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Crystal-structure refinement of high sanidine from the upper mantle

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ABSTRACT

The crystal structure of a high sanidine from a coesite-sanidine grospydite nodule from the Roberts Victor kimberlite in South Africa has been refined using 2150 independent X-ray reflections to a final R of 0.055 (R_{wt} = 0.047). Microprobe analyses of the same grain indicate a composition of $Or_{97.6}Ab_{1.8}An_{0.2}Cn_{0.4}$. Cell parameters ($a$ = 8.595(3) Å; b = 13.028(5) Å; c = 7.175(2) Å; β = 115.94(2)°) are consistent with the high Or content of the sanidine (Or_{calc} = 97.7%) and suggest very high Al-Si disorder. Mean T–O distances are 1.644 Å for T_1 and 1.639 Å for T_2, indicating an Al occupancy of 0.266 and 0.234 for T_1 and T_2, respectively; thus an apparent slight residual preference of Al for T_1 is observed. Madelung site energies were calculated based on this refinement and a tetrahedral-cation charge of 3.75. These indicate that the T_1 site has a slightly shallower potential well (~16 kcal/mol) than T_2. The very high disorder observed in this grain coupled with its long-term exposure to high P and T conditions in the upper mantle suggest that it may represent a more disordered state than is attainable at lower pressure.

INTRODUCTION

The petrologic significance of alkali feldspars and the relationship of their structural state and ordering to their thermal history have led to much study of Al-Si order-disorder in the structure (e.g., Ribbe and Gibbs, 1969; Smith, 1974; Kroll and Ribbe, 1983). In the past (Cole et al., 1949; Ribbe, 1963; Weitz, 1972), the most disordered state was obtained by heating natural or synthetic minerals above 1000°C for prolonged periods; recent experiments have subjected alkali feldspar to heating for thousands of hours (M. Sacerdoti, pers. comm.). Despite these attempts to synthesize very disordered alkali feldspars, residual ordering is always observed: the Al content of the T_1 site (t_1) has never been reported to be less than 0.27.

We report here on the structure of a natural high sanidine that, as a result of its unusual occurrence, equals or slightly exceeds previous heat-treated specimens in Al disorder. The mineral is a primary phase of a coesite-sanidine grospydite nodule found in the Roberts Victor kimberlite (Smyth and Hatton, 1977). Modal mineralogy of the nodule is Ca-Eskola–rich clinopyroxene, 56.8%; grossular-pyrope garnet, 22.7%; kyanite, 13.6%; coesite, 1.7%; quartz (after coesite), 3.5%; sanidine 0.9%; serpentine (alteration) 0.8%; sulfides 0.1%. Estimates of pressure and temperature of equilibration for this nodule are 48–50 kbar and 1050–1125°C (Wohletz and Smyth, 1984; McCormick and Smyth, 1986). Quenching was sufficiently rapid to preserve large crystals of coesite, so the nodule probably did not spend more than a few hours above 700°C during ascent (Smyth and Hatton, 1977). The occurrence of near end-member high sanidine in eclogite nodules, though rare, has also been reported by McGee and Hearn (1984) and Ater et al. (1984) in North American kimberlites.

Previously reported alkali feldspar structures show slightly lower Al-Si disorder and/or Or contents. This refinement is therefore submitted as a reference example of the end-member high sanidine structure at room temperature and pressure.

ANALYTICAL METHOD AND RESULTS

A crystal of sanidine was removed from the interior of the nodule. A fragment of the grain measuring 320 × 440 × 400 μm was used for the refinement. Initial optical examination revealed no fractures, twins, or inclusions. Microprobe analyses of fragments of the same grain as used in the refinement and several other grains of sanidine from the nodule (Table 1) indicate a near end-member composition (Or_{97-98}). Because of the unusual occurrence of the mineral, BaO, SrO, and Rb_2O were included in later analyses. BaO content is ~1400 ppm (a greater impurity than Ca); SrO and Rb_2O were below detection limits (<0.01 wt%). The grains are nearly uniform in composition, as evidenced by the low standard deviations for averages of analyses both among and within grains.

Measurements of optical parameters were generously provided by Shu-Chun Su and John Phelps at Virginia Polytechnic Institute and State University, using universal-stage data reduced by the EXCALIBUR computer program developed by F. Donald Bloss. The value of $2V_X$ for the grain used in the structure analysis is 48.1° at λ = 486 nm, 46.1° at λ = 589 nm, 45.1° at λ = 656 nm;

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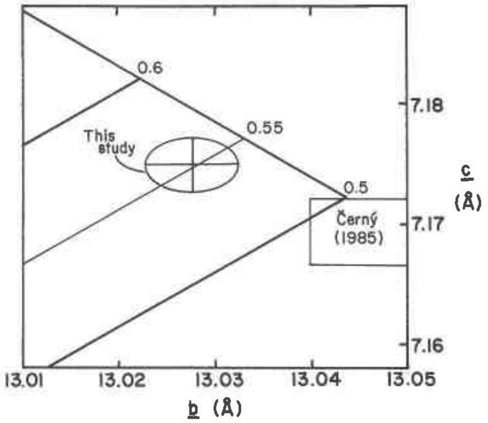

Fig. 1. *b-c* plot for monoclinic alkali feldspars in the region of high sanidine showing results of cell-edge refinement for the sanidine (figure adapted from Kroll and Ribbe, 1983). Numbers along the upper diagonal line refer to calculated $2t_1$ value. Recent cell-edge measurements of high-sanidine adularia (presumably quenched from a vapor phase) are shown for comparison (Černý, 1985; see also Černý and Chapman, 1986).

dispersion is $v > r$. The $2V_X$ parameter is very sensitive to ordering in alkali feldspar; a comparison of this value with those published in Kroll and Ribbe (1983) for other alkali feldspars indicates the grain is as disordered as any previously observed, within the scatter of the data.

Cell parameters obtained by least-squares refinement of 25 strong reflections of 2θ between 30° and 48° (Mo$K\alpha$ radiation) are reported in Table 2. The Or content calculated from cell volume (using the equation of Kroll and Ribbe, 1983) is 97.7%, in good agreement with microprobe data. Cell parameters indicate a near end-member $C2/m$ high sanidine structure in both composition and Al-Si disorder (see Fig. 1 and Table 2). However, vapor-deposited adularia with cell parameters (determined by powder techniques) even closer to the theoretical limits of high sanidine have recently been reported from pegmatite cavities and hydrothermal veins (Černý 1985; Černý and Chapman, 1986). The data are shown for comparison in Figure 1. As yet, no refinement exists for these grains.

TABLE 1. Averaged microprobe analyses of sanidines

	A: Grains in thin sections*		B: Grain used for refinement**	
Oxide	Wt%	Atoms/ formula unit	Wt%	Atoms/ formula unit
SiO_2	64.66(25)	3.000	65.07(36)	2.998
Al_2O_3	18.36(12)	1.004	18.54(27)	1.007
		4.004		4.005
FeO	0.05(4)	0.002	0.04(2)	0.002
TiO_2	0.02(1)	0.001	0.01(1)	0.000
Cr_2O_3	0.02(1)	0.001	0.02(1)	0.001
MgO	<0.01	0.0	0.02(1)	0.001
MnO	<0.01	0.0	0.03(1)	0.001
NiO	0.02(1)	0.001	0.02(1)	0.001
CaO	0.03(1)	0.002	0.03(1)	0.002
Na_2O	0.12(4)	0.011	0.19(16)	0.017
K_2O	16.25(17)	0.962	15.87(29)	0.933
BaO	0.14(7)	0.003	0.13(5)	0.004
	99.67	0.981	99.97	0.962

Composition: A = $Or_{98.5}Ab_{1.1}An_{0.1}Cn_{0.3}$
B = $Or_{97.6}Ab_{1.8}An_{0.2}Cn_{0.4}$

Orthoclase composition predicted from cell volume (Kroll and Ribbe, 1983):

$$n_{Or} = -584.668 + 2.587(V) - (3.835 \times 10^{-3})(V^2) + (1.9043 \times 10^{-6})(V^3)$$

$$V = 722.383\ \text{Å}^3$$

$$n_{Or}\ (\text{calc}) = 0.9767$$

Note: Estimated standard errors in last figure are shown in parentheses.

* Average of 24 analyses from Smyth and Hatton (1977), Smyth (unpub. data, 1980), Drexler (pers. comm., 1986) and Solberg (pers. comm., 1986). Solberg also reported <0.01% of Rb_2O, SrO, ZnO, P_2O_5, F and Cl.

** Average of 11 analyses taken from four fragments of the grain used for the structure refinement.

TABLE 2. High sanidine structural parameters

Unit cell

$a = 8.595(3)$ Å
$b = 13.028(5)$ Å
$c = 7.175(2)$ Å
$\beta = 115.94(2)°$
$V = 722.383$ Å³

Atomic coordinates

Atom	x	y	z
K	0.28660(9)	0	0.1380(1)
T_1	0.00991(7)	0.18560(4)	0.22381(8)
T_2	0.71075(7)	0.18813(4)	0.34438(8)
O_{A1}	0	0.1470(1)	0
O_{A2}	0.6400(3)	0	0.2849(3)
O_B	0.8302(2)	0.1476(1)	0.2269(2)
O_C	0.0351(2)	0.3105(1)	0.2569(2)
O_D	0.1789(2)	0.1265(1)	0.4038(2)

Anisotropic temperature factors (factors × 10^4)

Atom	β_{11}	β_{22}	β_{33}	β_{12}	β_{13}	β_{23}
K	68(1)	36.9(4)	150(2)	0	38(1)	0
T_1	44.2(7)	11.2(2)	54(1)	−3.8(3)	26.2(7)	−1.9(4)
T_2	43.5(8)	7.4(2)	62(1)	−1.0(3)	23.5(7)	0.0(3)
O_{A1}	101(4)	17.4(9)	88(4)	0	47(3)	0
O_{A2}	75(3)	12.3(8)	117(5)	0	22(3)	0
O_B	83(2)	31.3(8)	121(4)	−7(1)	57(3)	−0(1)
O_C	71(2)	15.6(7)	108(3)	−2(1)	35(2)	−5(1)
O_D	78(2)	19.2(7)	82(3)	3(1)	23(2)	1(1)

Note: Estimated standard errors in last figure are shown in parentheses.

Our structure refinement is based on 2150 observed independent reflections. Intensities of 6927 reflections, up to 80° 2θ, were measured on a Nicolet automated four-circle diffractometer. Corrections were made for polarization and Lorentz effects. An absorption correction derived from the variation of intensity of ten reflections with 2θ ranging from 8° to 65° through full rotations of psi was applied to the data. Transmission factors ranged from 0.529 to 0.316. Symmetrically equivalent reflections were combined to yield 2332 independent data points with an R for averaging of 0.020. From this set, 175 weak ($F_{obs} < 3\sigma$) and seven anomalous (high F_{obs}/F_{calc} ratio) structure factors were removed. Several of the latter group had anomalous peak profiles containing "notches" or dual peaks in the scans. This is tentatively attributed to submicroscopic twin lamellae in the crystal. However, examination of other sanidine crystals from the nodule using transmission-electron microscopy did not reveal any twinning or exsolution. Least-squares refinements of po-

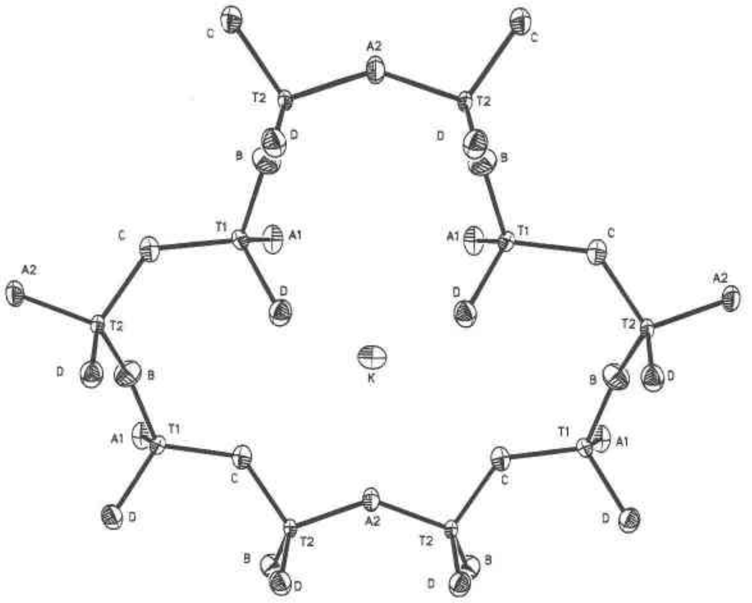

Fig. 2. Projection down c^* of sanidine from this refinement (inverted "dog-face" projection). The horizontal direction is parallel to b and the vertical is parallel to a. Anisotropic thermal-vibration ellipsoids are shown for each atom.

sitional and anisotropic thermal parameters using the RFINE program (Finger and Prince, 1975) gave an R value of 0.055 and an R_{wt} of 0.047. Observed and calculated structure factors from the final refinement cycle are presented in Table 3.[1] Atom positions and anisotropic temperature factors are reported in Table 2. A direct refinement of Al and Si tetrahedral-site occupancy was not attempted.

Anisotropic thermal-vibration ellipsoids are relatively large (Table 4). The sizes of the ellipsoids are the result of a combination of positional disorder, expected to be significant in this structure, and true thermal vibration. Positional disorder and thermal-vibration effects contribute to the refinement residual (R) of 0.055. An examination of Figure 2 shows that the calculated ellipsoids are not greatly distorted from spherical. Therefore no attempt was made to refine the structure using split atom positions. Although no difference Fourier calculations were done, the R value observed is consistent with previously reported values for disordered feldspar. We assume that most of the apparent misfit is due to positional disorder that is not properly modeled by thermal oscillations.

Bond lengths derived from the refinement are reported in Table 5. Potassium-oxygen distances (K-O) are slightly larger than those reported in previous studies (Phillips and Ribbe, 1973; Smith, 1974; Kroll and Ribbe, 1983) consistent with the more potassic composition of this specimen (Table 2). Assigning a definite coordination number to the large cation site is somewhat arbitrary. We report ten K-O distances less than 3.6 Å for the structure. Tetrahedral bond lengths overlap considerably between the two tetrahedra and indicate nearly equal tetrahedral size. Mean bond lengths are 1.644 Å for T_1 and 1.639 Å for T_2. A comparison of individual T-O distances with the order parameter $c - 0.4b$ (Hovis et al., 1970) for this grain and previous refinements (Fig. 3) shows close correlation among all analyses, with the sanidine of this study

TABLE 4. Thermal-vibration ellipsoids for high sanidine

Atom	Axis	RMS amplitude	Angle (°) with a	Angle (°) with b	Angle (°) with c	Equivalent isotropic B
K	1	0.143	23	90	93	2.259
	2	0.178	90	180	90	
	3	0.183	113	90	3	
T_1	1	0.093	62	29	104	0.874
	2	0.101	61	107	162	
	3	0.120	42	112	79	
T_2	1	0.080	85	5	92	0.851
	2	0.113	43	94	158	
	3	0.115	48	93	67	
O_{A1}	1	0.123	90	0	90	1.662
	2	0.131	71	90	173	
	3	0.176	19	90	97	
O_{A2}	1	0.103	90	0	90	1.669
	2	0.142	126	90	117	
	3	0.180	143	90	27	
O_B	1	0.134	147	112	44	1.946
	2	0.161	97	126	132	
	3	0.173	58	136	80	
O_C	1	0.114	88	12	80	1.545
	2	0.147	142	81	101	
	3	0.155	128	98	15	
O_D	1	0.125	78	143	66	1.603
	2	0.132	94	125	135	
	3	0.166	167	98	54	

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[1] To receive a copy of Table 3, order Document AM-87-357 from the Business Office, Mineralogical Society of America, 1625 I Street, N.W., Suite 414, Washington, D.C. 20006, U.S.A. Please remit $5.00 in advance for the microfiche.

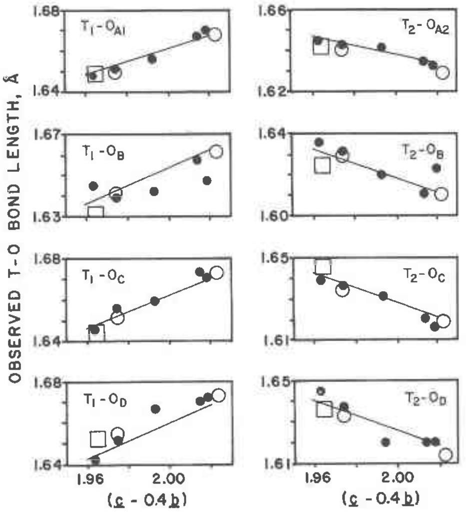

Fig. 3. Plot of T–O distances for each T–O pair for this sanidine and others reported in Phillips and Ribbe (1973) vs. the order parameter $c - 0.4b$. Square indicates this study; solid circles indicate X-ray work done by Phillips and Ribbe (1973), Colville and Ribbe (1968), and Ribbe (1963); open circles are data from neutron refinements by Brown et al. (1974) and Prince et al. (1972). Figure adapted from Phillips and Ribbe, 1973.

TABLE 5. Bond lengths and bond angles

	Tetrahedral bond lengths (Å)				
	Obs	Calc*		Obs	Calc
T_1–O_{A1}	1.649(1)	1.650	T_2–O_{A2}	1.641(2)	1.646
–O_B	1.631(2)	1.638	–O_B	1.634(2)	1.632
–O_C	1.644(2)	1.648	–O_C	1.646(2)	1.642
–O_D	1.652(2)	1.645	–O_D	1.636(2)	1.639
Average	1.644(1)			1.639(1)	
	Grand mean = 1.642(1)				
T–O–T angle		angle (°)		1/cos(T–O–T)	
T_1–O_{A1}–T_1		144.47		−1.2288	
T_2–O_{A2}–T_2		139.33		−1.3184	
T_1–O_B–T_2		152.96		−1.1227	
T_1–O_C–T_2		130.90		−1.5273	
T_1–O_D–T_2		141.36		−1.2803	
Average T_1		142.43		−1.2898	
Average T_2		141.13		−1.3122	
	K–O bond lengths (Å)				
K–O_{A2}	2.744(1)		K–O_B	3.042(1)	
–O_{A1}	2.929(1)		–O_C	3.129(1)	
–O_D	2.959(1)		–O_{A2}	3.358(1)	

Note: Estimated standard errors in last figure are shown in parentheses.
* Calculated T–O lengths are from formulae in Phillips and Ribbe, 1973.

plotting near the heated Spencer C values given in Phillips and Ribbe (1973). The equations derived by Phillips and Ribbe (1973) for calculation of individual T–O distances as a function of $c - 0.4b$ yield values in close agreement with those observed.

A plot of T–O bond length vs. 1/cos(T–O–T) shows a positive correlation, though much better for the T_2 tetrahedron than T_1 (Fig. 4). Correlation coefficients (r) for the two plots are 0.37 (T_1) and 0.95 (T_2). T–O–T angle has the second strongest correlation with T–O distances (after Al occupancy of the site; Phillips and Ribbe, 1973). Most of the angles measured agree within 0.3° of those reported by Phillips and Ribbe (1973); however, the T_2–O_{A2}–T_2 angle is more than 1.4° larger here.

Several independent methods suggest that the Al-Si disorder of this grain is exceedingly high. Applying the T–O distance techniques outlined by Kroll and Ribbe (1983), average Al occupancy in the T_1 site (t_1) is 0.266, and that in the T_2 site (t_2) is 0.234. Other methods (using

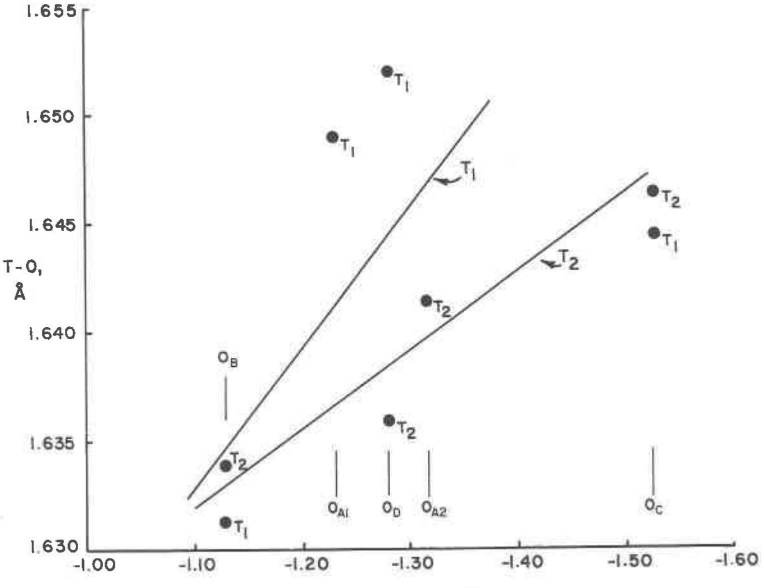

Fig. 4. T–O distance vs. 1/cos(T–O–T) for this sanidine. Correlation coefficients for the two tetrahedra are 0.37 (T_1) and 0.95 (T_2).

cell dimensions and optical data) resulted in t_1 values of 0.277 (*b-c* relationship; Stewart and Wright, 1974), 0.279 ($2V_X$ method, Su et al., 1983), and 0.291 (tr[110] method; Kroll, 1973; tr[1$\bar{1}$0] = 7.804 Å). These values agree with or slightly exceed the limits of disordering previously observed for refined structures (see review in Kroll and Ribbe, 1983). However, despite this grain's exposure to disordering conditions for geologically long periods, a slight residual preference of Al for the T_1 site is observed, as with all previous refinements.

TABLE 6. Madelung site-energy calculations

Structure site	kcal/mol
K	−271.0
T_1	−3 880.7
T_2	−3 896.5
O_{A1}	−1 326.5
O_{A2}	−1 317.5
O_B	−1 392.3
O_C	−1 349.4
O_D	−1 391.9
Formula unit	−13 368.3

T_1 site: −3880.7/3.75 = −1034.9 kcal/mol *e*
T_2 site: −3896.5/3.75 = −1039.1 kcal/mol *e*

$T_1 \times 3e$ = −3104.6 kcal/mol; $T_1 \times 4e$ = −4139.4 kcal/mol
$T_2 \times 3e$ = −3117.2 kcal/mol; $T_2 \times 4e$ = −4156.2 kcal/mol

Ordered state = $T_1(3+) + T_2(4+)$ = −7260.8 kcal/mol
Antiordered state = $T_1(4+) + T_2(3+)$ = −7256.6 kcal/mol

Note: Calculations were performed using Bertaut method (Y. Ohashi, pers. comm.) program; four shells about the unit cell were included.

DISCUSSION

The apparent residual preference of Al for T_1 in this grain and others exposed for long periods to disordering conditions raises several questions about the limit of Al-Si disorder observable in alkali feldspars. Two possible explanations are (a) the cation thermal energy available for randomizing position within the structure is limited by the melting temperature and (b) the method used for determining tetrahedral Al occupancy from X-ray refinements (based on T–O bond lengths) may be limited by the assumption of equal size of tetrahedral sites at full disorder.

To examine the possible causes of residual ordering in alkali feldspar, and the possibility of size differences independent of Al occupancy in T_1 and T_2, Madelung electrostatic site energies were calculated using the atom positions of this refinement and a model tetrahedral-cation charge of 3.75. The results (Table 6) indicate that the energy difference between T_1 and T_2 in the near-disordered structure is approximately 16 kcal/mol with the T_1 potential well being shallower, hence favoring Al partitioning. This amounts to approximately a 4.2-kcal/mol difference between ordered and antiordered states in a structure with tetrahedra of nearly identical size. The difference would increase dramatically with ordering (and resulting tetrahedral-site size changes). This gives a reasonable ionic explanation of the onset of ordering of Al into T_1 and a possible explanation of some of the residual size differences of tetrahedral sites noted in synthetically disordered alkali feldspars. The calculations suggest that even at high temperature and high disorder, significant potential differences exist between the tetrahedra. To completely disorder the structure, the ratio of cation thermal energy to site potential difference would need to be very high. Yet at the conditions of previous experiments, greater thermal energy would result in melting; most of the experimental runs were within 100°C of melting. The slightly greater disorder observed for this grain relative to synthetic high sanidines may be explained by its equilibration at temperatures above the low-pressure melting point. Although high pressure probably favors Al-Si ordering, previous experiments on a variety of crystal structures suggest that its effect, based on the compressibility of the tetrahedra, would be small (e.g., Hazen and Finger, 1979).

A shallower potential well for T_1 could result in a slightly larger T_1 site even though Al occupancy of both sites may be close to 0.25. The T–O technique for evaluating Al content assumes that at $t_1 = 0.25$ the tetrahedra will be exactly equal in average bond length. The Al occupancy equation for feldspars (Kroll and Ribbe, 1983) is $t_i = 0.25(1 + n_{An}) + (\langle T_i–O\rangle - \langle\langle T–O\rangle\rangle)/\text{const.}$, where n_{An} is the mole fraction of anorthite in the structure, $\langle T_i–O\rangle$ is average tetrahedral cation–oxygen bond length for the site in question, and $\langle\langle T–O\rangle\rangle$ is the grand mean bond length for all tetrahedral sites. The constant is determined by the mean difference betwen Al–O and Si–O bond lengths, taken as 0.130 in plagioclases and 0.125 in K-rich feldspars. The assumption of equivalent size at $t_1 = t_2 = 0.25$ is questionable; the two sites are not symmetrically related and exactly equal sizes would be fortuitous. Coesite, a structural polytype of the monoclinic feldspar tetrahedral framework (Megaw, 1970) has a single tetrahedral cation (Si) in both sites. Recent structure refinements of this mineral (Smyth et al., 1987) have shown tetrahedral-site size differences of about 0.11% ($\langle T_1–O\rangle$ = 1.6117(6) Å; $\langle T_2–O\rangle$ = 1.6134(7) Å at 292 K). The size difference in the sanidine structure reported here is about 0.3%. Our suggestion is that part of this size variation may be due to a larger T_1 site independent of Al occupancy as a result of a slightly shallower potential well.

In addition to Al occupancy, Kroll and Ribbe (1983) cited several secondary factors that correlate with T–O bond length; T–O–T angle, K–O distance, and Al occupancy of the adjacent site. Tetrahedral bond length increases with oxygen bond angle as a result of increased cation-cation repulsion effects (Smyth et al., 1987) or bond orbital overlap in a covalent model (Gibbs, 1982). Reduced distance to the extraframework cation or lower Al content in the adjacent site results in increased T–O bond lengths arising from reduced valence compensation of the oxygen. Yet in the (hypothetical) absence of any Al ordering between the two tetrahedra, the above considerations suggest that T_2, not T_1, should be the larger site. The average T–O–T angle for the oxygens surrounding T_1 is 142.43°, about 1.3° larger than T_2. The K–O distances for the two tetrahedra are identical except for K–O_{A1} (in T_1) vs. K–O_{A2} (in T_2), with the latter being 0.2 Å shorter. Mean Al content in the adjacent site will, of course, be identical for all sites in a completely disordered structure. Thus, the electrostatic potential appears to be a primary factor in initiating ordering in the structure.

CONCLUSIONS

Structural refinement of this natural near end-member high sanidine grain indicates that it has very high Al-Si disorder; however, as with all previous refinements of alkali feldspar, some residual preference for T_1 by Al is observed. A closer approach to complete disorder may be unattainable owing to a slight difference in the electrostatic potential of the two tetrahedral sites at any temperature below the melting point. The approach to complete disorder may be partly masked if Al occupancy is based on ⟨T–O⟩ calculations. Although some ordering is probably always present, the amount may be slightly exaggerated by an inherent tetrahedral-site size difference at high disorder, similar to that observed in coesite. A test of this idea would be to compare X-ray refinement ⟨T–O⟩ values of a very highly disordered alkali feldspar with neutron refinement data on the same grain and of sufficient quality to directly refine Al-Si occupancy. Similar experiments have been conducted before, but on low sanidine with $t_1 = 0.32$ (Brown et al., 1974).

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