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The Crystal Structure of Tugtupite - a New Mineral, $Na_8\,Al_2\,Be_2\,Si_8\,O_{24}\,(Cl,S)_2$

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The structure of the new mineral tugtupite $Na_8Al_2Be_2Si_8O_{24}(Cl,S)_2$ has been determined by single-crystal X-ray methods. The crystals are tetragonal with space group $I\bar{4}$. They are strongly piezoelectric but show no pyroelectric effect. Optically the mineral is orthorhombic with values of $2V_\gamma$ up to 10° and $n_\alpha \simeq n_\beta = 1{\cdot}496 \pm 0{\cdot}001$, $n_\gamma = 1{\cdot}502 \pm 0{\cdot}002$. The specific gravity is $2{\cdot}30 \pm 0{\cdot}02$. The unit-cell constants are $a = 8{\cdot}583 \pm 0{\cdot}004$, $c = 8{\cdot}817 \pm 0{\cdot}004$ Å. Atomic and thermal vibrational coordinates were refined to $R =$ 8·9 % by full-matrix least-squares methods and with three-dimensional data. The following bond lengths were found:

$$\begin{aligned} \text{Be–O} &= 1{\cdot}608 \pm 0{\cdot}012 \text{ Å} \\ \text{Al–O} &= 1{\cdot}762 \pm 0{\cdot}014 \\ \text{Si –O} &= 1{\cdot}601 \pm 0{\cdot}008 \end{aligned}$$

The last value is an average of four independent determinations.

Introduction

The mineral was described by Sørensen (1960, 1962) under the name of beryllium sodalite, and by Semenov & Bykov (1960), who used the name beryllo-sodalite. Its chemical and physical properties turned out to be so different from those of sodalite that a distinct name was justified. Tugtupite was suggested after the place where the mineral was originally found (Tugtup agtakôrfia in the Ilimaussaq intrusion, South Greenland), and this name was approved in 1965 by the I.M.A. Commission on New Minerals and Mineral Names.

Experimental

Chemical and physical properties

The result of a chemical analysis is given in Table 1. The formula of the mineral was calculated to be $Na_8Al_2Be_2Si_8O_{24}(Cl,S)_2$ with traces of K and Mg substituted for Na, the S content being about 5% of the Cl content.

Table 1. *Chemical analysis of tugtupite*

	Weight %	Metal atoms in 100 g	Metal atoms in $100\,.\,\frac{12{\cdot}00}{1{\cdot}295}$ g†
SiO_2	51·58	0·861	7·98
Al_2O_3	11·15	0·219	2·03
Na_2O	25·52	0·822	7·62
BeO	5·40	0·216	2·00
Cl	7·28	0·205	1·90
S*	0·33	0·010	0·09
K_2O	0·12	0·002	0·02
MgO	0·20	0·005	0·05

* Present as S^{2-}.

† The sum of Be, Al and Si was 1·295 in 100 g; in sodalite the sum of Al and Si is 12. The figures in the third column were therefore multiplied by the ratio $\frac{12{\cdot}00}{1.295}$ to give the last column.

The crystals are white when kept in darkness, but change to pink when exposed to daylight. Optically the mineral is orthorhombic with values of $2V_\gamma$ up to 10°.

$$n_\alpha \simeq n_\beta = 1{\cdot}496 \pm 0{\cdot}001$$
$$n_\gamma = 1{\cdot}502 \pm 0{\cdot}002;\ c \neq \gamma\,.$$

The cleavage is good parallel to {110} and {101}. (A more extensive crystallographic description will be given in *Medd. om Grønland*, vol. 181, No. 4).

Table 2. *Observed and calculated values of* $\sin^2\theta$ *up to* 0·2500

$\sin^2\theta_{obs}$	Intensity	Indices	$\sin^2\theta_{calc}$
0·0158	*s*	101	0·0157
0·0162	*vw*	110	0·0161
0·0306	*w*	002	0·0306
0·0323	*vvw*	200	0·0323
0·0467	*m*	112	0·0467
0·0480	*vs*	211	0·0480
0·0630	*vvw*?	202	0·0628
0·0647	*vvw*	220	0·0645
0·0770	*vw*	103	0·0769
0·0803	*vw*	301	0·0802
0·0808	*vvw*	310	0·0807
0·0952	*m*	222	0·0951
0·1093	*w*	213	0·1091
0·1113	*w*	312	0·1112
0·1126	*w*	321	0·1125
0·1384	*w*	114	0·1384
0·1413	*w*	303	0·1414
0·1451	*m*	330 411	0·1452 0·1448
0·1595	*vw*	402	0·1596
0·1612	*vvw*	420	0·1613
0·1738	*vw*	323	0·1737
0·1868	*vvw*	224	0·1869
0·1918	*vw*	422	0·1919
0·2026	*vvw*?	314	0·2030
0·2062	*vw*	413	0·2059
0·2093	*w*	431	0·2093
0·2314	*vvw*	215	0·2315
0·2410	*vvw*?	521 512	0·2416 0·2403

The specific gravity, as determined by hydrostatic weighing, is $2{\cdot}30 \pm 0{\cdot}02$, while the density calculated from the chemical analysis and the unit-cell volume is $2{\cdot}36$ g.cm^{-3}. By means of differential thermal analysis it was ascertained that no reaction takes place below 630 °C. X-ray powder diagrams showed no change in symmetry when the mineral was heated to the melting point ($\sim$950 °C).

The crystals are strongly piezoelectric, but no pyroelectric effect could be detected.

X-ray data

The axes of the unit cell were determined at room temperature by the Guinier technique with Cu $K\alpha$ radiation ($\lambda = 1{\cdot}5418$ Å):

$$a = b = 8{\cdot}583 \pm 0{\cdot}004 \text{ Å}$$
$$c = 8{\cdot}817 \pm 0{\cdot}004 \text{ Å}$$
$$V = 658 \text{ Å}^3$$
$$Z = 1$$

Table 2 gives the observed and calculated values of $\sin^2\theta$ with their roughly estimated intensities. NaCl has been used as a standard, $a = 5{\cdot}6400$ Å.

The symmetry of precession and Weissenberg films and the strong piezoelectric effect reduced the possible space groups to $I4$ and $I\bar{4}$. The only way of deciding between these two with certainty would be detection of a positive pyroelectric effect, which is allowed only for $I4$. The close relation with the sodalite structure (space group $P\bar{4}3m$ or $P\bar{4}3n$, see later) and the types of equivalent positions in the two space groups strongly favour $I\bar{4}$, and consequently the structure determination was started on the assumption of this space group. The final agreement between calculated and observed structure factors showed that the choice was correct.

Intensity data

An approximately equidimensional crystal ($\sim$0·3 mm) was rotated about the c axis, and the reciprocal layers $hk0-hk6$ were recorded with unfiltered Cu radiation and the Weissenberg technique.

Another crystal ($\sim 0{\cdot}4 \times 0{\cdot}1$ mm), ground to ellipsoidal shape, was rotated along the long axis of the ellipsoid, which was nearly parallel to the b axis of the crystal, and the $h0l-h6l$ reflexions were photographed. As the latter crystal turned out to be not quite perfect, only the equatorial reflexions were measured. The intensities were estimated visually by means of a calibrated strip. The multiple film technique was used and the conversion factors between the layers were determined experimentally. The exposure times for the packets were chosen so that one film from one packet should be more or less identical with a film in another packet.

As $I_{hkl} = I_{\bar{h}\bar{k}l}$ the same reflexions were measured on several films and on different positions within the film; in many cases β reflexions also gave valuable information. Due regard was paid to all measurements.

In case of $\alpha_1 - \alpha_2$ splitting a weighted mean was calculated. The fourfold symmetry was checked and found to be fulfilled within the experimental error. (Optically, however, the symmetry is lower; see above.) Mean values of I_{hkl} and $I_{k\bar{h}l}$ were used when different. The intensities were corrected for Lorentz and polarization factors, but not for absorption; see later*.

Structure determination and refinement

The two Patterson projections $P(uv)$ and $P(uw)$ were in good agreement with what could be expected from knowledge of the sodalite structure: Cl in 000, Al and Be in $0\frac{1}{2}\frac{1}{4}$ and $0\frac{1}{2}\frac{3}{4}$ (only the refinement could decide the distribution between the two positions; see later), and Si in a general position with $xyz \simeq 0\frac{1}{4}\frac{1}{2}$, the 12 metal atoms Be, Al, Si thus occupying the positions of Al and Si in sodalite. As Cl is in 000 the Patterson projections bear great resemblance to electron-density projections, and some information could be obtained about the other atoms. Two sets of O atoms stood out, but the last O was overlapped by Na and again use must be made of the sodalite structure, whose 24 O atoms can be divided into three groups corresponding to the three eightfold general positions in $I\bar{4}$. As the cubic space groups have cyclic rotation of the coordinates, a well resolved O atom in a projection will give information about the third coordinate of another O atom.

As the electron-density projection along the c axis is centrosymmetric the corresponding difference maps were calculated until R was 23%.

A minimum residual program (Bhuiya & Stanley, 1963) written by J. Danielsen refined the coordinates to $R = 14\%$ and $R = 9\%$ for the $hk0$ and $h0l$ reflexions respectively. A common isotropic B value of 1·0 was used, and no attempt was made to vary the temperature factor at this stage. In order to calculate F_{h0l} Al and Be had to be placed in the twofold positions. Both possibilities were tried; the one with Be in $0\frac{1}{2}\frac{1}{4}$ and Al in $0\frac{1}{2}\frac{3}{4}$ converged more rapidly and was therefore used for the three-dimensional R-minimization later on. (The final least-squares calculations proved this choice to be correct; see below.)

Data from the reciprocal layers $hk0-hk6$ were put on the same scale using the $h0l$ reflexions. For a given l the ratio between common F values from the two zones was not constant but varied with ξ because of absorption in the larger crystal used for recording the $hk0-hk6$ reflexions. The ratios were extrapolated to $\xi = 0$. These preliminary values for the conversion factors between the layers were later refined in the usual way using $F_{\text{obs}}/F_{\text{calc}}$ for each layer when more accurate coordinates were known. There seems to be a possibility of extinction, but no correction for this has been made. After a readjustment of the conversion factors the final

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* No allowance was made for spot shape distortion other than averaging the intensities of reflexions from the upper and lower half of the film.

Table 3. *Observed and calculated structure factors*

h	k	l	$10\|F_o\|$	$10\|F_c\|$
1	-11	0	89	95
0	-10	0	136	123
2	-10	0	200	217
4	-10	0	95	120
1	-9	0	156	146
3	-9	0	260	245
5	-9	0	206	223
0	-8	0	653	615
2	-8	0	61	56
4	-8	0	823	863
6	-8	0	190	191
1	-7	0	147	126
3	-7	0	179	137
5	-7	0	311	314
7	-7	0	140	148
0	-6	0	844	834
2	-6	0	144	115
4	-6	0	166	140
6	-6	0	160	133
1	-5	0	59	151
3	-5	0	225	197
5	-5	0	73	3
7	-5	0	440	395
9	-5	0	67	69
0	-4	0	385	387
2	-4	0	405	376
4	-4	0	894	1009
6	-4	0	362	333
8	-4	0	475	437
10	-4	0	154	166
1	-3	0	462	534
3	-3	0	981	1137
5	-3	0	373	337
7	-3	0	469	448
9	-3	0	251	260
0	-2	0	248	239
2	-2	0	338	338
4	-2	0	383	353
6	-2	0	446	399
8	-2	0	698	687
10	-2	0	115	116
1	-1	0	283	264
3	-1	0	135	137
5	-1	0	48	52
7	-1	0	127	124
9	-1	0	197	186
1	-10	1	446	479
3	-10	1	187	204
2	-9	1	196	225
4	-9	1	103	131
6	-9	1	174	180
1	-8	1	273	233
3	-8	1	80	54
5	-8	1	116	113
7	-8	1	395	474
2	-7	1	810	674
4	-7	1	95	112
6	-7	1	222	219
1	-6	1	571	509
3	-6	1	304	268
5	-6	1	606	576
2	-5	1	523	460
4	-5	1	560	505
1	-4	1	711	723
3	-4	1	767	803
2	-3	1	452	448
1	-2	1	800	1071
0	-1	1	444	518
1	2	1	800	1071
0	3	1	453	458
2	3	1	614	627
1	4	1	749	740
3	4	1	326	315
0	5	1	212	211
2	5	1	362	393
4	5	1	252	229
1	6	1	60	49
3	6	1	637	545
5	6	1	452	418
0	7	1	321	265
2	7	1	231	219
4	7	1	302	345
6	7	1	181	176
1	8	1	494	412
3	8	1	146	159
5	8	1	293	308
7	8	1	114	125
0	9	1	265	219
2	9	1	354	327
4	9	1	170	157
6	9	1	380	431
1	10	1	332	322
3	10	1	411	456
0	11	1	110	140
0	-10	2	154	157
2	-10	2	269	305
4	-10	2	100	131
1	-9	2	133	118
3	-9	2	335	313
5	-9	2	250	237
0	-8	2	624	587
2	-8	2	178	167
4	-8	2	158	151
6	-8	2	163	174
1	-7	2	268	236
3	-7	2	434	414
5	-7	2	157	148
7	-7	2	367	402
0	-6	2	226	215
2	-6	2	701	634
4	-6	2	156	143
6	-6	2	446	465
1	-5	2	127	104
3	-5	2	797	789
5	-5	2	462	443
0	-4	2	632	629
2	-4	2	553	553
4	-4	2	880	918
1	-3	2	401	398
3	-3	2	301	251
0	-2	2	153	154
2	-2	2	769	953
1	-1	2	621	871
1	3	2	441	446
2	4	2	203	179
1	5	2	437	428
3	5	2	249	234
2	6	2	439	390
4	6	2	391	373
1	7	2	815	771
3	7	2	351	304
5	7	2	260	266
2	8	2	267	225
4	8	2	406	386
6	8	2	158	142
1	9	2	199	212
3	9	2	86	76
5	9	2	315	311
2	10	2	360	378
4	10	2	95	72
1	-10	3	348	404
3	-10	3	97	89
0	-9	3	133	122
2	-9	3	341	297
4	-9	3	193	170
1	-8	3	417	439
3	-8	3	469	437
5	-8	3	138	107
7	-8	3	119	126
0	-7	3	536	469
2	-7	3	289	259
4	-7	3	95	71
6	-7	3	382	398
1	-6	3	572	516
3	-6	3	547	541
5	-6	3	517	511
0	-5	3	520	466
2	-5	3	354	326
4	-5	3	139	80
1	-4	3	185	165
3	-4	3	413	375
0	-3	3	843	1012
2	-3	3	601	623
1	-2	3	590	668
0	-1	3	330	421
1	2	3	398	425
2	3	3	333	323
1	4	3	469	476
3	4	3	520	497
2	5	3	751	778
4	5	3	114	104
1	6	3	556	521
3	6	3	692	728
5	6	3	67	39
2	7	3	399	325
4	7	3	271	253
6	7	3	80	75
1	8	3	447	428
3	8	3	150	120
5	8	3	148	139
7	8	3	135	175
2	9	3	327	322
4	9	3	135	139
1	10	3	27	35
3	10	3	218	238
0	-10	4	254	270
2	-10	4	43	51
1	-9	4	377	394
3	-9	4	145	144
5	-9	4	51	63
0	-8	4	698	702
2	-8	4	361	362
4	-8	4	450	433
6	-8	4	210	249
1	-7	4	197	179
3	-7	4	303	259
5	-7	4	219	218
7	-7	4	99	85
0	-6	4	281	242
2	-6	4	410	345
4	-6	4	130	127
6	-6	4	96	114
1	-5	4	390	328
3	-5	4	345	308
5	-5	4	106	112
0	-4	4	965	1117
2	-4	4	627	628
4	-4	4	866	951
1	-3	4	254	208
3	-3	4	248	215
0	-2	4	294	309
2	-2	4	475	492
1	-1	4	686	834
1	3	4	299	279
2	4	4	627	647
1	5	4	381	348
3	5	4	229	210
2	6	4	389	334
4	6	4	302	281
1	7	4	508	440
3	7	4	254	260
5	7	4	66	76
2	8	4	69	66
4	8	4	546	552
6	8	4	271	278
3	9	4	235	257
5	9	4	60	75
2	10	4	168	176
0	-9	5	98	85
2	-9	5	304	330
1	-8	5	131	128
3	-8	5	235	243
5	-8	5	210	213
0	-7	5	312	283
2	-7	5	266	278
4	-7	5	193	212
6	-7	5	363	368
1	-6	5	764	787
3	-6	5	118	109
5	-6	5	439	453
0	-5	5	109	75
2	-5	5	456	419
4	-5	5	370	364
1	-4	5	250	227
3	-4	5	388	340
0	-3	5	548	513
2	-3	5	687	684
1	-2	5	263	239
0	-1	5	174	191
1	2	5	453	467
2	3	5	641	645
1	4	5	611	537
3	4	5	154	126
2	5	5	641	585
4	5	5	196	178
1	6	5	351	321
3	6	5	284	244
5	6	5	395	395
2	7	5	239	219
4	7	5	186	179
6	7	5	279	283
1	8	5	131	140
3	8	5	99	86
5	8	5	270	262
2	9	5	442	450
4	9	5	99	122
1	-9	6	131	122
0	-8	6	221	224
2	-8	6	57	41
4	-8	6	483	558
1	-7	6	97	69
3	-7	6	361	365
5	-7	6	166	182
0	-6	6	124	125
2	-6	6	469	472
4	-6	6	117	93
6	-6	6	368	363
1	-5	6	434	380
3	-5	6	176	176
5	-5	6	217	210
0	-4	6	510	485
2	-4	6	234	205
4	-4	6	315	266
1	-3	6	319	317
3	-3	6	612	609
0	-2	6	148	154
2	-2	6	588	576
1	-1	6	166	167
1	3	6	578	551
2	4	6	198	141
1	5	6	319	280
3	5	6	358	335
2	6	6	581	570
4	6	6	287	274
1	7	6	194	199
3	7	6	120	126
5	7	6	531	567
2	8	6	184	181
4	8	6	244	249
1	9	6	350	357

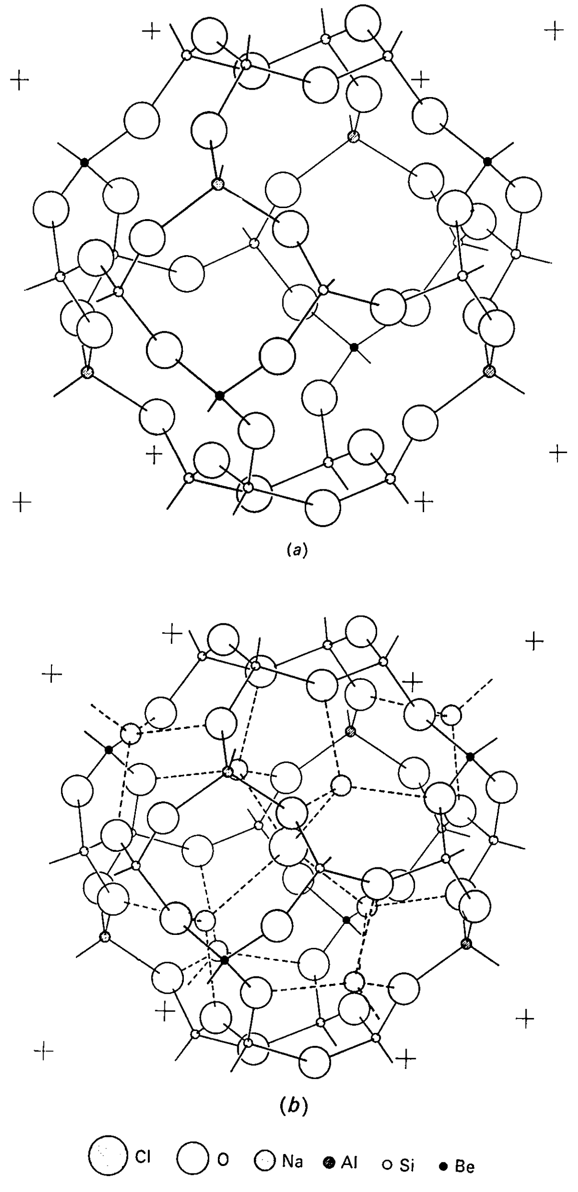

Fig. 1. Modified clinographic projection of tugtupite. $\varphi = 9°28'$ is the angle of elevation in the *a–c* plane of the lines of projection *after* the rotation $\theta = 18°26'$ about the *c* axis. In this special kind of projection the *b* and *c* axes remain in the plane of the paper and mutually perpendicular. The *a* axis points towards the reader to the left. The corners of the unit cell are indicated by crosses. In (*a*) only the Si, Be, Al and O are shown, while the complete structure is given in (*b*).

refinement of the parameters was done by using a full-matrix least-squares program (Busing, Martin & Levy, 1962). After two cycles new scale factors were calculated and three more cycles were computed until the shifts were less than 1% of the standard deviations. The final R was 8·9%. The weighting function was of the type

$$w = A_1^2 \qquad F_o \leq 2{\cdot}0$$
$$w = A_2^2 \cdot F_0^{2B_2}; \quad F_o > 2{\cdot}0$$

with

$$A_1 = 5{\cdot}0$$
$$A_2 = 10; \; B_2 = -1; \; F_{\min} \simeq 2{\cdot}0$$

All possible reflexions were observed, except five. These were not included in the least-squares calculations. *f* values were taken from *International Tables for X-ray Crystallography* (1962, pp. 202–3), and values for neutral atoms were used. Only isotropic temperature factors were introduced and refined with the positional parameters.

Results and conclusions

The observed and calculated structure factors are given in Table 3 as ten times the absolute values. The final atomic positions with their Debye temperature factors are found in Table 4.

As mentioned above, the crystal is not small enough for the absorption to be negligible ($\mu \sim 86$ cm^{-1}). The B values determined by the least-squares method are consequently too low. Especially the *hk*0 reflexions seem to be affected.

The structure consists of linked MO_4 tetrahedra with M = Be, Al and Si as the metallic cations (Fig. 1). These tetrahedra share corners, Cl and Na being placed in holes in the framework. Characteristic are the 8-rings with alternating metal and oxygen atoms. One third of the rings contain only Si, while the rest have Be, Si and Al alternating. Fig. 1(*a*) shows the arrangement of the 8-rings. Fig. 1(*b*) gives the complete structure. As Be and Al are placed on a fourfold axis the BeO_4 and AlO_4 tetrahedra are regular. The metal–oxygen distances are 1·608 ± 0·012 Å and 1·762 ± 0·014 Å for Be–O and Al–O respectively. The SiO_4 tetrahedra, however, are distorted. Of the four O atoms in the tetrahedron, two are bound to other Si atoms, one to Be and one to Al. The bond lengths with their standard deviations are given in Table 5. The Si–O distances in the pure rings are 1·646 (*A*) and 1·611 (*B*) alternating, while the mixed rings have distances of 1·588 (*C*) when O is linked to Be and 1·566 (*F*) when linked to Al.

Table 4. *Atomic coordinates and thermal parameters with their standard deviations*

	x/a	σ(*x/a*)	*y/b*	σ(*y/b*)	*z/c*	σ(*z/c*)	*B*	σ(*B*)
O(1)	0·1471	0·0008	0·1332	0·0008	0·4431	0·0013	0·63	0·14
O(2)	0·3467	0·0009	0·0362	0·0009	0·6512	0·0015	0·86	0·13
O(3)	0·4261	0·0008	0·1506	0·0008	0·1347	0·0014	0·79	0·13
Na	0·1575	0·0005	0·1970	0·0005	0·1815	0·0008	1·12	0·10
Si	0·0134	0·0003	0·2535	0·0003	0·4956	0·0005	0·22	0·08
Be	0·0000	—	0·5000	—	0·2500	—	0·66	0·41
Al	0·0000	—	0·5000	—	0·7500	—	0·26	0·10
Cl	0·0000	—	0·0000	—	0·0000	—	1·50	0·11

Table 5. *Bond lengths with their standard deviations*

	Bond	M–O Distance	σ
Si–O	*A*	1·646 Å	0·014 Å
Si–O	*B*	1·611	0·013
Si–O	*C*	1·580	0·018
Si–O	*D*	1·566	0·017
Average:		1·601	0·008*
Al–O	*E*	1·762	0·014
Be–O	*F*	1·608	0·012

* Taken as the average of σ divided by the square root of the numbers of independent determinations, as suggested by Smith & Bailey (1963).

Smith & Bailey (1963) give as best values for Si–O and Al–O 1·61 Å and 1·75 Å respectively, and our values agree within the experimental error. Only a few Be–O distances have been reported in the literature, but the value found in tugtupite falls within the interval given by *International Tables for X-ray Crystallography* (1962, p. 260). The question of the space group of sodalite, $Na_8Al_6Si_6O_{24}Cl_2$, is still open. In the paper of Pauling (1930) it was given as $P\bar{4}3n$, while Barth (1932) argued for $P\bar{4}3m$. Later Saalfeld (1961) discussed the matter in relation to other members of the sodalite group and proposed the space group $P\bar{4}3n$. With the technique used in the early structure determinations it was not possible to determine the Si–O and Al–O distances with sufficient accuracy to decide whether the 6 Al and 6 Si are in two different special positions ($P\bar{4}3n$) or statistically distributed in a 12-fold position ($P\bar{4}3m$).

In view of the ordered arrangement of the cations of tugtupite it seems worth while to re-examine the structure of sodalite. We hope to be able to do so in the near future.

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On the Equivalence of Structure Invariants*

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The triangle in reciprocal space associated with a given structure invariant is defined and the concept of the equivalence of structure invariants is introduced. It is assumed that many of the interatomic triangles (especially the smaller ones) in a crystal structure are congruent to each other and that the triangles in each collection of congruent interatomic triangles are more or less randomly oriented in space. Under these assumptions the values of equivalent structure invariants are approximately equal, especially if the sides of the associated triangle are small. This result facilitates the solution of the problem of direct phase determination for structures satisfying our assumptions.

1. Introduction

The structure invariants are those entities whose values are uniquely determined by a crystal structure. They play a fundamental role in the problem of direct phase determination. An important set of structure invariants consists of the linear combinations of the phases

$$\varphi_1+\varphi_2+\varphi_3\,, \tag{1·1}$$

in which the abbreviations

$$\varphi_i=\varphi_{\mathbf{h}_i}\,,\quad i=1,2,3\,, \tag{1·2}$$

have been used and the assumption

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