American Mineralogist, Volume 71, pages 1378–1383, 1986

Crystal structure of lisetite, $CaNa_2Al_4Si_4O_{16}$

Giuseppe Rossi, Roberta Oberti
C.N.R., Centro di Studio per la Cristallografia Strutturale, % Dipartimento di Scienze della Terra, Via A. Bassi 4,
27100 Pavia, Italy
David C. Smith
Laboratoire de Minéralogie, CNRS Unité Associé no. 286, Muséum National d'Histoire Naturelle, 61 rue Buffon,
75005 Paris, France

Abstract

The crystal structure of lisetite $CaNa_2Al_4Si_4O_{16}$, $a = 8.260$, $b = 17.086$, $c = 9.654$ Å, space group $Pbc2_1$, Z = 4, has been determined through direct methods using 1445 intensities measured with an automated X-ray diffractometer. The anisotropic least-squares refinement led to a final discrepancy index $R = 0.026$ for the 1450 observed reflections. Lisetite is a tectosilicate with a framework based upon the connection of four-membered rings of tetrahedra whose apical oxygens point alternately up (U) and down (D) with respect to the (100) plane (i.e., UDUD rings). The ordered distribution of Al and Si among the tetrahedra results in the lack of the symmetry center. Ca and Na are surrounded by seven and six oxygen atoms, respectively, at average distances of 2.53 and 2.48 Å and occur in cavities sandwiched between layers of four- and eight-membered rings of tetrahedra. The structure of lisetite is related to that of feldspars, which is also based on four-membered rings of tetrahedra; however, the rings in feldspars are of the UUDD type, and lisetite contains 1.5 more extra-framework cations. Whereas lisetite shares the same Al-Si framework with banalsite $BaNa_2Al_4Si_4O_{16}$, the latter has a different arrangement of the large cations. Other combinations of extra-framework cations should be possible in a tectosilicate family based upon UDUD rings of tetrahedra.

Introduction

The new Ca-Na-Al-Si-O mineral lisetite was described very briefly in Smith (1984) and Rossi et al. (1985) and in some detail in Smith et al. (1986). Lisetite occurs in the retrograde metamorphosed Na- and Al-rich, K- and Mg-poor Liset eclogite pod in Norway, and it is most probably stable in the highest-pressure part of the greenschist, amphibolite, and granulite facies. Electron-microprobe analyses show that it has almost the stoichiometric composition $CaNa_2Al_4Si_4O_{16}$, i.e., chemically midway between the composition of anorthite and the pure Na equivalent of nepheline, but it is neither a feldspar nor a feldspathoid.

The aims of this paper are to describe the structure determination and refinement by single-crystal X-ray diffraction carried out on the co-type crystal G201b7-LT2 and to compare the lisetite structure with that of feldspars and the rare minerals banalsite $BaNa_2Al_4Si_4O_{16}$ (Haga, 1973) and stronalsite $SrNa_2Al_4Si_4O_{16}$ (A. Kato, pers. comm.).

Determination and refinement of the crystal structure

The co-type crystal, a small fragment of lisetite detached from an uncovered petrographic thin section, was used for the crystal-structure analysis. The lattice parameters (Table 1) were determined by least-squares refinement using single-crystal X-ray data obtained from a Philips PW 1100 automatic diffractometer. Details of the X-ray data collection are given in Table 1. The intensities were corrected for absorption following the semiempirical method of North et al. (1968); no extinction correction was applied.

The space group determined from systematic absences is $Pbc2_1$. The nonstandard space group was preferred in order to take into account the marked *Pbcn* (standard setting) pseudosymmetry exhibited by the mineral (Smith et al., 1986). It will be shown that the lack of the symmetry center results from the ordered distribution of Si and Al among the tetrahedra of the silicate framework.

The crystal structure was determined by means of direct methods (program MULTAN78, Main et al., 1978). The least-squares isotropic refinement converged at an R factor of 0.05. The site occupancy refinement of the nontetrahedral cationic sites was carried out without chemical constraints and by assuming that they were occupied by Ca or Na and/or were vacant. The final discrepancy factor, after the anisotropic refinement, was 0.026 for the 1445 reflections with $I > 3\sigma(I)$ and 0.050 for all the measured reflections.

The troubles that arose in the simultaneous refinement of parameters belonging to pairs of atoms related by pseu-

Table 1. X-ray crystal and refinement data

a (Å)	8.260(1)
b (Å)	17.086(1)
c (Å)	9.654(1)
Unit-cell volume (Å^3)	1362.5
Space group	*Pbc*2$_1$
Crystal dimensions (mm)	0.26 × 0.16 × 0.07
Radiation	Mo*Kα*
Scan mode	*ω*
Scan width (°)	2.0
θ range (°)	2–30
Measured reflections	4441
Independent reflections	2096
Observed reflections*	1445
R (sym)**	0.036
R (obs)	0.026
R (all)	0.050

* Only the reflections with $I \geq 3\sigma(I)$ were considered as observed.

** $R\,(\mathrm{sym}) = \sum_{hkl} (I_{hkl} - \bar{I}) / \sum_{hkl} I$, where $\bar{I} = (I_{hkl} + I_{h\bar{k}l})/2$.

Table 2. Site occupancies, atomic coordinates (×10^4) and equivalent isotropic temperature factors

Atom					*x*/*a*	*y*/*b*	*z*/*c*	B_{eq}
Ca	Ca	0.92	Na	0.08	42(2)	4115(1)	2500(0)	0.66(2)
NaA	Na	0.94	Ca	0.06	5352(2)	3461(1)	4147(2)	1.73(5)
NaB	Na	0.95			4671(2)	3508(1)	811(2)	1.27(5)
T1A	Al	0.84	Si	0.16	6688(1)	907(1)	604(1)	0.43(2)
T2A	Al	0.11	Si	0.89	8174(1)	76(1)	3074(1)	0.53(2)
T3A	Al	0.88	Si	0.12	6969(1)	1525(1)	4557(1)	0.52(2)
T4A	Al	0.10	Si	0.90	8040(1)	2432(1)	2063(1)	0.48(2)
T1B	Al	0.08	Si	0.92	3263(1)	866(1)	4416(1)	0.57(2)
T2B	Al	0.91	Si	0.09	1722(1)	146(1)	1905(1)	0.54(2)
T3B	Al	0.12	Si	0.88	2994(1)	1554(1)	306(1)	0.58(2)
T4B	Al	0.92	Si	0.08	1915(2)	2365(1)	2815(1)	0.57(2)
O1A					7908(4)	1672(2)	1091(3)	1.04(7)
O2A					6807(4)	180(2)	1864(3)	0.63(6)
O3A					4727(4)	1126(2)	121(3)	0.86(6)
O4A					7438(4)	645(2)	−1032(3)	0.73(6)
O5A					8402(4)	852(2)	3997(3)	0.89(6)
O6A					7624(4)	1805(2)	6223(3)	0.89(6)
O7A					6934(4)	2326(2)	3434(3)	1.15(7)
O1B					2092(4)	1564(2)	3878(3)	0.75(6)
O2B					3178(4)	179(2)	3259(3)	0.88(6)
O3B					5088(4)	1108(2)	4791(4)	1.23(7)
O4B					2583(4)	615(2)	5921(3)	0.88(6)
O5B					1611(4)	980(2)	899(3)	0.87(6)
O6B					2441(4)	1797(2)	−1257(3)	0.70(6)
O7B					3125(4)	2305(2)	1347(3)	0.68(6)
O8					−115(7)	−221(1)	2457(8)	0.92(6)
O9					−103(7)	2641(1)	2464(8)	0.88(6)

Note: Atom pairs related by the pseudosymmetry have the same label plus an extra "A" and "B," respectively (e.g., T1A and T1B). Numbers in parentheses are e.s.d.'s referred to the last digit.

dosymmetry elements (high correlations, physically impossible thermal parameters, departures from the pseudosymmetry less than the e.s.d., etc.; see Dollase, 1970, for nepheline), were overcome by refining alternately only one half of the atoms at once. In this way, the refinement reached convergence easily, and in the final set of atomic parameters (Tables 2 and 3), refined simultaneously in the last cycle, only two coordinates show departures from the *Pbcn* pseudosymmetry that are less than five times their e.s.d.'s.

Half-ionized scattering factors for Al, Si, and O, and fully ionized scattering factors for Ca and Na, were used in the refinement (*International Tables for X-ray Crystallography,* 1974). The observed and calculated structure factors are compared in Table 4.[1]

DESCRIPTION AND DISCUSSION OF THE STRUCTURE

The tectosilicate framework

The basic structural unit of lisetite is a four-membered ring of tetrahedra lying in the (100) plane (Fig. 1). The apical oxygens of the tetrahedra point upward (U) and downward (D) alternately with respect to the plane of the ring, following the scheme UDUD, which is one of the four possible ways to build up a four-membered ring (Smith and Rinaldi, 1962). The connection of the rings along [100] through the apical oxygens produces chains of tetrahedra (Fig. 1) similar to those that have been found isolated in the mineral narsarsukite $Na_4(TiO)_2Si_8O_{20}$ (Pyatenko and Pudovkina, 1960). The lateral linking of these chains gives rise to a three-dimensional framework of tetrahedra. Thus lisetite is a tectosilicate and exhibits the same framework type as that found in banalsite Ba-

Table 3. Anisotropic thermal parameters

Atom	β_{11}	β_{22}	β_{33}	β_{23}	β_{13}	β_{12}
Ca	23(1)	5(1)	20(1)	1(1)	4(1)	1(1)
NaA	39(3)	17(1)	58(3)	−4(1)	−1(2)	−2(1)
NaB	30(3)	13(1)	40(2)	−2(1)	−12(2)	10(1)
T1A	14(2)	5(1)	9(1)	0(1)	−1(1)	1(1)
T2A	20(1)	5(1)	13(1)	1(1)	1(1)	0(1)
T3A	12(1)	5(1)	16(1)	0(1)	3(1)	0(1)
T4A	16(1)	4(1)	13(1)	1(1)	3(1)	1(1)
T1B	22(1)	4(1)	16(1)	1(1)	0(1)	0(1)
T2B	14(1)	5(1)	18(1)	0(1)	3(1)	0(1)
T3B	22(1)	6(1)	12(1)	0(1)	3(1)	2(1)
T4B	24(2)	4(1)	15(1)	0(1)	−7(1)	2(1)
O1A	56(5)	6(1)	25(3)	1(2)	2(3)	−4(1)
O2A	28(4)	6(1)	13(3)	4(2)	−4(3)	0(1)
O3A	23(4)	11(1)	17(3)	0(2)	−3(3)	3(1)
O4A	23(4)	9(1)	13(3)	−3(2)	4(3)	3(1)
O5A	28(4)	8(1)	26(3)	0(2)	8(3)	1(1)
O6A	29(4)	9(1)	22(3)	−2(2)	0(3)	3(1)
O7A	56(4)	7(1)	30(3)	2(2)	10(3)	1(1)
O1B	32(4)	6(1)	17(3)	1(2)	4(3)	1(1)
O2B	29(4)	8(1)	24(3)	0(2)	0(3)	1(1)
O3B	34(4)	11(1)	41(4)	0(2)	6(3)	−8(2)
O4B	43(4)	7(1)	17(3)	0(2)	6(3)	1(1)
O5B	34(4)	8(1)	21(3)	3(2)	−1(3)	0(1)
O6B	20(4)	7(1)	20(3)	2(2)	−1(3)	2(1)
O7B	26(4)	5(1)	20(3)	−2(2)	5(3)	−2(1)
O8	29(4)	7(1)	32(3)	−2(2)	13(3)	0(3)
O9	20(4)	7(1)	35(3)	0(2)	−8(3)	−1(3)

Note: The anisotropic thermal parameters are defined by

$$\exp - (h^2\beta_{11} + k^2\beta_{22} + l^2\beta_{33} + 2hk\beta_{12} + 2hl\beta_{13} + 2kl\beta_{23}).$$

Numbers in parentheses are e.s.d.'s referred to the last digit.

---

[1] To obtain a copy of Table 4, order Document AM-86-316 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.

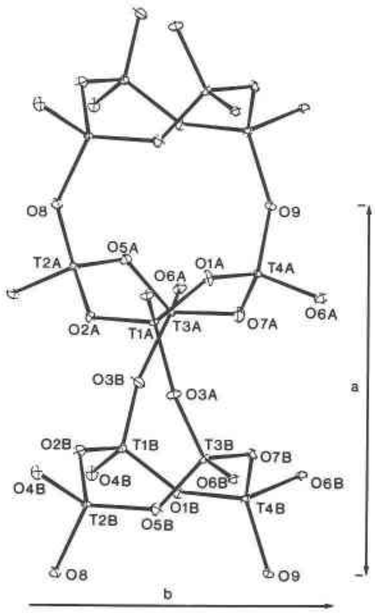

Fig. 1. ORTEP plot (Johnson, 1976) of the four-membered rings of tetrahedra lying in the plane (100) and connected through the apical oxygen atoms O3A, O3B, O8, and O9 to form chains parallel to the **a** axis.

$Na_2Al_4Si_4O_{16}$ (Campbell Smith et al., 1944; Haga, 1973). The recently discovered mineral stronalsite $SrNa_2Al_4Si_4O_{16}$ (A. Kato, pers. comm.) should also belong to the same structure type. The tectosilicate framework of lisetite (together with that of banalsite) is among the four framework types based upon twisted UDUD rings suggested by Smith (1978).

The lateral connection of the four-membered rings in the plane (100) produces layers of tetrahedra in which rings of eight tetrahedra can also be observed (Fig. 2). These layers are connected along [100] through the apical oxygens of the tetrahedra. The extra-framework cations, Ca and Na, are sandwiched between two successive layers of this kind and occur at about the same x coordinate as that of the apical oxygens (Fig. 3).

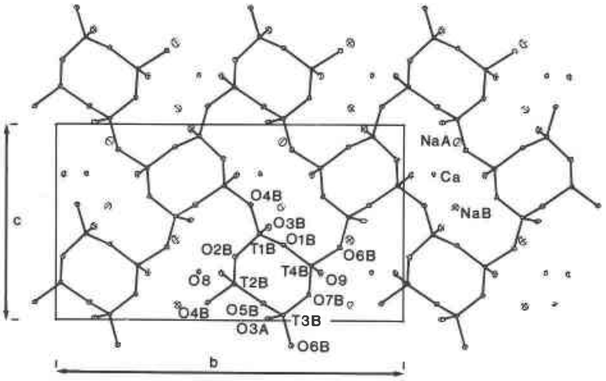

Fig. 2. ORTEP plot of one layer of four- and eight-membered rings of tetrahedra; one half of the structure is projected down the **a**-axis. Ca and Na occur at about the same level of the apical oxygen atoms, i.e., at $x = 0$ and 0.5. Only one of the two crystallographically independent rings of tetrahedra is shown here; the other, related to this by the pseudo–center of symmetry, forms the layer occurring between $x = 0.5$ and $x = 1.0$.

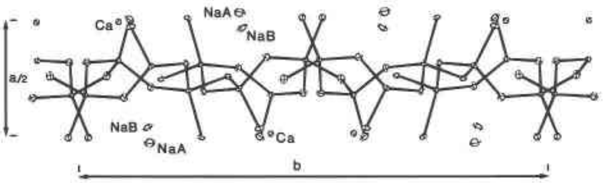

Fig. 3. Partial projection of the structure along the **c** axis to show the layers of extra-framework cations and the tetrahedral layer edge on.

The description of the lisetite structure clearly suggests a close relationship between the framework of lisetite and that of banalsite and also that of feldspars; the latter relationship was already observed by Haga (1973). In effect the structure of feldspars is also based upon four-membered rings of tetrahedra, but in these rings the apical oxygens of two adjacent tetrahedra point upward and the others point downward; hence the rings are arranged following the UUDD scheme of Smith and Rinaldi (1962). The connection of the UUDD rings through the apical oxygens gives rise to other four-membered rings perpendicular to the former ones: in this way the double-crankshaft typical of feldspars is formed. Also in these minerals the layers of four- and eight-membered rings are present.

The relationships of lisetite and banalsite with feldspars are not immediately evident if the actual unit-cell parameters are considered. However, Campbell Smith et al. (1944) observed that the cell dimensions of feldspars and banalsite could be compared by using the alternative cell of sanidine suggested by Taylor (1933). More generally, if the idealized conventional cells devised by Smith and Rinaldi (1962) to describe the structures of the framework silicates based upon four-membered rings are considered, those relationships appear clearly: lisetite—$a' = b/2 = 8.543$, $b' = c = 9.654$, $c' = a = 8.260$ Å, $V = 682.4$ Å^3, $\alpha' = \beta' = \gamma' = 90°$; stronalsite—$a' = a = 8.407$, $b' = b = 9.886$, $c' = c/2 = 8.345$ Å, $V = 693.5$ Å^3, $\alpha' = \beta' = \gamma' = 90°$; banalsite—$a' = a = 8.496$, $b' = b = 9.983$, $c' = c/2 = 8.378$ Å, $V = 710.6$ Å^3, $\alpha' = \beta' = \gamma' = 90°$; and sanidine—$a' = 1/2[012] = 9.160$, $b' = 1/2[01\bar{2}] = 9.160$, $c' = [100] = 8.564$ Å, $V = 716.5$ Å^3, $\alpha' = \beta' = 90°$, $\gamma' = 90.66°$.

The tetrahedra

Eight independent tetrahedral cations are contained in the lisetite asymmetric unit and, as expected from the Si:Al ratio, their distribution is ordered. Ordering of Si and Al accounts for the lack of a symmetry center; the structure is topologically nearly centrosymmetric and the oxygen atoms occur in slightly different arrangements depending upon the nature (Si or Al) of the tetrahedral cation.

The distribution of Si and Al among the eight indepen-

Table 5a. Bond distances (Å)

T1A–O1A	1.716	T1B–O1B	1.620
–O2A	1.742	–O2B	1.623
–O3A	1.726	–O3B	1.604
–O4A	1.754	–O4B	1.616
Mean	1.736	Mean	1.616
TQE	1.0147	TQE	1.0089
TAV	54.75	TAV	34.01
T2A–O2A	1.634	T2B–O2B	1.777
–O4A	1.622	–O4B	1.760
–O5A	1.609	–O5B	1.728
–O8	1.615	–O8	1.726
Mean	1.620	Mean	1.747
TQE	1.0049	TQE	1.0115
TAV	18.92	TAV	43.38
T3A–O3B	1.725	T3B–O3A	1.618
–O5A	1.737	–O5B	1.610
–O6A	1.763	–O6B	1.631
–O7A	1.745	–O7B	1.633
Mean	1.742	Mean	1.623
TQE	1.0031	TQE	1.0030
TAV	12.16	TAV	11.52
T4A–O1A	1.607	T4B–O1B	1.717
–O6A	1.630	–O6B	1.771
–O7A	1.618	–O7B	1.737
–O9	1.622	–O9	1.765
Mean	1.619	Mean	1.748
TQE	1.0017	TQE	1.0084
TAV	6.81	TAV	32.23
NaA–O1A	2.375	NaB–O1B	2.370
–O4A	2.386	–O4B	2.392
–O5B	2.530	–O5A	2.607
–O8	2.787	–O8	2.716
–O6B	2.381	–O6A	2.332
–O7A	2.439	–O7B	2.474
Mean	2.483	Mean	2.482
Ca–O2A	2.453		
–O2B	2.449		
–O3A	2.571		
–O3B	2.645		
–O4A	2.524		
–O4B	2.527		
–O9	2.521		
Mean	2.527		

Note: The mean e.s.d. is 0.001 Å. TQE = tetrahedral quadratic elongation and TAV = tetrahedral angle variance as defined by Robinson et al. (1971).

Table 5b. Bond angles (°)

O1A–T1A–O2A	108.6	O1B–T1B–O2B	106.6
O1A–T1A–O4A	103.5	O1B–T1B–O4B	106.0
O2A–T1A–O4A	115.3	O2B–T1B–O4B	114.3
O3A–T1A–O4A	98.2	O3B–T1B–O4B	101.1
O1A–T1A–O3A	117.4	O1B–T1B–O3B	116.4
O2A–T1A–O3A	113.3	O2B–T1B–O3B	112.5
O2A–T2A–O4A	101.7	O2B–T2B–O4B	98.4
O2A–T2A–O8	112.0	O2B–T2B–O8	112.3
O2A–T2A–O5A	112.8	O2B–T2B–O5B	115.0
O4A–T2A–O8	106.6	O4B–T2B–O8	104.7
O4A–T2A–O5A	112.0	O4B–T2B–O5B	109.1
O5A–T2A–O8	111.1	O5B–T2B–O8	115.3
O5A–T3A–O3B	112.4	O5B–T3B–O3B	113.0
O5A–T3A–O6A	104.7	O5B–T3B–O6B	106.6
O5A–T3A–O7A	109.7	O5B–T3B–O7B	107.9
O6A–T3A–O3B	105.6	O6B–T3B–O3B	105.1
O6A–T3A–O7A	111.1	O6B–T3B–O7B	112.8
O7A–T3A–O3B	113.0	O7B–T3B–O3A	111.4
O1A–T4A–O6A	109.5	O1B–T4B–O6B	108.5
O1A–T4A–O7A	110.4	O1B–T4B–O7B	113.1
O1A–T4A–O9	112.4	O1B–T4B–O9	114.1
O6A–T4A–O7A	107.9	O6B–T4B–O7B	106.7
O6A–T4A–O9	105.1	O6B–T4B–O9	99.5
O7A–T4A–O9	111.3	O7B–T4B–O9	113.7
T1A–O1A–T4A	144.7	T1B–O1B–T4B	145.9
T1A–O2A–T2A	128.0	T1B–O2B–T2B	123.9
T2A–O5A–T3A	129.7	T2B–O5B–T3B	131.7
T3A–O7A–T4A	125.9	T3B–O7B–T4B	120.7
T1A–O3A–T3B	153.9	T3A–O3B–T1B	157.5
T2A–O8 –T2B	140.3	T4A–O9 –T4B	151.7

Note: The mean e.s.d. is 0.1°.

dent tetrahedra has been computed with the equation given by Jones (1968) for feldspars: $y = 6.3481x - 10.178$, where $y = \mathrm{Al}/(\mathrm{Si} + \mathrm{Al})$ and $x = \langle \mathrm{T–O} \rangle$, the average bond distance (Table 5). Ordering calculated in this way appears to be not as high as expected from an overall Si:Al ratio of 1:1, which would imply complete accord with the aluminum avoidance rule. On the other hand it could be observed that in both anorthite (Megaw et al., 1962) and low albite (Ribbe et al., 1969) 0.09 Si atoms and 0.07 Al atoms apparently occur in the Al and Si tetrahedra, respectively, when the same equation is used. The apparent incomplete ordering in lisetite could be explained either by invoking, as suggested by Haga (1973) for banalsite, the presence of domains in which submicroscopic twinning of perfectly ordered lamellae simulates a disordered distribution, or by the inadequacy of the Jones's (1968) equation, which was devised for feldspars and is applied here to a mineral which is related to, but not identical with, feldspars. However, the distribution given in Table 2 leads to total amounts of Si (4.036) and Al (3.964) that are very close to the values obtained with the electron-microprobe (EMP) analysis (4.021 and 3.997, respectively; Smith et al., 1986).

The tetrahedra exhibit different degrees of distortion as measured by the tetrahedral angle variance (TAV) as defined by Robinson et al. (1971): the family of Al-rich tetrahedra (T1A, T2B, T3A, T4B) are on average more distorted than the family of Si-rich tetrahedra (Table 5). Within each of the two families the distortion increases with the number of those oxygen atoms of the tetrahedron that are also bonded to Ca. For instance, T1A and T1B, which have the largest TAVs in their respective family, have three oxygens bonded to Ca, whereas T3A and T4A, which have the smallest TAVs, have only one oxygen bonded to Ca plus one oxygen at a long distance (~2.9 Å) from the same cation. In low albite and anorthite the largest TAVs are those of the Al tetrahedra, and TAVs in anorthite (Wainwright and Starkey, 1971) are larger than those in low albite (Ribbe et al., 1969). All these observations can be explained by the fact that the oxygen atoms bonded to the lower-charged Al are more influenced by the nontetrahedral cations and that, among these, the higher-charged Ca exerts more influence on oxygens than the lower-charged Na.

The extra-framework cations

Ca and Na are distributed over three independent positions. In the Ca position a small amount (0.08 atoms) of Na is also present. One of the two Na positions (Na1) contains some Ca (0.06 atoms), whereas the other is not completely occupied (0.95 Na atoms occur in Na2). The

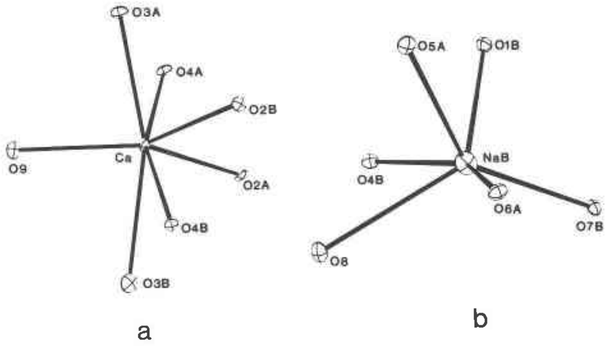

Fig. 4. The co-ordination polyhedra of the extra-framework cations projected along the **a** axis. (a) Ca is linked to three apical oxygen atoms (O3A, O3B, and O9) at the same x level and to four more oxygens, two of which (O2A and O4A) lie in one tetrahedral layer and two (O2B and O4B) in the adjacent one. (b) Only the co-ordination of NaB is shown since that of NaA is quite similar due to the pseudosymmetry. NaB is connected to one apical oxygen O8 and to three oxygens of the tetrahedral layer above (O1B, O4B, and O7B) and two of the layer below it (O5A and O6A).

total amounts of Ca and Na resulting from the unconstrained X-ray structure refinement (XRef) are in good agreement with those determined with EMP (respectively, 0.98 and 0.98 atoms per formula unit (pfu) for Ca and 1.97 and 1.96 atoms pfu for Na). The global amount of extra-framework cation charges fits the total (Al + Si) charges very well: the overall charge balance by XRef indicates a difference of 0.04 valence units over a total of 32 unit charges to be balanced.

Ca is surrounded by seven oxygen atoms at distances ranging from 2.45 to 2.65 Å and by two more oxygens at longer distances (2.86 and 2.97 Å, Table 5). The coordination polyhedron is irregular (Fig. 4a). NaA and NaB have an irregular six-fold coordination (Fig. 4b). The average Na–O distances (2.48 Å) of both polyhedra are shorter than the average Na–O distances in albite (2.60 Å; Ribbe et al., 1969). This is not surprising since lisetite, which has a framework structure similar to that of feldspars, possesses 1.5 times the number of extra-framework cations. The structure of lisetite is therefore more compact as is witnessed, for instance, by the lower coordination number of Na, and, hence, by the shorter Na–O bond distances.

Comparison with banalsite

Banalsite (Bs) (Haga, 1973) has the same three-dimensional framework as lisetite (Lt). Banalsite is orthorhombic, space group *Ibam*; the lattice parameters are a = 8.496 Å, b = 9.983 Å, c = 16.755 Å, and their relationships with those of lisetite are as follows: $a_{Lt} \cong c_{Bs}/2$, $b_{Lt} \cong 2a_{Bs}$, $c_{Lt} \cong b_{Bs}$. A close inspection of the structures of the two minerals reveals that the similarity is restricted to the fact that they have the same type of tetrahedral framework. The cell parameter corresponding to the direction normal to the plane of the four-membered rings and to the layers of extra-framework cations is doubled in banalsite because two successive layers are not equivalent: one layer contains only Ba atoms, the other only Na atoms. In this way the former layer contains only four cations and the latter as many as eight cations. Owing to these features the coordination of Na in banalsite is different from that of lisetite even if the average Na-O distance (2.49 Å) is similar. The segregation of Ba and Na into different layers is due to the large difference in their ionic radii: this difference would produce an excessive distortion in the tetrahedral framework if the two cations occurred in the same layer. In lisetite two successive layers are equivalent and contain six cations (2Ca + 4Na) (Fig. 3). The overcrowding of Na cations in one layer of banalsite can explain the relative expansion of b, whereas the presence of the large Ba atoms causes the c cell parameter to increase with respect to lisetite.

The features described above are an excellent demonstration of the remarkable flexibility of this kind of tetrahedral framework and of the possibility to have arrangements of the extra-framework cations other than those found in banalsite and lisetite. For instance, if we assume a Si:Al ratio of 1:1, the only apparent requirement is that the sum of the positive charges in each layer is 8, no matter which is the number of cations. Thus we can hypothesize other minerals with 1Ca + 6Na, or 3Ca + 2Na, or even 4Ca or 8Na in each layer. Moreover, if the Si:Al ratio could be different from 1:1 (e.g., 5:3), a further series of arrangements of large cations could be imagined. However, only mineral synthesis experiments could confirm whether or not a whole new mineral family, parallel to that of feldspars but based upon four-membered rings of the UDUD type, can exist. Lisetite and banalsite, and presumably also stronalsite, are the members of this family which have so far been found in nature.

REFERENCES

Campbell Smith, W., Bannister, E.A., and Hey, M.H. (1944) Banalsite, a new barium feldspar from Wales. Mineralogical Magazine, 27, 33–48.

Dollase, W.A. (1970) Least-squares refinement of the structure of a plutonic nepheline. Zeitschrift für Kristallographie, 132, 27–44.

Haga, N. (1973) The crystal structure of banalsite, BaNa$_2$Al$_4$Si$_4$O$_{16}$, and its relation to the feldspar structure. Mineralogical Journal, 7, 262–281.

International tables for X-ray crystallography. (1974) Volume IV, 99–101. Kynoch Press, Birmingham, England.

Johnson, C.K. (1976) ORTEP II. Report ORNL-5138, Oak Ridge National Laboratory, Tennessee, U.S.A.

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

Main, P., Hull, S.E., Lessinger, L., Germain, G., Declercq, J.-P., and Woolfson, M.M. (1978) MULTAN78, a system of computer programs for the automatic solution of crystal structures from X-ray diffraction data. Universities of York, England, and Louvain, Belgium.

Megaw, H.D., Kempster, C.J.E., and Radoslovich, E.W. (1962) The structure of anorthite, CaAl$_2$Si$_2$O$_8$. II. Description and discussion. Acta Crystallographica, 15, 1017–1035.

North, A.C.T., Phillips, D.C., and Mathews, F.S. (1968) A semiempirical method of absorption correction. Acta Crystallographica, A24, 351–359.

Pyatenko, Yu.A., and Pudovkina, Z.V. (1960) Crystal structure of narsarsukite. Kristallografija, 5, 563–573 (transl. Soviet Physics–Crystallography, 5, 540–548).

Ribbe, P.H., Megaw, H.D., Taylor, W.H., Ferguson, R.B., and Traill, R.J. (1969) The albite structures. Acta Crystallographica, B25, 1503–1518.

Robinson, K., Gibbs, G.V., and Ribbe, P.H. (1971) Quadratic elongation, a quantitative measure of distortion in co-ordination polyhedra. Science, 172, 567–570.

Rossi, G., Smith, D.C., Oberti, R., and Kechid, S.-A. (1985) Some crystal-chemical and petrological relationships between two new minerals in the system anorthite-nepheline. (abs.) Rendiconti Società Italiana Mineralogia e Petrologia, 40, 424–425.

Smith, D.C. (1984) Remarques cristallochimiques et pétrogenetiques sur des minéraux inhabituels dans les éclogites de Liset et Rekvika, Norvège. X Réunion Annuelle des Sciences de la Terre, Bordeaux, 1984, Société Géologique de France, Paris, 511.

Smith, D.C., Kechid, S.-A., and Rossi, G. (1986) Occurrence and properties of lisetite, $CaNa_2Al_4Si_4O_{16}$, a new tectosilicate in the system Ca-Na-Al-Si-O. American Mineralogist, 71, 1372–1377.

Smith, J.V. (1978) Enumeration of 4-connected 3-dimensional nets and classification of framework silicates. II. Perpendicular and near-perpendicular linkages from 4.8^2, 3.12^2 and 4.6.12 nets. American Mineralogist, 63, 960–969.

Smith, J.V., and Rinaldi, F. (1962) Framework structures formed from parallel four- and eight-membered rings. Mineralogical Magazine, 33, 202–212.

Taylor, W.H. (1933) The structure of sanidine and other feldspars. Zeitschrift für Kristallographie, 85, 425–442.

Wainwright, J.E., and Starkey, J. (1971) A refinement of the structure of anorthite. Zeitschrift für Kristallographie, 133, 75–84.

Manuscript received August 22, 1985
Manuscript accepted July 8, 1986