The crystal structure of naujakasite,
a double sheet silicate

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Abstract

The crystal structure of naujakasite from Tuperssuatsiait has been determined by X-ray data from four-circle computer controlled Philips PW 1100 diffractometer (Mo Kα radiation).

Naujakasite crystallizes in the space group $C2/m$ with cell dimensions $a = 15.025(1)$, $b = 7.991(2)$, $c = 10.486(1)$ Å, $\beta = 113°40'(5')$; the structural formula is $Na_6FeAl_4Si_8O_{26}$, $Z = 2$.

The structure has been solved by Patterson methods and refined by full matrix least-squares method to $R_w = 0.027$.

Naujakasite is a sheet silicate with double layers of tetrahedra perpendicular to the c direction. All the oxygen atoms of the structure are shared between two tetrahedra except one that interrupts the three-dimensional linking. Each single layer is formed by rings of six tetrahedra and the linkage between two single layers gives rise to rings of four and six tetrahedra. Out of the three independent tetrahedral sites present in the structure one is occupied by silicon and the other two by (0.5 Si + 0.5 Al).

The Na-O polyhedra (quite irregular) and the Fe-O polyhedron (a tetragonal bipyramid) are all linked together forming a three-dimensional framework in which all the oxygen atoms of the structure are involved.

Introduction

The crystal structure analysis of naujakasite has been undertaken on the basis of the exhaustive description made by Petersen (1967) with essentially three aims: (1) the determination of the space group out of the three ($C2$, Cm, $C2/m$) consistent with the systematic absences; (2) the fitting of the chemical analysis to the structural results in order to settle some points of interest like the presence or the lack of water molecules in the structure, the FeO/Fe_2O_3 ratio and the amount of cation diadochy that were slightly doubtful owing to the great difficulty in obtaining sufficiently pure material; (3) the relationships between naujakasite and other silicate minerals.

Experimental procedure

The structural formula of naujakasite, the cell dimensions and other related data are given in table 1.

Cell dimensions were re-determined by least-squares from 20 high-angle reflections carefully centered with a General Electric four circle diffractometer using Cu Kα radiation ($\lambda = 1.54051$ Å). They are in excellent agreement with the earlier determination made by Petersen (1967) using Guinier photographs. From the three space groups consistent with the systematic absences, the centrosymmetric one ($C2/m$) was chosen

according to statistical averages and distribution of the normalized structure factors.

The calculated density (2.714) is slightly different from the density measured by Petersen (2.622) suspending the mineral in heavy liquids; the difference is probably due to the thin layers of air and/or analcite along the basal cleavage, as pointed out by Petersen himself.

For the structure determination a single platy crystal (0.22 × 0.16 × 0.03 mm) of naujakasite from Tuperssuatsiait in the Ilímaussaq intrusion, South Greenland, has been used. Intensities were measured by ω-scans with a Philips PW 1100 computer-controlled four circle diffractometer, using Mo $K\alpha$ radiation ($\lambda = 0.71069$ Å) mono-chromatized with a graphite crystal. The rate of scanning was 0.064°/sec and the scan range was 2°. The background was measured, on either side of the scan range, for a time T according to the equation: $T = \frac{1}{2} T_{scan} . \sqrt{I_{bck}/I_{int}}$, where T_{scan} is the total scantime, I_{bck} is the mean of two preliminary background measurements of 5 sec. at each side of the scan interval in which the total number of counts (I_{int}) was memorized. When the condition $I_{top} - 2 \sqrt{I_{top}} < I_{bck}$ happened during the scan the reflection was skipped; at the end of the refinement these weak reflections were re-introduced with $F_0 = 0$.

Three standard reflections were measured every hour to check the crystal alignment during the data collection. No significant variation in their intensity was observed, and no automatic re-orientation of the crystal occurred. All reflections in the hemisphere of reciprocal space ±h, ±k, +1 were collected out to a ϑ angle of 30°. 1809 independent reflections were inspected; 212 out of these were skipped and 1496, with $I > \sigma(I)$, were used in the refinement.

Net intensities and their standard deviations were calculated according to the formulae:

(1) $\quad I = C - T_c/2T_b (B_1 + B_2);$ (2) $\quad \sigma(I) = \sqrt{[C + (T_c/2T_b)^2 (B_1 + B_2)]}$

where C is the total number of counts recorded during the scan time T_c and B_1, B_2 are the background counts, each measured for a time T_b. When the two background intensities were different in such a way that $(B_1 + B_2)$ was less than $(B_1 - B_2)^2/4$, the former quantity was replaced by the latter in the formula (2). Intensities of equivalent reflections and those measured more than once were averaged. The intensities were corrected for Lorentz and polarization effects, but not for absorption ($\mu = 14.8$ cm^{-1}).

The weighting scheme used throughout the refinement gave zero weight if $F^2 < \sigma(F^2)$ and $w = 4F^2/\sigma^2(F^2)$ if $F^2 \geqslant \sigma (F^2)$.

Structure determination and refinement

The data were placed on an approximately absolute scale and $|E|$ values were calculated using Wilson's (1942) method. The statistical averages and distribution of the normalized structure factors are in very good agreement with the theoretical

Table 1. Cell dimensions of naujakasite and other related data

a	15.025($\pm$0.001) Å
b	7.991($\pm$0.002) Å
c	10.486($\pm$0.001) Å
β	113°40'($\pm$6')
Space group	C2/m (N.12)
Cell volume	1153 Å^3
Cell contents	$2Na_6FeAl_4Si_8O_{26}$
Specific gravity calc.	2.714
Specific gravity obs.	2.622
Linear total absorption coefficient	$\mu = 14.8$ cm^{-1}
Total number of reflections collected ($\vartheta_{max} = 30°$, Mo Kα radiation)	2911
Total number of independent reflections inspected	1809
Total number of independent reflections with I > σ (I) used in the refinement	1496

values for centrosymmetric distribution of atoms in the unit cell (Karle *et al.*, 1965); therefore the space group *C2/m* was chosen and afterwards confirmed by the results of the crystal structure determination.

The structure was solved by inspection of the three-dimensional Patterson map that gave the position of the iron atom and of three complete Si-O tetrahedra. A three-dimensional Fourier map computed with the coordinates of these atoms allowed to locate the sodium atoms. Since no other prominent peaks were evident in the Fourier maps, it was decided to refine the coordinates of the atoms found so far, even if one water molecule was expected to be present, according to the chemical analyses made by C. R. Dethlefsen and by E. I. Semenov (Petersen, 1967). Several determinations of the weight percent of H_2O have been made also in our laboratory, but the results were always doubtful due to the difficulty in obtaining a sufficiently pure material.

The isotropic refinement of the structural model obtained from the Fourier maps, considering at first the tetrahedral positions to be fully occupied by silicon, converged to $R_w = \sqrt{\Sigma w (|F_0| - |F_c|)^2/\Sigma w |F_0|^2} = 0.08$, using the atomic scattering factors listed by Hanson *et al.*, (1964).

It was possible to deduce, from the oxygen–tetrahedral cation distances, that one tetrahedral position, $T(1)$, was fully occupied by silicon, while the other two positions, $T(2)$ and $T(3)$, were (0.5 Si + 0.5 Al), corresponding to an overall amount of aluminium that is in good agreement with the chemical formula tentatively proposed by Petersen. According to this conclusion the atomic scattering curve for the two tetrahedral cations, $T(2)$ and $T(3)$, was obtained by averaging the values of (Si + Al)/2. One additional isotropic least-square cycle converged to $R_w = 0.068$.

At this point anisotropic thermal factors were included in the refinement and the multipliers of the cations were allowed to vary, in order to check the occupancy and the isomorphic substitution of the cations. The anisotropic refinement converged to $R_w = 0.027$ without significant variation from complete occupancy of the sodium and iron atoms and with a full confirmation of the Si, Al distribution used throughout the anisotropic refinement. The conventional R factor, at the end of the refinement, was $R = 0.041$ and the final parameter shifts were less than 0.01σ.

The secondary extinction was negligible, so no extinction factor was taken into account.

A three-dimensional difference Fourier synthesis was carried out which did not show any significant peak.

It is possible to conclude, from the results of the refinement, that naujakasite has the following chemical formula:

$$Na_6FeAl_4Si_8O_{26}, Z = 2$$

Table 2. Idealized chemical analysis corresponding to the structural formula compared with the chemical analysis

	Chemical analysis calculated from structural formula		Wet chemical analysis†	
	Weight per cent	Number of cations in the unit cell	Weight per cent*	Number of cations in the unit cell
SiO_2	51.00	16	52.11	16.26
TiO_2			0.03	0.01 } 7.82
Al_2O_3	21.64	8	21.24	7.81
FeO	7.63	2	5.70	1.49
MnO			1.13	0.30 } 1.89
CaO			0.31	0.10
Na_2O	19.73	12	18.90	11.43
K_2O			0.51	0.20 } 11.63
P_2O_5	———	——	0.07	0.02
	100.00	38	100.00	

†Analyst: Ib Sørensen, GGU.
*Weight per cent recalculated on the basis that iron contents are entirely present as FeO.

without significant diadochy.

The idealized chemical analysis corresponding to the structural formula, apart from small isomorphic substitution of the cations (that, however, should be less than 1 % in weight), is reported in table 2, where it is compared with the chemical analysis made by I. Sørensen and recalculated disregarding the results of the thermogravimetric analysis. It clearly appears that the chemical results are substantially in good agreement with the structural analysis, with only a few small differences. The assumption that trivalent iron hardly can be present is confirmed by the facts that the tetrahedral sites are fully occupied by the amount of silicon and aluminium resulted from the chemical analysis, and that the iron on the origin, for the electrostatic neutrality of the structure, must be divalent.

The final fractional atomic coordinates and the anisotropic thermal parameters, as well as their standard deviations, are listed in table 3 and in table 4. The analysis of the anisotropic thermal parameters is reported in table 5.

Observed and calculated structure factors may be requested directly from the authors.

Table 3. Fractional atomic coordinates with their standard deviations in parentheses and equivalent isotropic temperature factors after Hamilton (1959)

Atom	x/a	y/b	z/c	$B_H Å^2$
Fe	0.0000	0.0000	0.0000	1.01
T(1)	0.1505(1)	0.3081(1)	0.1315(1)	0.65
T(2)	0.0584(1)	0.1953(1)	0.3415(1)	0.81
T(3)	0.1463(1)	0.3014(1)	0.6507(1)	0.73
O(1)	0.1010(1)	0.1789(3)	0.0102(2)	1.64
O(2)	0.2681(1)	0.2937(3)	0.2103(2)	1.22
O(3)	0.1070(1)	0.3120(3)	0.2509(2)	1.22
O(4)	0.1318(1)	0.5000	0.0647(3)	1.09
O(5)	0.1393(1)	0.1973(3)	0.5071(2)	1.72
O(6)	0.0360(2)	0.0000	0.2759(3)	1.82
O(7)	0.0445(1)	0.2932(3)	0.6771(2)	1.26
O(8)	0.1769(2)	0.5000	0.6338(3)	1.60
Na(1)	0.2299(1)	0.5000	0.4403(2)	1.60
Na(2)	0.3430(1)	0.5000	0.1126(2)	1.85
Na(3)	0.4643(1)	0.0000	0.1650(2)	1.88

Table 4. Final anisotropic thermal parameters ($\times 10^4$)* and their standard deviations in parentheses

Atom	β_{11}	β_{22}	β_{33}	β_{12}	β_{13}	β_{23}
Fe	8(1)	11(1)	59(1)	0	12(1)	0
T(1)	7(1)	17 (1)	26(1)	−1(1)	5(1)	−3(1)
T(2)	8(1)	28 (1)	30(1)	−1(1)	7(1)	−8(1)
T(3)	7(1)	22 (1)	28(1)	−2(1)	5(1)	−3(1)
O(1)	18(1)	59 (4)	61(3)	−20(2)	19(2)	−37(3)
O(2)	11(1)	47 (4)	37(2)	2(2)	4(1)	12(3)
O(3)	18(1)	36 (3)	46(3)	−3(2)	18(1)	−1(3)
O(4)	15(2)	40 (5)	25(3)	0	4(2)	0
O(5)	14(1)	61 (4)	65(3)	2(2)	11(2)	−33(3)
O(6)	19(2)	73 (6)	44(4)	0	1(2)	0
O(7)	15(1)	42 (4)	45(3)	−4(2)	12(1)	−1(3)
O(8)	15(2)	70 (6)	57(4)	0	16(2)	0
Na(1)	16(1)	59 (3)	50(2)	0	8(1)	0
Na(2)	30(1)	49 (3)	75(3)	0	34(1)	0
Na(3)	20(1)	104 (4)	32(2)	0	4(1)	0

* In the form: $\exp\left[-(h^2\beta_{11}+k^2\beta_{22}+l^2\beta_{33}+2hk\beta_{12}+2hl\beta_{13}+2kl\beta_{23})\right]$.

Table 5. Analysis of the anisotropic thermal parameters*

Atom	r.m.s.	$U_i a$	$U_i b$	$U_i c$
Fe	0.059 (4)	90	8	81
	0.081 (3)	180	90	90
	0.168 (2)	90	105	164
T(1)	0.072 (3)	105	20	76
	0.081 (2)	160	108	81
	0.113 (2)	94	102	166
T(2)	0.085 (2)	158	109	81
	0.087 (3)	104	29	65
	0.126 (2)	82	62	151
T(3)	0.079 (3)	132	45	75
	0.089 (3)	133	135	81
	0.117 (2)	89	102	167
O(1)	0.079 (7)	119	31	99
	0.126 (5)	138	107	53
	0.200 (4)	102	136	130
O(2)	0.098 (6)	128	47	66
	0.117 (5)	63	44	121
	0.151 (4)	109	114	148
O(3)	0.099 (6)	135	53	112
	0.115 (5)	131	137	84
	0.153 (4)	60	122	133
O(4)	0.104 (8)	108	90	161
	0.114 (7)	90	0	90
	0.133 (6)	137	90	47
O(5)	0.095 (6)	126	42	72
	0.122 (5)	41	68	56
	0.204 (4)	59	77	146
O(6)	0.120 (7)	127	90	143
	0.154 (6)	90	0	90
	0.176 (6)	119	90	29
O(7)	0.105 (6)	136	46	88
	0.126 (5)	134	136	88
	0.145 (4)	75	106	157
O(8)	0.108 (7)	180	90	90
	0.150 (6)	90	0	90
	0.163 (6)	66	90	156
Na(1)	0.125 (4)	150	90	60
	0.138 (4)	90	0	90
	0.161 (3)	95	90	174
Na(2)	0.120 (4)	154	90	115
	0.126 (4)	90	0	90
	0.199 (3)	40	90	130
Na(3)	0.116 (4)	110	20	90
	0.155 (4)	90	90	180
	0.183 (3)	135	134	90

* Root mean squares thermal vibrations along the ellipsoid axes (Å), with their standard deviations in parentheses, and angles (in degrees) between the crystallographic axes and the principal axes (U_i) of the vibration ellipsoids.

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Description and discussion of the structure

Naujakasite is a sheet silicate characterized by the presence of a double layer of tetrahedra perpendicular to the c direction. In figure 1 the projection of the double layer down the b direction is shown. Each single layer (fig. 2) is formed by three different rings of six tetrahedra; the rings are built up by two mirror-related wollastonite-like chains (i.e. with repeat unit of three tetrahedra) which are connected through the $O(4)$, $O(6)$, $O(8)$ oxygen atoms. Two centrosymmetric layers are linked to each other through the oxygen atom $O(5)$ to form the double sheet; in this way all the oxygen atoms are shared except $O(1)$ that interrupts the linkage of the tetrahedra along the c direction.
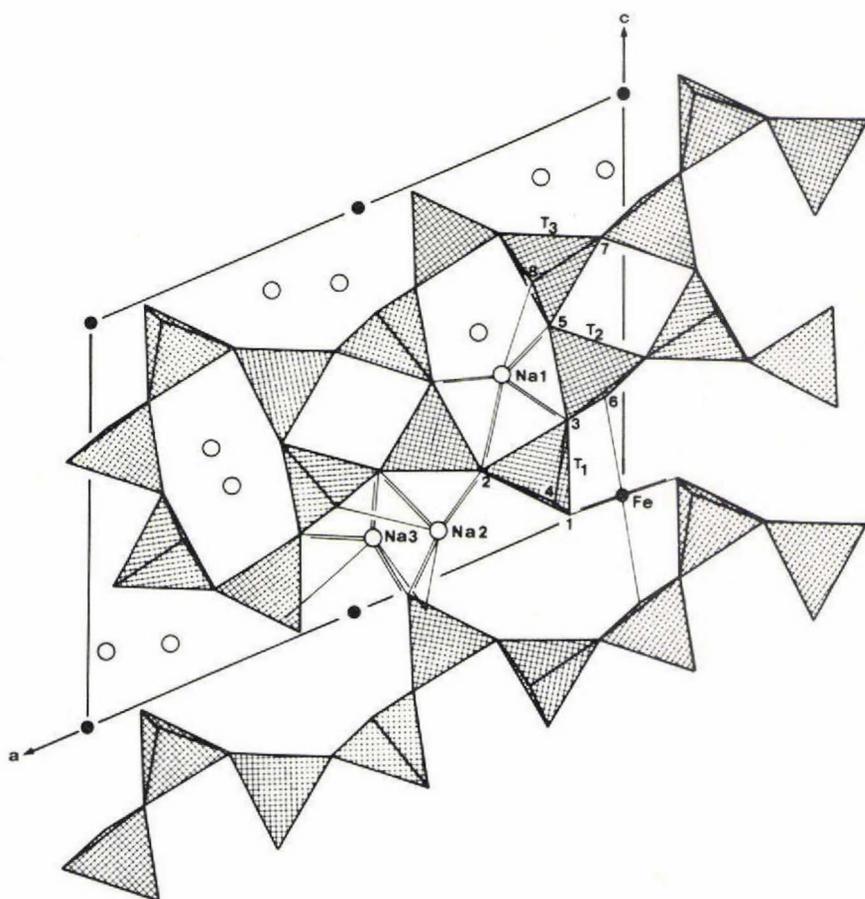
Fig. 1. The double layer of tetrahedra of naujakasite projected along [010]. The cations are connected by thin lines with the oxygen atoms of the tetrahedral framework; double lines are referred to a pair of equivalent, mirror-related oxygen atoms.
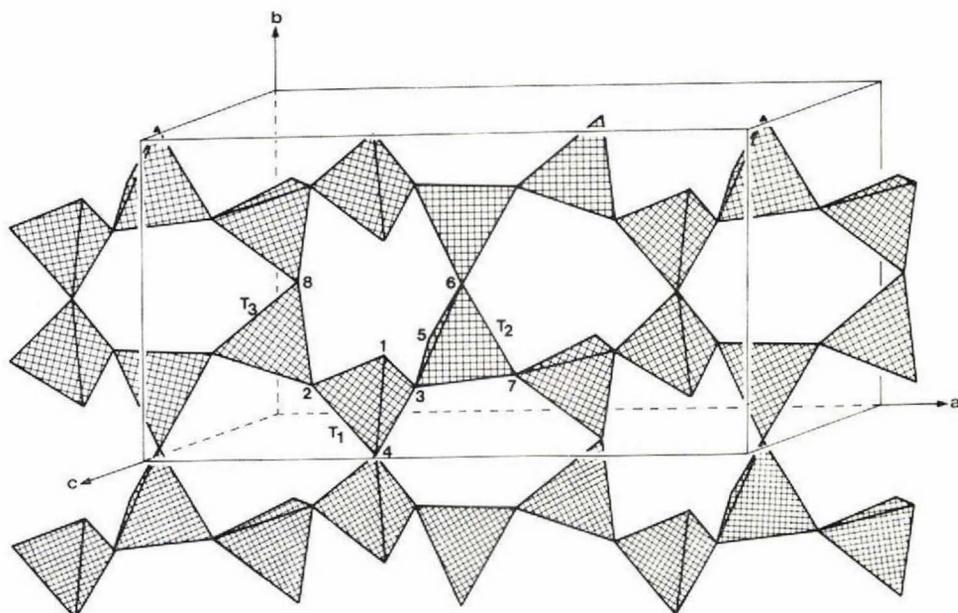
Fig. 2. Clinographic projection of a single layer of tetrahedra of naujakasite.

The linkage between the two single layers gives rise to rings of four and six tetrahedra (fig. 3) which form infinite channels running along the b direction. The Na(1) atoms have places in the channels formed by the six-membered rings; Na(2), Na(3) and Fe atoms can be considered as interlayer cations connecting double layers of tetrahedra along the c direction.

From these findings the connection of the {001} mica-like cleavage with the double sheet structure of naujakasite is obvious.

The iron atom has a six-fold coordination, which corresponds to a fairly regular tetragonal bipyramid with two centrosymmetric O(6) atoms in the apical positions. It is worth while pointing out the unusually long Fe-O(6) distance (2.722 Å), which cannot be neglected due to charge balance considerations (see later).

The three independent sodium atoms Na(1), Na(2), Na(3) form, with the oxygen atoms of the tetrahedral framework, irregular polyhedra with respectively $5 + 4$, $5 + 3$, $5 + 3$ coordination number (see table 6). The Na-O and Fe-O polyhedra are all linked together in a rather complicated way forming a three-dimensional framework in which all the oxygen atoms of the structure are involved.

The naujakasite structure is the sixth sheet silicate with double layers of tetrahedra known so far. In macdonaldite (Cannillo et al., 1968), in delhayelite (Cannillo et al., 1970) and in carletonite (Chao, 1972) each single layer is built up with rings of four and eight tetrahedra; in latiumite structure (Cannillo et al., 1973) the layers are made
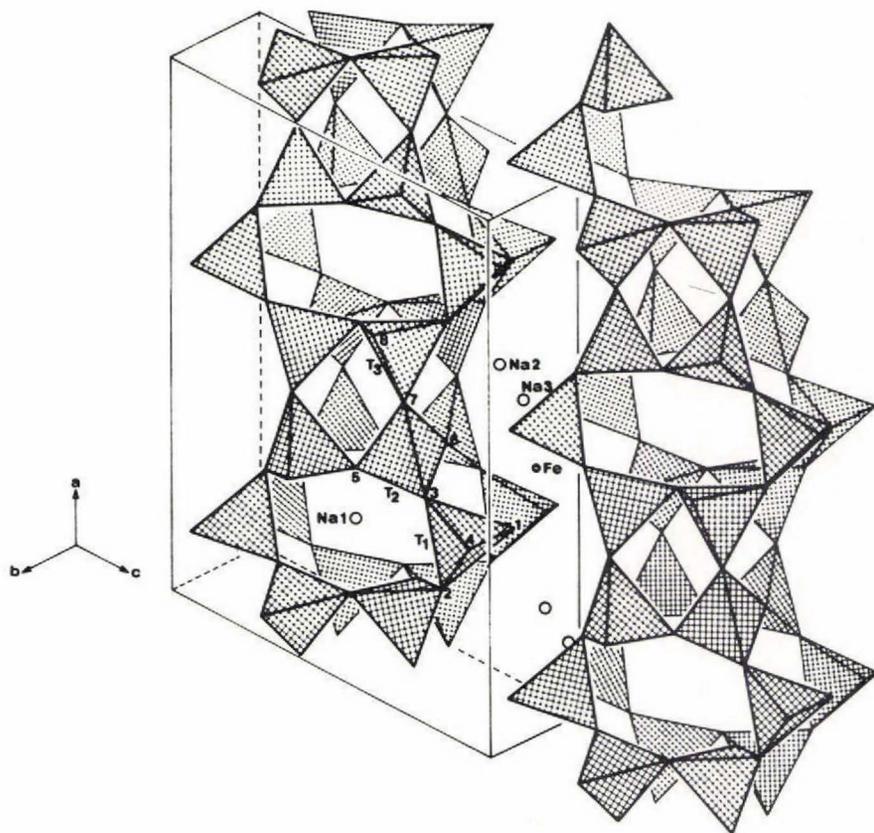
Fig. 3. Clinographic projection of the crystal structure of naujakasite, showing two complete double layers of tetrahedra and the interlayer cations.

with rings of six and eight tetrahedra. Major similarities occur between naujakasite and hexagonal $CaAl_2Si_2O_8$ (Takeuchi & Donnay, 1959) in which each single layer is formed with rings of six tetrahedra too. However in hexagonal $CaAl_2Si_2O_8$ each tetrahedron shares all its corners with neighbouring tetrahedra thus making the ratio $O/(Si, Al) = 2$, which corresponds to the Zoltai's (1960) sharing coefficient $c = 2$ or to the modified (Coda, 1969) sharing coefficient $C = 4$; in naujakasite the corresponding figures are: $O/(Si,Al) = 2.167$, $c = 1.917$ and $C = 3.667$. In this way in hexagonal $CaAl_2Si_2O_8$ each tetrahedron of a single sheet shares its apical oxygen with the apical oxygen of another sheet, thus forming the double layer of tetrahedra; in naujakasite only four oxygen atoms, $O(5)$, in each ring of six tetrahedra, are shared with the adjacent sheet to form the double layer, leaving unshared the remaining two oxygen atoms, $O(1)$.

Table 6. Interatomic distances (Å) with their standard deviations in parentheses

Atoms	Bond lengths	Symmetry operation
T(1)-O(1)	1.574 (2)	
-O(2)	1.626 (2)	
-O(3)	1.629 (2)	
-O(4)	1.662 (2)	
Average	1.623	
T(2)-O(3)	1.692 (2)	
-O(5)	1.673 (2)	
-O(6)	1.684 (2)	
-O(7)'	1.673 (2)	-x , y , 1-z
Average	1.680	
T(3)-O(2)'	1.689 (2)	1/2-x, 1/2-y,1-z
-O(5)	1.687 (2)	
-O(7)	1.660 (2)	
-O(8)	1.681 (2)	
Average	1.679	
Fe-O(1)	**2.056 (2)	
-O(6)	*2.722 (3)	
Na(1)-O(2)	*3.158 (3)	
-O(3)	*2.582 (3)	
-O(5)	*2.993 (3)	
-O(5)'	*2.405 (3)	1/2-x, 1/2+y,1-z
-O(8)	2.459 (3)	
Na(2)-O(1)'	*2.298 (3)	1/2-x, 1/2+y, -z
-O(2)	*2.441 (3)	
-O(4)	3.006 (3)	
-O(6)'	2.713 (3)	1/2+x, 1/2+y, z
-O(7)'	*3.196 (3)	1/2-x, 1/2+y,1-z
Na(3)-O(1)'	*3.078 (3)	1/2-x, 1/2-y, -z
-O(3)	*2.472 (3)	
-O(4)'	2.258 (3)	1/2+x, 1/2-y, z
-O(4)''	3.093 (3)	1/2-x, 1/2+y, -z
-O(7)'	*2.380 (3)	1/2-x, 1/2-y,1-z

A sign ′ is used to distinguish equivalent atoms. The distances preceded by one asterisk occur twice; those preceded by two asterisks occur four times

Table 7. Angles with their standard deviations in parentheses

Atoms	Angles	Symmetry operation
O(1)-T(1)-O(2)	115°26' (7')	
O(1)-T(1)-O(3)	115°21' (7')	
O(1)-T(1)-O(4)	108°37' (7')	
O(2)-T(1)-O(3)	107°27' (7')	
O(2)-T(1)-O(4)	104° 8' (7')	
O(3)-T(1)-O(4)	107°42' (7')	
Average	109°17'	
O(3)-T(2)-O(5)	106°14' (7')	
O(3)-T(2)-O(6)	109°58' (7')	
O(3)-T(2)-O(7)''	105°16' (7')	-x , y, -z
O(5)-T(2)-O(6)	112° 2' (7')	
O(5)-T(2)-O(7)''	111°40' (7')	-x , y, -z
O(6)-T(2)-O(7)''	111°16' (7')	-x , y, -z
Average	109°25'	
O(5)-T(3)-O(2)'''	107°30' (7')	1/2-x , 1/2-y,1-z
O(5)-T(3)-O(7)	113°27' (7')	
O(5)-T(3)-O(8)	107° 2' (7')	
O(7)-T(3)-O(2)'''	105°48' (7')	1/2-x , 1/2-y,1-z
O(7)-T(3)-O(8)	111°20' (7')	
O(8)-T(3)-O(2)'''	111°43' (7')	1/2-x , 1/2-y,1-z
Average	109°29'	
T(1)-O(2)-T(3)	140° 1' (7')	
T(1)-O(3)-T(2)	144°52' (9')	
T(1)-O(4)-T(1)'	134°37' (11')	x , -y, z
T(2)-O(5)-T(3)	133°38' (7')	
T(2)-O(6)-T(2)'	135°52' (13')	x , -y, z
T(3)-O(7)-T(2)	150°15' (9')	
T(3)-O(8)-T(3)'	141°22' (11')	x , -y, z
O(1)-Fe-O(1)'	88° 7' (7')	x , -y, z
O(1)-Fe-O(1)''	91°52' (7')	-x , y, -z
O(1)-Fe-O(6)	96°42' (5')	
O(1)-Fe-O(6)''	83°17' (5')	-x , y, -z

As pointed out before, the distribution of Si and Al atoms in the three independent tetrahedral sites has been determined on the basis of the relationship between T-O distances (table 6) and Al contents given by the chemical analysis. The T(2)-O and T(3)-O mean bond lengths are in perfect agreement with a half and half Si, Al distribution.

The T(1)-O(1) short bond length and the relatively high O(1)-T(1)-O angles (table 7) are those expected from an unshared oxygen atom.

Table 8. Charge balance

	T(1)	T(2)	T(3)	Na(1)	Na(2)	Na(3)	Fe	
O(1)	1.15				0.23	0.05	0.45	1.88
O(2)	0.98		0.85	0.03	0.16			2.02
O(3)	0.98	0.84		0.13		0.14		2.09
O(4)	0.89				0.05	0.23+0.03		2.09
O(5)		0.89	0.86	0.19+0.06				2.00
O(6)		0.88			0.11		0.10	1.97
O(7)		0.89	0.91		0.03	0.18		2.01
O(8)			0.88	0.18				1.94
	4.00	3.50	3.50	1.00	1.00	1.00	2.00	16.00

On the basis of the suggestions given by Brown & Shannon (1973), bond-strength – bond-length relationships have been derived by using the formula $s = s_0 (R/R_0)^{-N}$ and by requiring that the sum of the bond strengths around the cations be equal to their valences. The results shown in table 8 are considered very satisfactory and provide an additional evidence of the correctness of both the crystal structure and the chemical formula proposed for naujakasite. The best charge balance has been achieved taking into account the contribution of all the Na-O and Fe-O distances listed in table 6.

The thermal situation is in perfect agreement with the structural results; the major part of the atoms have the maximum thermal displacement (table 5) along the c direction, according to the mica-like {001} cleavage observed.

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