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THE CRYSTAL STRUCTURE OF THE NATURAL STRONTIUM BORATE, p-VEATCHITE, $Sr_2[B_5O_8(OH)]_2 \cdot B(OH)_3 \cdot H_2O$

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The monoclinic cell of p-veatchite, with dimensions a = 6.70, b = 20.80, c = 6.60 Å, β = 119°15', contains two units of $Sr_2B_{11}O_{16}(OH)_5 \cdot H_2O$. The space group is the acentric enantiomorphous $C_2^2 = P2_1$. The structure was determined from the three-dimensional Patterson function and successive electron density difference syntheses. The refinement was carried out with three-dimensional Fourier syntheses, by the method of least squares, and by the method of random search. Hydrogen bonds were deduced from analysis of the distances between corresponding oxygen atoms. The structure is characterized by 104 coordinate parameters (without H atoms). The disagreement index is R_{hkl} = 15.2% for an isotropic temperature factor B_{hkl} = 1.6 Å^2 for the 1100 nonzero reflections. p-veatchite is a mixed-type borate with boron-oxygen radicals $[B_5O_8(OH)]_n^{-2n}$ which are infinite in two directions, and independent island triangles of $B(OH)_3$ complexes. This is the first known example of a mixed borate. The Sr atoms are located inside oxygen ten- and eleven-coordinate polyhedra, which are linked to each other by common edges. The structure has a layer character. Each layer is an open network of Sr polyhedra, to one side of which a boron–oxygen network $[B_5O_8(OH)]_n^{-2n}$ is joined, and to the other side a similar network in addition to solitary $B(OH)_3$ triangles is linked. Successive layers are joined by hydrogen bonds. The $[B_5O_8(OH)]_n^{-2n}$ radicals are found for the first time in p-veatchite.

The object of the study is the strontium mineral p-veatchite, which is a member of the class of aqueous borates. It was first found in England [1, 2], and then in the Federal Republic of Germany [3] and the Soviet Union [4]. It was named because of its similarity to the previously discovered mineral, veatchite [5-7], whose properties and chemical composition are very close to those of p-veatchite. However, the cell dimensions and space group of veatchite are different from those of p-veatchite [2, 7, 8]. The English and German samples had the chemical formula $SrO \cdot 3B_2O_3 \cdot 2H_2O = SrB_6O_{10} \cdot 2H_2O$ [1-3], while native samples had the formula $4SrO \cdot 11B_2O_3 \cdot 7H_2O = Sr_4B_{22}O_{37} \cdot 7H_2O$ [4]. In the first x-ray diffraction work on p-veatchite, the parameters of the monoclinic cell were determined and the diffraction group of the crystal was established: a = 6.72, b = 20.81, c = 6.64, β = 119°04', V = 813 Å^3, $2/mP2_1/-$. These data agree with the results of other workers [3, 4, 8] within the limits of experimental error. p-veatchite exhibits perfect cleavage parallel to (010). The density is within the limits 2.60-2.69 g/cm^3 [1, 2, 4]. A preliminary communication about the structure was published in 1968 [9].

Small, orange-red, platelike crystals from the Inderskii formation (Kazakh SSR) served as the objects of study. The monoclinic cell parameters which we determined are: a = 6.70 ± 0.02, b = 20.80 ± 0.05, c = 6.60 ± 0.02 Å, β = 119°15', V = 797 Å^3 (RKV-86 camera, Cu Kα radiation; the β angle was determined from the $h0l$ layer with a comparator). For a density of 2.69 g/cm^3 [4], the cell contains one unit of $Sr_4B_{22}O_{37} \cdot 7H_2O$; d_{calc} = 2.70

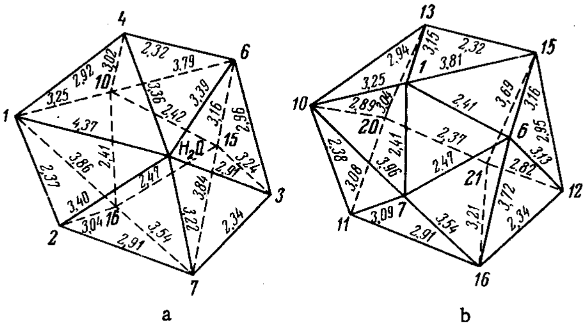

Fig. 1. The oxygen polyhedra around the Sr atoms. a) Sr_I ten-coordinate polyhedron; b) Sr_{II} eleven-coordinate polyhedron. Lengths of the O–O edges are given in Å.

g/cm³. Because the wavelength of the Sr K-series absorption edge is close to Mo Kα, the photographs were taken with Cu Kα radiation. The strong tendency of the crystals to split precluded the preparation of spherical samples. Weissenberg patterns of the zero and three upper layers were taken for rotations about *a* and c, and also the zero and first layers were obtained for rotation about b. The reflection intensities were estimated by comparison with an intensity strip (in steps of $2^{1/4}$). The multiple film method was used for measuring the high-intensity reflections. In all, 1100 independent nonzero reflections were obtained. A correction for spot shape [10] was introduced into the I_{hk3} and I_{3kl} intensities, in addition to polarization and kinematic corrections. The acentric space group $C_2^2 = P2_1$ was established on the basis of the statistics of the intensities [11]: the quantities $|F_{h0l}|^2$ corresponded to a centrosymmetric distribution, but $|F_{hk0}|^2$ and $|F_{0kl}|^2$ corresponded to an acentric distribution.

The structure was solved with the help of the Patterson function in conjunction with successive Fourier syntheses. The three-dimensional P(uvw) diagram yielded the positions of the two Sr basis atoms. The light O and B atoms were located from difference three-dimensional Fourier syntheses (Sr contributions subtracted). In the calculation of each Δ synthesis were included the largest peaks from the previous Δ synthesis. The number of such peaks was limited by the proposed number of atoms in the structure (according to chemical analysis [1-3], it was expected that there would be 36 light atoms, not counting hydrogens, in the independent part of the cell), and also by consideration of the statistical distribution of the peaks with respect to height: the value below which the number of peaks sharply increased was taken as a critical one and smaller peaks were considered to reflect errors in the background. In the first stage, the peaks chosen were used as O atoms; subsequently their heights and relative positions were analyzed, and they were identified. As a result, the false peaks (several fairly large ones among this number) gradually disappeared, and the peaks corresponding to real atoms appeared on succeeding Δ diagrams. The model of the structure was revealed fairly clearly. In the final Δ synthesis, the smallest oxygen peak was three times larger, and the smallest boron peak two times larger, than the highest peak in the background (estimate made without F_{000}). The disagreement index R_{hkl} dropped to 21% upon inclusion of all 33 light atoms found in the calculations. It thus appeared that there were not 38, but 35 atoms in the independent part of the cell. The

TABLE 1. Coordinates of the Basis Atoms in the Structure of p-Veatchite

Atom	*x/a*	*y/b*	*z/c*	Atom	*x/a*	*y/b*	*z/c*
Sr_I	0.073	0	$0\ 020_5$	O_{17}	0.050	0.792	0.984
Sr_{II}	0.379	0.887_2	0.689_5	O_{18}*	0.235	0.690_5	0.105
O_1	0.599	0.010	0.900	O_{19}*	0.428	0.668	0.682
O_2	0.906	0.014	0.287	O_{20}*	0.610	0.770	0.760
O_3	0.514	0.023	0.200	O_{21}*	0.207	0.765	0.597
O_4	0.805	0.021	0.600	H_2O	0.141	0.115	0.056
O_5	0.982	0.109	0.516	B_1	0.672	0.016	0.131
O_6	0.186	0.008	0.699	B_2	0.962	0.036_5	0.516
O_7	0.400	0.016_5	0.483	B_3	0.585	0.021	0.435
O_8	0.393	0.106_5	0.727	B_4	0.394	0.039	0.698
O_9*	0.180	0.205_5	0.604	B_5	0.190	0.139	0.583
O_{10}	0.852	0.889	0.809	B_6	0.779	0.867	0.578
O_{11}	0.545	0.880_5	0.422	B_7	0.489	0.854	0.193
O_{12}	0.937	0.876_5	0.509	B_8	0.866	0.874	0.274
O_{13}	0.646	0.871	0.109	B_9	0.057	0.861_5	0.011
O_{14}	0.458	0.786	0.193	B_{10}	0.248	0.756	0.083
O_{15}	0.265	0.885	0.010	B_{11}	0.412	0.734	0.673
O_{16}	0.051	0.880	0.226				

*O atom in an OH group.

formula of the compound obtained exactly confirms the chemical analysis in [4].

The structure was refined by the method of least squares on the M-20 and BÉSM-4 computers with the full set of $|F_{hkl}|$. The refinement was carried out in stages: only 55 parameters [12] could be refined in each stage, and the structure of p-veatchite is characterized by 104 coordinate parameters (not counting temperature factors and absolute scaling coefficient). The refinement was divided into three stages, each of which was repeated until the parameter changes remained fairly small ($\Delta x, \Delta y, \Delta z \leq 10^{-4}, \Delta K, \Delta B \leq 10^{-3}$). After the first least squares refinement, the disagreement index dropped to 18.2%. At this point interatomic distances were calculated; they deviated noticeably from the average numbers known for other borates [13-17]. Therefore a large number of least squares cycles was carried out with different groups of atoms. These alternated with three-dimensional Fourier Δ syntheses. The coordinates obtained from the separate least squares refinements varied over intervals which reached 0.1 Å in several cases. The R_{hkl} factor for the average values of these coordinates, with all nonzero reflections, was 15.5% (B_{hkl} = 1.6 Å^2). However, the interatomic distances even for the averaged version of the structure were not completely satisfactory.

In contrast to the least squares results, the values of the coordinates determined from successive three-dimensional Fourier Δ syntheses converged to certain values. These differed from the ones obtained by least squares, while the interatomic distances derived from them still left something to be desired.[1]

The "random search" program, written for the Ural-2 computer in the Institute of Crystallography, Academy of Sciences of the USSR by V. I. Burdina and L. A. Muradyan, was used as a supplement to the above refinement. Refinement was carried out for each of the three zonal sets of structure factors and the results were averaged. The final disagreement factors are: R_{h0l} = 10.9, R_{hk0} = 8.3, R_{0kl} = 11.0, R_{hkl} = 15.8%. Again, the coordinates found differed from the ones determined by least squares and Fourier syntheses. The average interatomic distances calculated from them seemed to be closer to the standard values than the ones calculated from data obtained on the last Fourier synthesis.

Because the coordinates obtained by the three refinement methods did not agree with each other and did not give completely acceptable interatomic distances, and the R_{hkl} factors corresponding to them differed little from each other ($16.4\% \leq R_{hkl} \leq 15.5\%$), the most probable values of the coordinates were taken as the ones which gave interatomic distances closest to the standard ones. These values were within the limits of the results obtained by the three methods of refinement: $(x_j)_{max} \leq x_j \leq (x_j)_{min}$, where $(x_j)_{max}$ and $(x_j)_{min}$ are the maximum and minimum value of each coordinate obtained at the end of the refinement by one of the three methods. The results of such a selection procedure are shown in Table 1. The corresponding disagreement factor was less than the three previous ones: R_{hkl} = 15.2% (B_{hkl} = 1.6 Å^2, $\sin\vartheta/\lambda \leq 0.61$ Å^{-1}). With consideration of the individual temperature factors U_j, R_{hkl} = 14.2%.

The basic structural details can be seen in Figs. 1-4. The Sr atoms are located inside ten- and eleven-coordinate polyhedra of oxygen atoms. The configurations of nine of the oxygen atoms in both polyhedra is practically the same, but the first polyhedron is completed with an H_2O particle, while the second has two OH groups (Fig. 1a,b). Each Sr_I ten-coordinate polyhedron is joined to three close Sr_{II} eleven-coordinate polyhedra by common edges, and in turn each Sr_{II} eleven-coordinate polyhedron has common edges with three neighboring Sr_I ten-coordinate polyhedra. The interlinked Sr_I and Sr_{II} polyhedra form open walls perpendicular to the b axis, with indented cavities (Fig. 2a). Each indented cavity is surrounded by six mutually alternating Sr_I and Sr_{II} polyhedra.

On both sides of the walls of Sr polyhedra there are pairs of boron–oxygen network-radicals associated to the wall. These are not related by the elements of the symmetry group, but they do have the same formula, $[B_5O_8(OH)]_n^{-2n}$ and configuration (Fig. 2b,c). The two $[B_5O_8(OH)]_n^{-2n}$ networks are rotated 180° with respect to each other, about an axis parallel to the b axis ($x = 0.224 \pm 0.002$, $z = 0.354_5 \pm 0.000_2$), followed by mirror reflection in the plane $y = -0.052 \pm 0.001$. The repeating link of each boron-oxygen network is a pair of BO_3 triangles joined at a common vertex and two BO_4 tetrahedra which are also linked together. A $BO_2(OH)$ triangle is connected to the two free vertices of the latter, and its plane is almost perpendicular to the plane of the network. Together with the two BO_4 tetrahedra, this triangle forms the

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[1] The reflections obtained with Cu radiation were insufficient, but Mo radiation could not be used for the reason indicated above.

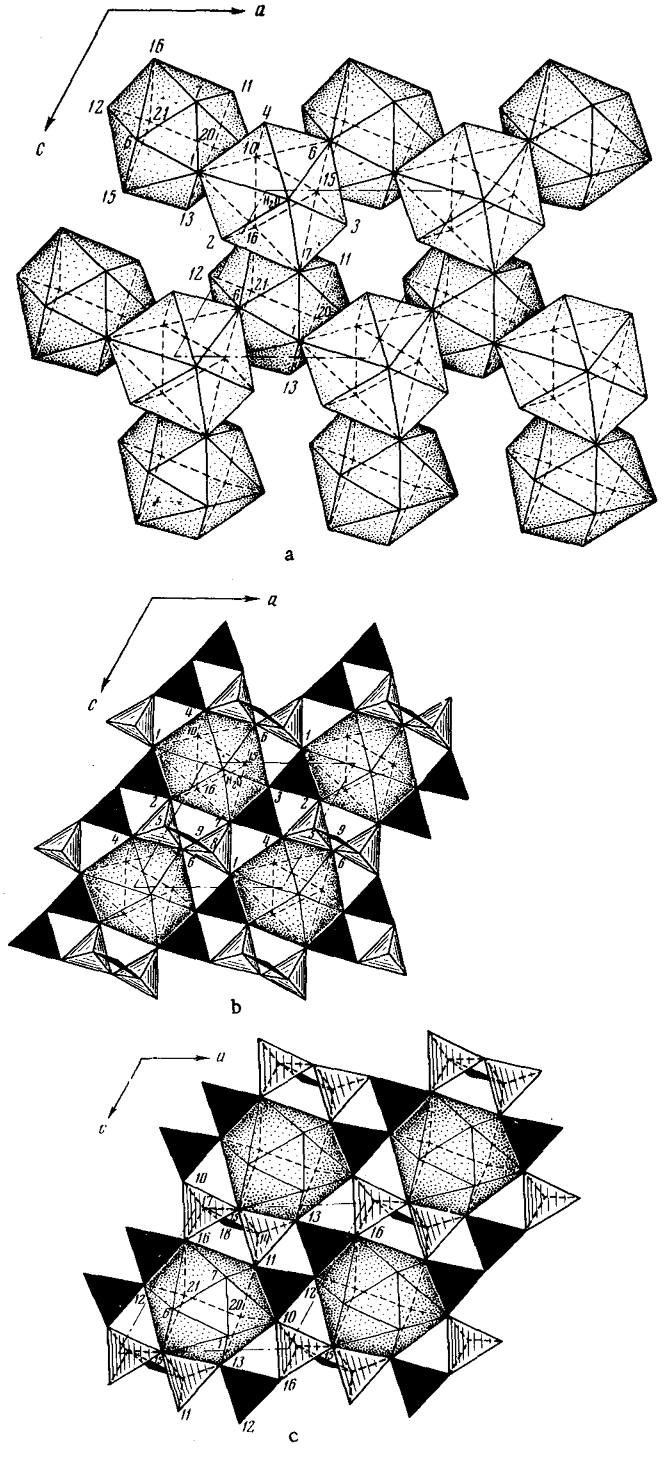

Fig. 2. Layer of Sr polyhedra and boron–oxygen network $[B_5O_8 \cdot (OH)]_n^{-2n}$ in the xz projection. a) Wall of interlinked Sr_I and Sr_{II} polyhedra; b) upper part of the layer: Sr_I ten-coordinate polyhedra positioned in the holes of the first network; c) lower part of the layer: Sr_{II} eleven-coordinate polyhedra filling the meshes of the second network. The B triangles are black. The numbers indicate the basis O atoms.

threefold ring $[B_3O_7(OH)]-(2t, \Delta)$,[2] which is very frequently met in borates [13-18]. Yet another trinuclear boron-oxygen ring $(2\Delta, t)$, parallel to the plane of the network, is obtained because of linking of the first pair of BO_3 triangles to one of the BO_4 tetrahedra (a similar ring has not been observed before in isolated form). As a result, an individual link of $[B_5O_8(OH)]^{-2}$ consists of two rings $(2\Delta, t)$ and $(2t, \Delta)$, linked by a common tetrahedron, with the planes of the rings mutually perpendicular. Each link is joined to four identical links [related by the translations $\pm a$, $\pm(a + c)$] by common vertices. The boron-oxygen network is formed as a result. The borate radicals $[B_5O_8(OH)]_n^{-2n}$, infinite in two directions, have been found for the first time in p-veatchite.

Quartets of neighboring links of $[B_5O_8(OH)]^{-2}$ are joined to give large loops almost triangular in shape. In the centers of these loops are located the Sr atoms. The sides of these loops are not identical, and the sequence of tetrahedra and triangles in them is as follows: $\Delta-t-t$, $\Delta-\Delta-t$, $t-\Delta-t$ (Fig. 2b). Each indented cavity in the wall of Sr polyhedra is filled by a pair of threefold rings $(2\Delta, t)$ from two adjoining networks. The second tetrahedron of the boron-oxygen link $[B_5O_8(OH)]^{-2}$ has a face in common with the Sr polyhedron, and each vertex of this face is linked to three $(2\Delta, t)$ rings from three cavities. In this case, the tetrahedron of the upper network (1-6-7-8 in Fig. 2b) has a face in common with the Sr_{II} eleven-coordinate polyhedron located beneath it (Fig. 2c), and a similar tetrahedron in the lower network (10-15-16-17 in Fig. 2c) shares a face with the Sr_I ten-coordinate polyhedron (Fig. 2b).

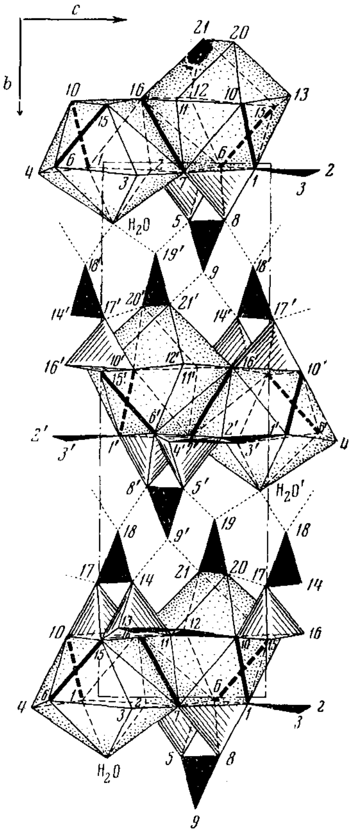

Fig. 3. Projection of the structure of p-veatchite, in polyhedral form, along the *a* axis. Dotted lines indicate hydrogen bonds. The heavy lines correspond to the common sides of two neighboring Sr polyhedra. The primed numbers designate atoms related to the basis atoms by a screw axis.

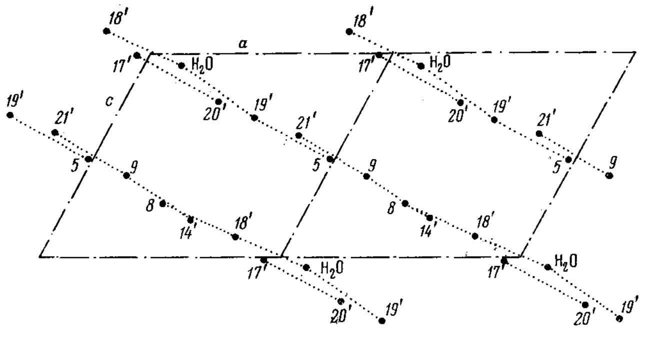

Fig. 4. Hydrogen bonds in the structure of p-veatchite. Projection along the b axis.

Besides the association of the boron-oxygen network to the Sr_{II} eleven-coordinate polyhedron, there is also associated an isolated $B(OH)_3$ triangle along a common OH edge. The plane of this triangle is almost parallel to the $BO_2(OH)$ triangle from the $(2t, \Delta)$ ring (Fig. 3). Thus, there are two types of boron-oxygen radicals in the structure of p-veatchite: boron-oxygen layers $[B_5O_8(OH)]_n^{-2n}$ and isolated $B(OH)_3$ triangles, i.e., p-veatchite is a mixed-type borate. It is evident that the four major classes of borates (island, chain, layer, and skeletal) should be expanded to include a fifth class of "mixed" borates. The first example of this last type is p-veatchite.

Along the b axis of the cell, two mica-like packets of Sr polyhedra and boron-oxygen radicals (Fig. 3) can be distinguished. These are crystallographically related by the 2_1 screw axes. Each packet is described by the formula $Sr_2 \cdot [B_5O_8(OH)]_2 \cdot B(OH)_3 \cdot H_2O$, which should be considered to be the derived chemical formula of p-veatchite. Successive packets are linked to each other by hydrogen bonds (Fig. 3).

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[2] The symbol t designates BO_4 tetrahedra, while Δ refers to BO_3 triangles.

TABLE 2. Interatomic Distances (Å) in the Structure of p-Veatchite

B_1 triangle		B_3 triangle		B_5 triangle	
$B_1 - O_1$	1.36	$B_3 - O_3$	1.38	$B_5 - O_5$	1.39
$B_1 - O_2$	1.39	$B_3 - O_4$	1.34	$B_5 - O_8$	1.39
$B_1 - O_3$	1.35	$B_3 - O_7$	1.42	$B_5 - O_9^*$	1.39
Av.	1.37	Av.	1.38	Av.	1.39
$O_1 - O_2$	2.37	$O_3 - O_4$	2.39	$O_5 - O_8$	2.40
$O_1 - O_3$	2.33	$O_3 - O_7$	2.34	$O_5 - O_9^*$	2.32
$O_2 - O_3$	2.40	$O_4 - O_7$	2.41	$O_8 - O_9^*$	2.40
Av.	2.37	Av.	2.38	Av.	2.37
B_6 triangle		B_8 triangle		B_{10} triangle	
$B_6 - O_{10}$	1.41	$B_8 - O_{12}$	1.38	$B_{10} - O_{14}$	1.36
$B_6 - O_{11}$	1.42	$B_8 - O_{13}$	1.35	$B_{10} - O_{17}$	1.38
$B_6 - O_{12}$	1.36	$B_8 - O_{16}$	1.41	$B_{10} - O_{18}^*$	1.37
Av.	1.40	Av.	1.38	Av.	1.37
$O_{10} - O_{11}$	2.38	$O_{12} - O_{13}$	2.39	$O_{14} - O_{17}$	2.38
$O_{10} - O_{12}$	2.33	$O_{12} - O_{16}$	2.34	$O_{14} - O_{18}^*$	2.38
$O_{11} - O_{12}$	2.40	$O_{13} - O_{16}$	2.42	$O_{17} - O_{18}^*$	2.39
Av.	2.37	Av.	2.38	Av.	2.38
B_2 tetrahedron		B_4 tetrahedron		B_7 tetrahedron	
$B_2 - O_2$	1.45	$B_4 - O_1$	1.49	$B_7 - O_{11}$	1.47
$B_2 - O_4$	1.45	$B_4 - O_6$	1.54	$B_7 - O_{13}$	1.45
$B_2 - O_5$	1.51	$B_4 - O_7$	1.51	$B_7 - O_{14}$	1.43
$B_2 - O_6$	1.51	$B_4 - O_8$	1.41	$B_7 - O_{15}$	1.53
Av.	1.48	Av.	1.49	Av.	1.47
$O_2 - O_4$	2.46	$O_1 - O_6$	2.41	$O_{11} - O_{13}$	2.47
$O_2 - O_5$	2.39	$O_1 - O_7$	2.40	$O_{11} - O_{14}$	2.37
$O_2 - O_6$	2.41	$O_1 - O_8$	2.39	$O_{11} - O_{15}$	2.42
$O_4 - O_5$	2.39	$O_6 - O_7$	2.46	$O_{13} - O_{14}$	2.39
$O_4 - O_6$	2.32	$O_6 - O_8$	2.42	$O_{13} - O_{15}$	2.35
$O_5 - O_6$	2.47	$O_7 - O_8$	2.46	$O_{14} - O_{15}$	2.41
Av.	2.41	Av.	2.42	Av.	2.40
B_9 tetrahedron		Sr_I polyhedron		Sr_{II} polyhedron	
$B_9 - O_{10}$	1.48	$Sr_I - O_1$	2.87	$Sr_{II} - O_{10}$	2.87
$B_9 - O_{15}$	1.48	$Sr_I - O_2$	2.52	$Sr_{II} - O_{11}$	2.51
$B_9 - O_{16}$	1.49	$Sr_I - O_3$	2.64	$Sr_{II} - O_{12}$	2.61
$B_9 - O_{17}$	1.45	$Sr_I - O_4$	2.50	$Sr_{II} - O_{13}$	2.48
Av.	1.47	$Sr_I - O_6$	2.59	$Sr_{II} - O_{15}$	2.58
$O_{10} - O_{15}$	2.42	$Sr_I - O_7$	2.78	$Sr_{II} - O_{16}$	2.76
$O_{10} - O_{16}$	2.41	$Sr_I - O_{10}$	2.73	$Sr_{II} - O_4$	2.94
$O_{10} - O_{17}$	2.37	$Sr_I - O_{15}$	2.73	$Sr_{II} - O_6$	2.84
$O_{15} - O_{16}$	2.46	$Sr_I - O_{16}$	2.88	$Sr_{II} - O_7$	3.05
$O_{15} - O_{17}$	2.37	$Sr_I - H_2O$	2.42	$Sr_{II} - O_{20}^*$	2.80
$O_{16} - O_{17}$	2.42			$Sr_{II} - O_{21}^*$	2.73
Av.	2.41				
		B_{11} triangle			
		$B_{11} - O_{19}^*$	1.37	$O_{19}^* - O_{20}^*$	2.37
		$B_{11} - O_{20}^*$	1.38	$O_{19}^* - O_{21}^*$	2.40
		$B_{11} - O_{21}^*$	1.37	$O_{20}^* - O_{21}^*$	2.37
		Av.	1.37	Av.	2.38

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*O atom in the OH group.

Table 2 gives the interatomic distances in the structure of p-veatchite. The average B–O distances in the BO_4 tetrahedra lie within the limits 1.47-1.49 Å, with the O–O sides 2.40-2.42 Å long. In the triangles, the average B–O distances are within the limits 1.37-1.40 Å with average O–O sides of 2.37-2.38 Å. The Sr–O distances in the Sr_I ten-coordinate polyhedron are within the interval 2.42-2.88 Å; in the Sr_{II} eleven-coordinate polyhedron they range from 2.48 to 3.05 Å. Other Sr–O distances exceed 3.8 Å. The shortest Sr–Sr vector (between atoms in the same layer) is 4.35 Å long. The lengths of the oxygen edges in the Sr polyhedra are shown in Fig. 1.

The hydrogen bonds were deduced from analysis of the lengths of those O–O vectors, at least one of whose O atoms was an OH or an H_2O group, and which do not correspond to sides in the coor-

TABLE 3. The Shortest Vectors between Oxygen Atoms Which Are Not Edges of Coordination Polyhedra

O–O vector	Vector length, Å	OH(H_2O) proton donor
$O_9{}^* - O_{21}{}^{*\prime}$	2,60	$O_{21}{}^{*\prime}$
$O_{17}{}' - O_{20}{}^{*\prime}$	2,61	$O_{20}{}^{*\prime}$
$O_5 - O_{19}{}^{*\prime}$	2,69	$O_{19}{}^{*\prime}$
$O_{14}{}' - O_9{}^*$	2,70	$O_9{}^*$
$O_{18}{}^{*\prime} - O_{22}$	2,71	O_{22}
$O_{19}{}^{*\prime} - O_{22}$	2,78	O_{22}
$O_8 - O_{18}{}^{*\prime}$	2,79	$O_{18}{}^{*\prime}$

Note: O_{22} is an O atom in an H_2O molecule. The primes designate atoms related to the basis atoms by a screw axis.

dination polyhedra. The shortest such distances are given in Table 3. They lie within the range 2.60-2.79 Å, and other O–O vector lengths exceed 3.15 Å. The great difference in these values, and also the unequivocal identification made of hydrogen bonds with an indication of the corresponding proton donors, permits us to consider that the distances given in Table 3 actually do correspond to hydrogen bonds. The locations of the H bonds are shown in Fig. 4. They are all located near the $(20\bar{1})$ plane, and cement together the separate layers of $Sr_2[B_5O_8(OH)]_2 \cdot B(OH)_3 \cdot H_2O$.

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