Crystallography

Crystal structure of sorensenite

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An alkaline silicate of tin – sorensenite – was first found in southern Greenland[1] in association with zeolite, sodalite, aegirine, microcline, and neptunite. The mineral is transparent, colorless or pinkish, biaxial, negative 2V ≈75°; n_g = 1.584-1.586, n_m = 1.581-1.585; n_p = 1.576-1.572. For prismatic and acicular crystals, cleavage along two directions is characteristic: The most perfect is along $\{10\bar{1}\}$, the other along $\{100\}$. The result of testing for a piezoelectric effect is negative.

From the initial investigation[1] the parameters of the monoclinic cell are: a = 20.78; b = 7.45; c = 12.05 Å; β = 117°06'; Federov group C2/c or Cc.

The complete chemical analysis of the mineral (analyzed by M. E. Kazakov) leads to the equation $Na_4SnBe_2 \cdot [Si_6O_{18}] \cdot 2H_2O$; for density 2.96, Z = 4 of the above-indicated units are contained in the cell.

X-ray data based on sorensenite, obtained on unfaceted fragments of dimensions 0.2 × 0.1 × 0.3 mm, gave Weissenberg patterns of the layer lines $h0l-h6l$, hk0 [Mo Kα radiation, max$(\sin\theta/\lambda)$ = 1 $Å^{-1}$]. An estimate of the intensities (fourfold) is made from a blackening scale with a step of $2^{1/4}$.

A total of 1150 nonzero reflections were used to construct the three-dimensional Patterson function P(uvw). An analysis of the rhombuses based on ref. 2 was insufficient for unambiguously assigning the mineral to a holohedron, and further analysis was carried out in the framework of the Federov group Cc. Based on the equations of refs. 2 and 3 we isolated 10 atoms of the structure: the heavier Sn and Si, and some anions. Their coordinates became the starting points for a series of syntheses of electron density [weighted projections σ_{h1l}, σ_{h2l}, σ_{h3l}, and $\rho(xyz)$], on which the remaining atoms of the structure were localized. Least-squares refinement of the layer factors, the isotropic thermal corrections, and the position parameters lead to R = 0.099.

The coordinates of the basis atoms at this stage of interpretation of the structure are presented in Table 1.

The tetravalent tin is located in a slightly stretched octahedron: The four Sn–O distances in the mean cross section of the octahedron [∥(001)] are close in value: 1.95-2.06 Å – for two polar stretched octahedra up to 2.12-2.16 Å. The edges of the Sn octahedra are within the limits 2.81-3.06 Å. In the tetrahedra: Si_1-O = 1.55-1.63 Å; Si_2-O = 1.61-1.69 Å; Si_3-O = 1.55-1.70 Å; Si_4-O = 1.58-1.74 Å; Si_5-O = 1.53-1.72 Å; Si_6-O = 1.60-1.75 Å; the edges of the tetrahedra fall outside the limits 2.50-2.80 Å.

Each of the two independent Be^{2+} is surrounded by four ligands at distances: Be_1-O = 1.60-1.70 Å and Be_2-O = 1.61-1.68 Å. Both Be tetrahedra are joined in a diorthogroup, not through the vertex, but along an edge, which explains the crystal chemical peculiarity of the structure. The common edge of the diortho group (formula Be_2O_6) is shortened to 2.37 Å (compare 2.42 Å in ref. 4), but the Be–O distances to the general vertices increase: 1.70 as compared to 1.60 Å in the Be_1 tetrahedron, and 1.68 as compared to 1.61 Å in the Be_2 tetrahedron, respectively.

We separate the coordination polyhedra at four types of independent Na with great difficulty. In their surroundings the general features appear: One distance (two in Na_2) is considerably shorter than the remaining distances in the intermediate coordination group of the ligand at distances 2.47-2.65 Å and, finally, in the external sphere 2.76-2.97 Å (the remaining atoms are oxygen). With the indicated reservations the Na_1 polyhedron becomes a distorted seven-vertex body with five ligands at distances 2.22-2.59 Å, and two at 2.78-2.82 Å, for the following neighbors spaced at a distance 3.28 Å and greater. At Na_2 in the first coordination sphere of four neighbors: 2.28, 2.32, 2.46, 2.62 Å for the four following 2.77, 2.90, 2.92, and 2.97 Å. In the Na_3 polyhedron there are fixed one distance 2.40, three distances 2.52, 2.62, 2.65, and three more, 2.78, 2.81, and 2.88 Å.

Finally, in the neighborhood of the last cation Na_4 for one short distance 2.22, two intermediate distances 2.47, 2.53 Å, there are fixed four more distances 2.60-2.76 Å; two ligands enter only into the coordination sphere of the cations of Na and they can be taken for neutral molecules of H_2O.

TABLE 1. Sorensenite. Coordinates of the Basis Atoms

Atom	x/a	y/b	z/c	Atom	x/a	y/b	z/c	Atom	x/a	y/b	z/c
Sn	0,4998	0.2371	0.2465	O_5	0.136	0.081	0,134	O_{16}	0,337	0,248	0.270
Si_1	0.3534	0.0527	0.2382	O_6	0.355	0.933	0.352	O_{17}	0,306	0,255	0.988
Si_2	0.1469	0.5366	0,2469	O_7	0.168	0.747	0.220	O_{18}	0.449	0.259	0.058
Si_3	0.3544	0.4445	0.2450	O_8	0.198	0.254	0.014	$O_{19}(=H_2O)$	0,073	0.212	0.392
Si_4	0.1453	0.9605	0.2509	O_9	0,049	0,738	0.438	$O_{20}(=H_2O)$	0.438	0.747	0.096
Si_5	0.1348	0.2388	0.0539	O_{10}	0,436	0.449	0.261	Na_1	0.304	0.227	0.452
Si_6	0.3684	0.7624	0.4454	O_{11}	0.431	0.039	0.237	Na_2	0.198	0.771	0.059
O_1	0.067	0.956	0.244	O_{12}	0.209	0.474	0.381	Na_3	0.511	−0,052	0.473
O_2	0.065	0.561	0.234	O_{13}	0.212	0.036	0.375	Na_4	0.999	0,048	0.487
O_3	0.292	0.965	0.110	O_{14}	0.366	0.578	0.367	Be_1	0.248	0.093	0.989
O_4	0.298	0.523	0.119	O_{15}	0.150	0.431	0.127	Be_2	0.251	0.408	0.010

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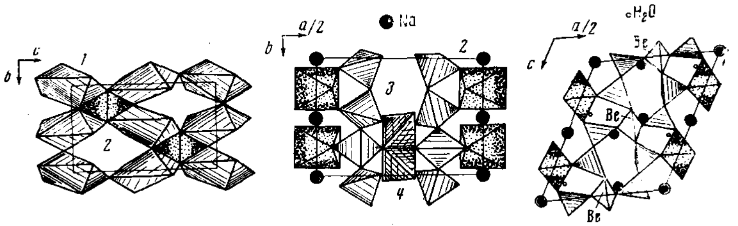

a b c

Fig. 1. Sorensenite: a) lattice wall ∥ (100). The vibrating columns of Na octahedra (1) and the Sn octahedra that cement them are separated (2). b) Projection of the structure in the polyhedra on the xy plane. The filling of the partition is shown: Two wollastonite $[Si_3O_9]_\infty$ chains (3) are joined by the Be_2O_6 diorthogroup (4) into a single beryllium—silicon—oxygen skeleton. c) Projection of the structure in polyhedra on the xz plane; the filled circles are the Na cations in the walls of the channels of the skeleton; the double circles are Na atoms of the lattice wall; the Be tetrahedra are left empty.

In the description of the structure of sorensenite we can proceed from the cation walls parallel to (100). The walls (Fig. 1a) are not solid, but are perforated lattices. They can be described in two ways. If we assume the Na_3 and Na_4 cations to be localized in the octahedra then the available columns of Na octahedra, oscillating without bound along (010), are joined at the vertices (the addition of a seventh vertex makes the joining more rigid, without changing the general architecture). The columns – the original columns and those derived from them (through reflection in the glide plane c) – are cemented by individual Sn octahedra; as a result there arises a perforated wall, similar to such a wall in calcium hydrosilicate – phase Y. This wall can be described as the result of the coupling through Na octahedra of infinite (in the direction [011] or [01$\bar{1}$], which is equivalent) composite chains of alternating Na and Sn octahedra (compare the natro-titanium columns in ramsayite and tinaksite); the unit cell is cleaved by two coupled C translations of such plane walls. Between them there is enclosed a silicon–beryllium–oxygen skeleton: two independent wollastonite chains of $[Si_3O_9]_\infty$ with axis along [010], which are fastened by the abovementioned diorthogroups of Be_2O_6 (Fig. 1b and c). In the skeleton obtained one should pay attention to the channels (along the z axis), in the walls of which are placed the Na_1 and Na_2 cations, without particpating in the construction of the cation wall.

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