4	6	2.4	2.4
-6	6	23.1	22.6
-8	6	15.0	14.4
-10	6	3.8	3.9
-1	7	20.3	20.3
-3	7	16.7	17.1
-5	7	12.7	12.6
-7	7	11.9	11.0
-9	7	14.0	13.4
-2	8	16.6	15.9
-4	8	20.8	20.8
-8	8	27.7	27.4
-10	8	6.1	7.0
-1	9	6.8	7.0
-3	9	35.3	34.4
-5	9	13.0	12.2
-7	9	16.4	16.2
-9	9	2.4	2.2
-2	10	7.7	7.3
-6	10	17.0	11.5
-8	10	1.5	1.9
-1	11	19.3	18.9
-3	11	2.6	2.6
-5	11	24.3	23.5
-7	11	7.0	7.2
-2	12	27.2	27.2
-6	12	10.6	9.2
-3	13	13.1	13.3
-5	13	19.1	18.5

h	k	F_{obs}	F_{calc}
	ℓ = 16		
0	0	28.5	30.5
2	0	4.0	4.0
1	1	17.5	19.2
0	2	12.6	12.5
2	2	19.9	22.1
1	3	4.5	3.9
0	4	13.8	14.4
2	4	21.4	22.3
1	5	7.5	7.7
0	6	20.3	21.3
1	7	9.5	9.0
0	8	11.6	11.2
-2	0	12.6	12.4
-4	0	39.9	41.5
-6	0	17.1	16.2
-8	0	20.0	20.0
-10	0	5.0	4.7
-1	1	23.1	24.3
-3	1	9.2	9.3
-5	1	9.8	10.9
-7	1	27.0	27.7
-9	1	23.7	22.8
-2	2	24.6	26.0
-4	2	20.2	20.0
-6	2	24.0	24.0
-8	2	10.9	10.1
-10	2	12.4	12.0
-1	3	14.9	15.1
-3	3	4.9	4.8
-5	3	3.6	3.8
-2	4	16.7	16.7
-4	4	13.0	13.1
-6	4	15.3	15.4
-8	4	9.3	8.7
-10	4	16.2	15.2
-1	5	17.3	19.4
-3	5	4.9	4.6
-5	5	4.5	4.9
-7	5	8.8	8.7
-2	6	8.5	8.6
-4	6	19.7	20.3
-6	6	10.8	10.5
-8	6	12.6	12.4
-10	6	11.5	10.9
-1	7	16.9	17.9
-3	7	2.7	2.4
-5	7	4.8	4.6
-7	7	20.5	20.6
-9	7	15.2	13.6
-2	8	20.0	20.7
-4	8	20.9	20.7
-6	8	19.9	19.9
-8	8	11.0	10.1
-1	9	17.1	16.9
-3	9	9.9	10.2
-5	9	9.4	9.8
-7	9	23.1	22.9
-2	10	13.5	13.4
-4	10	24.3	23.9
-6	10	14.5	13.7
-5	11	5.6	5.4
	ℓ = 18		
0	0	29.7	31.8
-2	0	10.6	11.1
-4	0	26.1	26.7
-6	0	16.9	17.7
-8	0	23.0	23.1
-1	1	14.6	15.6
-3	1	7.2	6.9
-5	1	7.2	7.3
-7	1	12.3	11.9
-2	2	20.3	22.1
-4	2	5.5	4.5
-6	2	21.1	22.1

h	k	F_{obs}	F_{calc}
-3	2	6.5	6.8
-1	3	8.7	9.4
-3	3	32.8	34.0
-7	3	18.3	18.7
-9	3	13.2	12.6
-2	4	13.5	14.9
-4	4	13.3	14.7
-6	4	30.2	30.9
-8	4	20.7	20.8
-1	5	29.2	30.9
-3	5	16.7	17.3
-5	5	19.7	19.8
-9	5	2.3	2.4
-4	6	26.1	26.6
-6	6	3.4	3.8
-8	6	27.6	27.8
-1	7	7.2	7.1
-2	8	19.3	20.4
-6	8	8.5	8.4
-5	9	8.8	10.0
-4	0	1.2	1.3
-6	0	4.1	3.8
-3	1	17.7	18.8
-5	1	32.4	34.2
-7	1	13.6	10.1
-4	2	7.5	5.2
-3	3	11.1	11.2
-7	3	9.7	10.0
-6	4	8.1	8.0
	ℓ = 1		
0	1	0.9	1.2
4	1	0.3	0.4
6	1	4.2	4.1
1	2	4.4	4.8
0	3	4.0	5.0
2	3	1.5	1.5
6	3	1.0	0.8
1	4	2.1	2.0
3	4	1.1	1.1
5	4	2.8	2.7
0	5	2.1	2.5
2	5	4.2	4.0
6	5	2.9	2.9
1	6	5.7	6.1
3	6	2.0	1.6
0	7	0.4	0.3
4	7	5.4	5.1
1	8	1.7	2.5
3	8	8.4	8.5
5	8	2.3	2.4
0	9	4.4	4.9
2	9	1.7	2.4
4	9	2.8	3.4
1	10	5.1	5.9
0	11	4.9	4.6
2	11	1.8	1.7
1	12	1.0	0.7
-2	1	1.2	1.0
-4	1	1.8	1.2
-6	1	3.0	3.9
-1	2	3.0	4.1
-3	2	3.6	3.6
-5	2	3.5	3.9
-7	2	2.0	2.1
-2	3	2.9	3.9
-6	3	3.2	4.0
-1	4	2.8	2.0
-3	4	1.8	2.3
-5	4	5.4	5.8
-2	5	3.7	4.1
-6	5	2.1	2.3
-3	6	3.0	3.0

h	k	F_{obs}	F_{calc}
-5	6	2.9	4.1
-2	7	5.0	4.9
-4	7	1.3	1.2
-6	7	2.9	2.7
-1	8	6.3	6.2
-3	8	1.9	2.0
-4	9	1.4	1.3
-1	10	1.6	2.6
-3	10	4.7	4.6
-2	11	4.1	3.3
-1	12	3.1	3.4
	ℓ = 3		
0	1	4.6	5.5
2	1	4.4	4.8
4	1	3.3	3.3
6	1	2.2	2.0
1	2	1.4	1.7
3	2	4.9	4.1
0	3	1.5	1.7
2	3	1.4	1.2
4	3	4.0	3.7
1	4	2.4	1.9
5	4	2.6	2.5
0	5	3.5	3.6
2	5	2.5	2.8
4	5	5.7	5.7
1	6	3.2	3.2
3	6	4.0	4.3
0	7	4.4	4.6
2	7	2.8	2.6
4	7	1.4	1.3
1	8	6.0	6.8
3	8	2.9	3.5
0	9	3.9	3.6
1	10	2.5	2.2
3	10	3.6	3.8
0	11	3.7	2.9
2	11	4.3	4.1
-2	1	3.8	3.8
-4	1	3.8	2.4
-6	1	5.4	5.4
-1	2	5.6	7.0
-3	2	2.0	1.7
-5	2	2.7	2.4
-7	2	5.5	5.5
-2	3	3.1	2.7
-4	3	3.1	3.4
-6	3	1.6	2.6
-1	4	1.4	1.2
-3	4	3.1	2.9
-5	4	1.7	1.5
-7	4	1.0	1.9
-4	5	3.6	4.0
-6	5	3.7	3.1
-1	6	2.0	2.8
-3	6	3.6	3.5
-5	6	4.4	5.4
-2	7	6.0	6.6
-4	7	3.6	3.7
-1	8	3.0	2.9
-3	8	2.3	2.5
-5	8	7.8	8.0
-2	9	7.7	7.6
-4	9	8.0	8.4
-1	10	4.3	3.0
-3	10	4.7	5.3
-1	12	4.7	5.2
	ℓ = 5		
0	1	4.8	4.8
2	1	6.5	6.1
4	1	1.2	1.0
1	2	1.1	0.8
3	2	4.8	4.6
5	2	2.4	2.2

h	k	F_{obs}	F_{calc}
0	3	2.1	1.8
3	4	1.0	0.7
5	4	1.2	1.0
0	5	4.4	4.2
2	5	4.8	5.2
4	5	1.3	1.0
1	6	3.5	3.4
3	6	4.8	4.9
0	7	2.0	1.5
2	7	7.6	7.7
4	7	1.9	1.2
1	8	2.6	2.1
3	8	7.0	6.7
0	9	9.0	9.0
2	9	5.4	4.3
1	10	1.5	2.3
-2	1	6.3	6.3
-4	1	3.0	3.3
-6	1	7.5	7.2
-8	1	1.6	1.5
-1	2	1.1	1.5
-3	2	1.9	1.9
-5	2	10.2	9.6
-7	2	2.9	3.8
-2	3	0.9	0.7
-4	3	6.9	6.8
-6	3	4.2	3.8
-1	4	2.8	3.8
-3	4	1.4	1.0
-5	4	4.2	4.1
-7	4	3.1	3.6
-4	5	6.1	6.2
-3	6	5.0	5.2
-5	6	5.0	5.3
-7	6	6.0	6.4
-2	7	7.6	7.3
-4	7	5.7	6.4
-6	7	3.2	2.5
-1	8	1.2	0.8
-3	8	1.8	2.0
-5	8	2.1	2.3
-2	9	1.9	1.4
-4	9	3.6	3.6
-1	10	2.1	2.1
-3	10	3.1	3.3
-2	11	4.4	3.9
	ℓ = 7		
0	1	2.7	3.3
2	1	4.5	5.0
4	1	3.0	3.0
1	2	4.4	4.4
3	2	2.9	3.1
0	3	2.1	1.3
4	3	2.6	2.9
1	4	3.4	3.0
3	4	4.1	4.6
0	5	2.1	1.9
2	5	2.2	2.4
1	6	3.8	3.0
3	6	2.2	1.6
2	7	4.3	3.6
1	8	5.3	4.9
0	9	5.2	4.6
-2	1	7.7	7.5
-4	1	3.7	3.3
-6	1	5.7	5.6
-8	1	1.9	1.3
-1	2	4.0	4.1
-3	2	2.2	2.2
-7	2	3.1	2.6
-4	3	6.4	5.7
-6	3	4.6	4.3
-1	4	2.7	2.9
-5	4	1.4	1.3
-7	4	3.8	2.3
-3	5	3.8	3.7
-5	5	3.9	3.5

h	k	F_{obs}	F_{calc}
-6	3	4.4	4.3
-1	4	1.4	1.3
-3	6	6.8	6.3
-5	6	1.7	1.8
-2	7	0.7	0.5
-4	7	5.4	5.6
-6	7	7.9	7.8
-1	8	7.6	7.4
-3	8	2.0	1.3
-5	8	8.1	8.3
-2	9	4.8	4.2
-1	10	0.7	0.6
-3	10	6.8	6.1
	ℓ = 9		
0	1	5.3	5.9
1	2	4.6	5.2
3	2	2.1	1.4
0	3	2.1	2.4
1	4	1.7	1.9
0	5	8.6	8.6
2	5	2.4	2.6
1	6	2.1	2.4
0	7	5.2	5.6
-2	1	7.6	7.7
-4	1	10.5	9.9
-6	1	9.6	9.3
-1	2	2.9	3.7
-3	2	4.1	3.2
-5	2	13.4	12.9
-7	2	3.8	3.1
-4	3	2.9	3.2
-6	3	1.1	1.4
-1	4	4.1	4.4
-3	4	4.4	4.5
-7	4	8.0	7.7
-2	5	1.4	1.0
-4	5	8.6	8.4
-6	5	5.4	5.5
-1	6	3.5	2.2
-3	6	3.1	3.2
-5	6	3.9	3.6
-2	7	7.7	8.1
-4	7	8.1	7.7
-1	8	8.5	8.3
-5	8	4.3	4.6
-2	9	6.3	6.6
	ℓ = 11		
0	1	2.0	1.8
0	3	1.2	0.9
0	5	3.8	3.1
-2	1	3.5	3.7
-4	1	3.2	3.2
-6	1	1.5	1.7
-1	2	2.1	2.3
-3	2	2.3	1.7
-4	3	4.1	3.6
-3	4	5.6	4.8
-5	4	1.7	1.0
-2	5	3.0	3.2
-4	5	5.2	5.2
-1	6	2.5	2.3
-3	6	2.2	2.3
-5	6	3.1	2.8
-2	7	5.1	5.6
-4	7	5.0	5.0
	ℓ = 13		
-2	1	7.1	7.1
-4	1	9.8	9.3
-3	2	3.5	3.2
-5	2	6.7	6.5
-2	3	3.6	3.8
-4	3	1.1	1.1

of its highly ordered Al/Si arrangement, has a doubled cell ($c \simeq 14$ 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, O_A2 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 ($\langle T_1O\text{–O}\rangle = 1.627$, $\langle T_1z\text{–O}\rangle = 1.732$, $\langle T_2O\text{–O}\rangle = 1.736$, $\langle T_2z\text{–O}\rangle = 1.630$ Å), when compared with $\langle$Si–O$\rangle$ = 1.613 Å and $\langle$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 ($\langle T_1\text{–O}\rangle = 1.670$, $\langle T_2\text{–O}\rangle = 1.657$ 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 $I2/c$ $SrAl_2Si_2O_8$ and a Listing of Parameter Shifts from the Positions of the Atoms in the "Average" $C2/m$ Structure*

Atom	x	y	z
	Atomic Coordinates		
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)
$T_2(0)$	.6934(2)	.1200(1)	.1706(1)
$T_2(z)$	.6845(2)	.1137(1)	.6716(1)
$O_A(1)$	.0045(4)	.1289(4)	.0003(2)
$O_A(2)$	.5911(7)	.0002(3)	.1427(4)
$O_B(0)$	.8267(6)	.1266(4)	.1054(3)
$O_B(z)$	.8104(6)	.1263(4)	.6113(3)
$O_C(0)$	.0132(6)	.2984(4)	.1186(3)
$O_C(z)$	.0188(6)	.3090(4)	.6304(3)
$O_D(0)$	.1876(6)	.1245(4)	.1955(3)
$O_D(z)$	.1960(6)	.1190(4)	.7027(3)
	Parameter Shifts		
Sr	---	-0.0020(1)	---
T_1	+0.0017(2)	-.0014(1)	-0.0040(1)
T_2	+.0044(2)	+.0031(1)	-.0005(1)
O_A1	+.0045(4)	---	+.0003(2)
O_A2	---	+.0002(3)	---
O_B	+.0081(6)	+.0003(4)	-.0029(3)
O_C	-.0028(6)	-.0053(4)	-.0059(3)
O_D	-.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 $SrAl_2Si_2O_8$, 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-feldspars 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 (⟨Sr–O⟩ = 2.691 Å) and celsian (⟨Ba,K–O⟩ = 2.863 Å; Newnham and Megaw, 1960) are monoclinic, and $P\bar{1}$ anorthite with its smaller M cation (⟨Ca^{VII}–O⟩ = 2.517 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 $SrAl_2Si_2O_8$*

Atom	B(Å^2)	Anisotropic temperature factors (× 10^4)					
		β_{11}	β_{22}	β_{33}	β_{12}	β_{13}	β_{23}
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)
$T_1(z)$	0.69(5)	36(3)	16(1)	4(1)	-2(2)	6(1)	0(1)
$T_2(0)$	0.64(5)	19(3)	16(1)	4(1)	-2(1)	1(1)	-1(1)
$T_2(z)$	0.67(4)	35(3)	12(1)	6(2)	1(1)	5(1)	1(1)
$O_A(1)$	0.9(1)	39(7)	23(3)	6(3)	9(3)	8(3)	-2(2)
$O_A(2)$	0.9(1)	30(8)	17(3)	13(2)	8(3)	-3(4)	4(2)
$O_B(0)$	1.2(1)	57(8)	28(3)	12(2)	-2(4)	17(4)	-2(2)
$O_B(z)$	1.2(1)	36(8)	31(3)	17(3)	-13(4)	16(4)	0(2)
$O_C(0)$	1.1(1)	43(7)	26(3)	7(3)	-11(4)	0(3)	-4(2)
$O_C(z)$	1.2(1)	43(8)	21(3)	18(3)	-5(4)	13(4)	-2(2)
$O_D(0)$	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 *I*2/*c* $SrAl_2Si_2O_8$*

	T-O distances		O-O distances	O-*T*-O angles
***T*$_1$(0) tetrahedron**				
$T_1(0)$-$O_A(1)$	1.644	$O_A(1)$-$O_B(0)$	2.525	101.5
-$O_B(0)$	1.617	-$O_C(0)$	2.754	115.5
-$O_C(0)$	1.612	-$O_D(0)$	2.544	101.9
-$O_D(0)$	1.633	$O_B(0)$-$O_C(0)$	2.683	112.4
		-$O_D(0)$	2.739	114.9
		$O_C(0)$-$O_D(0)$	2.658	110.0
Mean	1.627		2.651	109.4
***T*$_1$(z) tetrahedron**				
$T_1(z)$-$O_A(1)$	1.755	$O_A(1)$-$O_B(z)$	2.655	99.6
-$O_B(z)$	1.721	-$O_C(z)$	2.943	115.9
-$O_C(z)$	1.716	-$O_D(z)$	2.661	99.4
-$O_D(z)$	1.735	$O_B(z)$-$O_C(z)$	2.888	114.3
		-$O_D(z)$	2.929	115.9
		$O_C(z)$-$O_D(z)$	2.836	110.5
Mean	1.732		2.819	109.3
***T*$_2$(0) tetrahedron**				
$T_2(0)$-$O_A(2)$	1.738	$O_A(2)$-$O_B(0)$	2.788	106.8
-$O_B(0)$	1.734	-$O_C(0)$	2.680	101.1
-$O_C(0)$	1.732	-$O_D(0)$	2.779	106.1
-$O_D(0)$	1.739	$O_B(0)$-$O_C(0)$	2.884	112.6
		-$O_D(0)$	2.893	112.8
		$O_C(0)$-$O_D(0)$	2.944	116.0
Mean	1.736		2.828	109.2
***T*$_2$(z) tetrahedron**				
$T_2(z)$-$O_A(2)$	1.641	$O_A(2)$-$O_B(z)$	2.642	107.8
-$O_B(z)$	1.629	-$O_C(z)$	2.542	102.9
-$O_C(z)$	1.609	-$O_D(z)$	2.663	108.5
-$O_D(z)$	1.641	$O_B(z)$-$O_C(z)$	2.707	113.4
		-$O_D(z)$	2.678	109.9
		$O_C(z)$-$O_D(z)$	2.723	113.8
Mean	1.630		2.659	109.4

	Sr-O distances		*T*-O-*T* angles
Sr-$O_A(1)$	2.630	$T_1(0)$-$O_A(1)$-$T_1(z)$	137.8
-$O_A(1)$	2.650	$T_2(0)$-$O_A(2)$-$T_2(z)$	127.7
-$O_A(2)$	2.445	$T_1(0)$-$O_B(0)$-$T_2(0)$	144.4
-$O_B(0)$	2.746	$T_1(z)$-$O_B(z)$-$T_2(z)$	145.6
-$O_B(z)$	2.855	$T_1(0)$-$O_C(0)$-$T_2(0)$	129.6
-$O_D(0)$	2.769	$T_1(z)$-$O_C(z)$-$T_2(z)$	132.3
-$O_D(z)$	2.743	$T_1(0)$-$O_D(0)$-$T_2(0)$	139.7
-$O_C(0)$	3.229	$T_1(z)$-$O_D(z)$-$T_2(z)$	138.1
-$O_C(z)$	3.010	Mean	136.9

*Estimated standard error for all *T*-O and Sr-O bond lengths is 0.005 Å, for O-O distances 0.007 Å, and for O-*T*-O and *T*-O-*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.

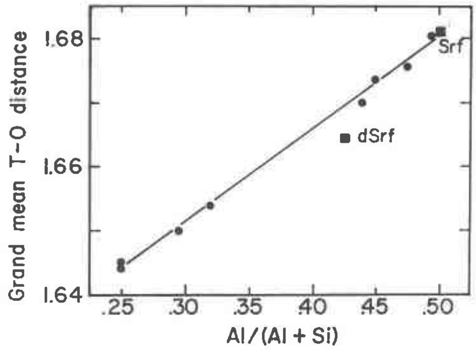

FIG. 2. Grand mean *T–O* distances *versus* Al/(Al + Si) for a variety of feldspars. In order of increasing ⟨⟨*T*–O⟩⟩, they are high and low albite, An_{16}, An_{28}, dSrf, An_{78}, An_{80}, celsian *P*$\bar{1}$ anorthite, and Srf. See Ribbe *et al* (1974) for references.

Phillips, Kroll, Pentinghaus, and Ribbe (1975) have found that the parameter ⟨*M*–O⟩/⟨⟨*T*–O⟩⟩ 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 $M^{2+}Al_2Si_2O_8$ (Fig. 4), except that the slope of the feldspar line is only one-fourth as great as that of the paracelsian line, and ⟨*T*–O–*T*⟩ 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

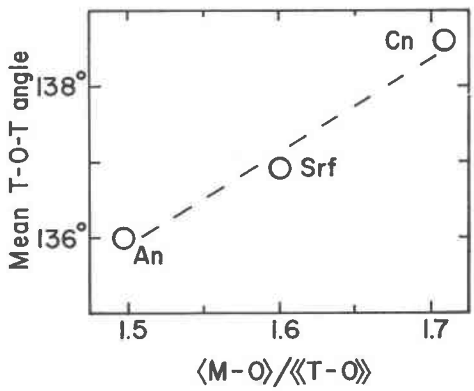

FIG. 3. Mean *T–O–T* angle *versus* the mean *M–O* distance (assuming 7-coordination) divided by the grand mean *T–O* distance for three feldspar structures: An (anorthite, Wainwright and Starkey, 1971), Srf ($SrAl_2Si_2O_8$, this paper), Cn (celsian, Newnham and Megaw, 1960).

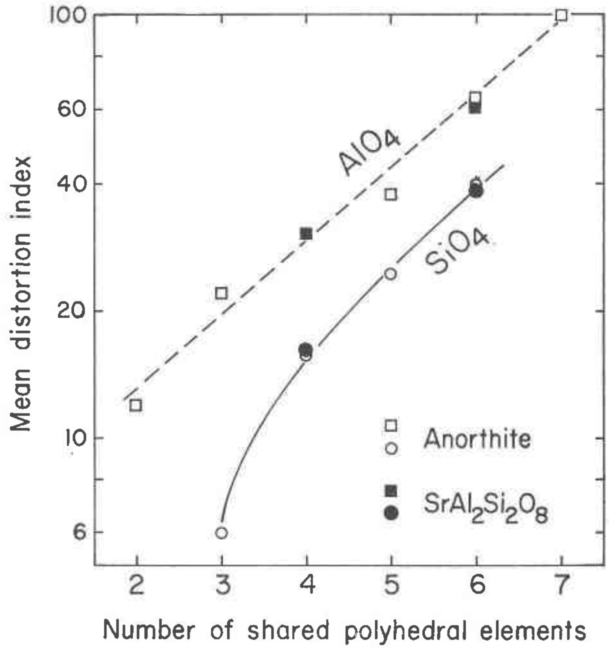

FIG. 4. Mean distortion index σ_{tet}^2, as defined by Robinson *et al* (1970), plotted against the number of shared polyhedral elements (edges plus corners) for AlO_4 and SiO_4 tetrahedra in anorthite (open symbols) and Srf (dark symbols). *Cf* Fig. 8, p. 41, in Ribbe *et al* (1974).

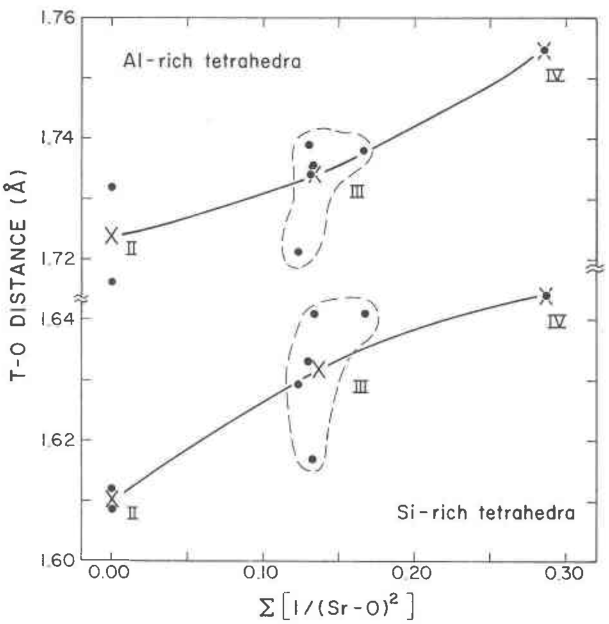

FIG. 5. Individual T–O distances in Srf plotted against the parameter $\Sigma[1/(\text{Sr–O})^2]$ and grouped according to whether the oxygen atom involved in the T–O bond is 2-, 3-, or 4-coordinated (Roman numerals). Large X's indicate mean values for each coordination number.

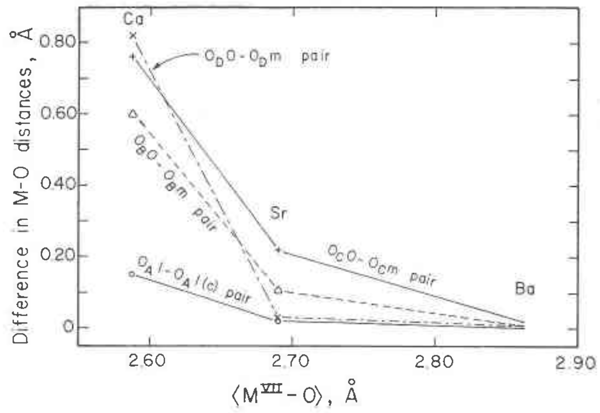

FIG. 6. Differences in interatomic distances for the pseudo-symmetrically related pairs of M–O bonds plotted against mean M–O distances for the seven-coordinated polyhedra in anorthite (Ca; values represent the means for 4 M atoms), in Srf, and in celsian (Ba).

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 O_C0 and O_Cm atoms. It is ~0.28 for the 4-coordinated O_A1 atom and 0.12 to 0.16 for the 3-coordinated O_A2, 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 (O_A1) 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 $C2/m$ ($c \simeq 7$ 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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