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The crystal structure of kelyanite, $(Hg_2)_6(SbO_6)BrCl_2$

Natalie V. Pervukhina,[1,*] Stanislav V. Borisov,[1] Svetlana A. Magarill,[1] Dmitrii Yu. Naumov,[1] and Vladimir I. Vasil'ev[2]

[1]Nikolaev Institute of Inorganic Chemistry, Siberian Branch of Russian Academy of Sciences, Lavrentiev Av. 3, Novosibirsk, 630090, Russia
[2]United Institute of Geology, Geophysics and Mineralogy, Siberian Branch of Russian Academy of Sciences, Koptyug Av. 3, Novosibirsk, 630090, Russia

Abstract

The crystal structure of kelyanite, a rare mercury mineral that was found in oxidized mercury-antimony ores in the Kelyana deposit (Buryatia, Russia), has been determined. The preliminary formula of kelyanite was $Hg_{34}Sb_3Cl_3Br_1O_{28}$ (assuming the presence of both the Hg^{1+} and Hg^{2+}). In contrast to this assumption, kelyanite appears to contain only monovalent Hg and its revised formula is $(Hg_2)_6(SbO_6)BrCl_2$. Kelyanite is trigonal, space group $P3$, $a = 13.560(4)$, $c = 10.004(6)$ Å, $V = 1593(1)$ Å^3, and $Z = 3$. In the structure, Hg atoms form six crystallographically independent pairs [dumbbells of composition $(Hg_2)^{2+}$] with Hg-Hg distances of 2.482(3)–2.519(2) Å. The Hg and O atoms form O-Hg-Hg-O systems with Hg-O bond lengths of 1.98(3)–2.33(3) Å and HgHgO angles of 140.3(7)–168.3(9)°. Mercury atoms in the $(Hg_2)^{2+}$ dumbbells have additional coordination to O, Cl, and Br atoms [Hg-O 2.62(2) Å, Hg-Cl 2.68(1)–2.97(1) Å, and Hg-Br 3.00(1)–3.55(1) Å]. Three crystallographically independent Sb atoms are octahedrally coordinated by O atoms with Sb-O distances of 1.96–2.14 Å. The $(Hg_2)^{2+}$ dumbbells link the (SbO_6) octahedra in a 3D structure.

Keywords: Kelyana mercury deposit, Hg mineral, mercury-antimony oxide-halide, $(Hg_2)^{2+}$ dumbbell, crystal structure, X-ray diffraction

Introduction

As a part of the general study of the crystal chemistry of minerals containing low-valence Hg, we have studied the crystal structure of kelyanite. Kelyanite is an Hg-Sb-O mineral containing chlorine and bromine from the Kelyana mercury deposit (Buryatia, Russia) described by Vasil'ev et al. (1982). This rare supergene mineral is probably the result of decomposition of primary Sb and Hg sulfides such as cinnabar and stibnite. Kelyanite occurs as irregular grains. Its brown-red or cherry-red aggregates are closely associated with calomel, eglestonite, shakhovite, and antimony oxides.

At present, there are about 30 known minerals of low-valence Hg such as calomel, Hg_2Cl_2 (Calos et al. 1989), eglestonite, $(Hg_2)_3O_2Cl_2H$ (Mereiter et al. 1991), edgarbaileyite, $Hg_6Si_2O_7$ (Angel et al. 1990), vasilyevite, $(Hg_2)_{10}O_6I_3(Br,Cl)_3(CO_3)$ (Cooper and Hawthorne 2003), etc., but only one of them, namely, shakhovite, $Hg_4Sb(OH)_3O_3$ (Tillmanns et al. 1982), contains Hg and Sb. The main features of the structures of these minerals and related synthetic compounds is the presence of cluster groups: $(Hg_2)^{2+}$ dumbbells and more rarely $(Hg_3)^{4+}$ triangles (Pervukhina et al. 1999a, 1999b).

Mercury minerals are particularly difficult to characterize with regard to their correct chemical formula because of the high atomic weight of Hg in comparison to lighter elements. Crystal-structure analysis plays an important role in the determination of the valence states of Hg and in detecting light elements.

Physical and optical properties, composition, and X-ray characteristics of kelyanite were originally studied using a natural specimen, but the structure of this mineral could not been solved at that time. Preliminary structural work showed the possible space groups $C2/m$, $C2$, Cm, Cc, and $C2/c$ with the unit-cell parameters: $a_m = 23.50 \pm 0.12$ Å, $b_m = 13.62 \pm 0.06$ Å, $c_m = 10.31 \pm 0.05$ Å, $\beta_m = 97.01 \pm 0.12°$ (Vasil'ev et al. 1982). Using data obtained by elemental analysis (JXA-5A and JSM-35 electron microprobe), the composition of kelyanite was determined as: Hg = 85.6, Sb = 4.7, Cl = 3.31, Br = 0.91, and O = 5.35 wt% (Vasil'ev et al. 1982), which leads to the formula $Hg_{4.106}Sb_{0.375}(Cl_{0.894},Br_{0.106})_{1.00}O_{3.21}$. With regard to the experimental density (8.51–8.69 g/cm^3), the preliminary formula of kelyanite, according to experimental data, could be written as $Hg_{34}Sb_3Cl_3Br_1O_{28}$ with $Z = 2$ (assuming the presence of both the Hg^+ and Hg^{2+}).

Single-crystal X-ray diffraction

A single crystal of dimensions $0.10 \times 0.05 \times 0.03$ mm was selected for X-ray diffraction measurement. The unit-cell parameters and diffraction intensity data were measured at room temperature, using a single-crystal Bruker X8 Apex diffractometer equipped with a 4K CCD detector. The crystallographic data, data collection parameters, and refinement parameters are summarized in Table 1. Kelyanite crystallizes in the trigonal space group $P3$ and exhibits the following unit-cell parameters (from 2815 reflections): $a = 13.560(4)$ Å, $c = 10.004(6)$ Å, and $V = 1593(1)$ Å^3. The calculated density, assuming a cell content of

* Present address: Nikolaev Institute of Inorganic Chemistry, Siberian Branch of Russian Academy of Sciences, Lavrentiev Av. 3, Novosibirsk, 630090, Russia. E-mail: pervukh@che.nsk.su

TABLE 1. Data, experimental, and refinement details for kelyanite, $(Hg_2)_6(SbO_6)BrCl_2$

Chemical formula	$(Hg_2)_6(SbO_6)BrCl_2$	Step size (°)	0.5
Space group	*P*3	No. of frames	739
Unit-cell dimensions	$a = 13.560(4)$ Å	Time/frame (s)	100
	$c = 10.004(6)$ Å	No. measured refl.	9920
	$V = 1593.0(11)$ Å^3	No. independent refl.	2241
Z	3	No. observed refl.	1727
Density (calc.)	8.680 g/cm^3	No. parameters	199
Absorption coefficient μ	89.748 mm^{-1}	R_{int}	0.0214
Crystal size (mm)	0.10 × 0.05 × 0.03	R_1	0.0390
Diffractometer type	Bruker Nonius X8 Apex 4K CCD detector	wR_2	0.0450
Radiation	Mo*K*α (graphite monochr.)	GOOF	1.397
θ range (°)	1.73–27.51	Largest diff. peak and hole	2.598 and –2.719
Scan type	φ		

$(Hg_2)_6(SbO_6)BrCl_2$, is $d_c = 8.680$ g/cm^3, $Z = 3$. Transformation of the monoclinic cell (*m*) proposed earlier by Vasil'ev et al. (1982) to a hexagonal cell (*h*) is defined by vector relationships $\boldsymbol{a}_h = ½ (\boldsymbol{a}_m + \boldsymbol{b}_m)$; $\boldsymbol{b}_h = ½(-\boldsymbol{a}_m + \boldsymbol{b}_m)$; $\boldsymbol{c}_h = \boldsymbol{c}_m$. It appeared that the only parameter that did not satisfy the hexagonal cell was β_m, which should be 90° rather than 97.01°.

An absorption correction was applied using XPREP (Bruker AXS Inc. 2004) (analytical method) according to the habit. The structure was solved by direct methods using the SIR2004 program package (Burla et al. 2005) and the subsequent structure refinement proceeded by means of the full-matrix least-squares program SHELX97 (Sheldrick 1998). The final atomic coordinates and equivalent isotropic displacement parameters for kelyanite are given in Table 2. Interatomic distances and selected angles for kelyanite, $(Hg_2)_6(SbO_6)BrCl_2$ are given in Table 3.

The agreement of our cell dimensions with those reported by Vasil'ev et al. (1982) suggests the identity of the minerals, which is also confirmed by the good agreement of the powder X-ray diffraction data (Table 4) calculated with our atomic coordinates and powder X-ray diffraction data of the kelyanite obtained by those authors. Observed and calculated structure factors and anisotropic displacement parameters for kelyanite are listed in the Supplementary Table 1[1].

RESULTS AND DISCUSSION

In contrast to the previous assumption (Vasil'ev et al. 1982), kelyanite contains entirely monovalent Hg and has the formula $(Hg_2)_6(SbO_6)BrCl_2$. The asymmetric unit contains 12 independent Hg atoms forming six $(Hg_2)^{2+}$ dumbbells, with the Hg-Hg distances in the range 2.482(3)–2.519(2) Å, in good agreement with the Hg-Hg bond lengths found in the structures of other known Hg minerals (Pervukhina et al. 1999a, 1999b). The $(Hg_2)^{2+}$ dumbbells have strong covalent bonds to the O atoms at each end [Hg-O 1.98(3)–2.33(3) Å]. The Hg and O atoms form O-Hg-Hg-O systems close to linear, with most HgHgO angles in the range 160.4(8)–168.3(9)°. For two dumbbells of the six, we should note a considerable deviation of the HgHgO angles from 180° [the O4-Hg5-Hg6 and O2-Hg9-Hg10 angles are 140.3(7) and 142.3(8)°, respectively; see Table 3], which was earlier observed in some natural and synthetic compounds, e.g., poyarkovite, Hg_3OCl (Vasil'ev et al. 1999), $Hg_5Re_2O_{10}$ (Schriewer-Pottgen and Jeitschko 1995), and a synthetic analog of chursinite, $(Hg_2)_3(AsO_4)_2$ (Kamenar and Kaitner 1973). Moreover, the mercury atoms in $(Hg_2)^{2+}$ dumbbells have an additional coordination to more remote O, Cl, and Br atoms [Hg7-O1 2.62(2) Å, Hg-Cl 2.68(1)–2.97(1) Å, and Hg-Br 3.00(1)–3.55(1) Å]. in refining the structure of kelyanite, we analyzed versions of statistical occupation of halogen positions by Cl and Br atoms simultaneously. We found that practically 100% of Cl1 and Cl2 positions are occupied by Cl atoms, as well as nearly 100% of Br1, Br2, and Br3 positions are occupied by Br atoms. This result is in good agreement with the Hg-Cl and Hg-Br distances and the anisotropic displacement parameters Cl and Br.

TABLE 2. Fractional atomic parameters and displacement parameters (Å^2) for the kelyanite, $(Hg_2)_6(SbO_6)BrCl_2$

Atom	Wyckoff site	*x*	*y*	*z*	U_{eq}
Sb1	1*a*	0	0	0.6629(7)	0.034(1)
Sb2	1*c*	0.6667	0.3333	1.0015(7)	0.033(1)
Sb3	1*b*	0.3333	0.6667	0.3325(7)	0.034(1)
Hg1	3*d*	0.2082(1)	–0.1482(1)	0.2704(1)	0.023(1)
Hg2	3*d*	0.1502(1)	–0.0239(1)	0.3950(1)	0.024(1)
Hg3	3*d*	0.4591(1)	–0.0228(1)	0.3926(1)	0.022(1)
Hg4	3*d*	0.5156(1)	0.1587(1)	0.2674(1)	0.025(1)
Hg5	3*d*	0.3490(2)	0.2160(2)	0.0625(2)	0.040(1)
Hg6	3*d*	0.1912(1)	0.0731(1)	–0.0789(2)	0.033(1)
Hg7	3*d*	0.3752(1)	0.5262(1)	0.0651(2)	0.037(1)
Hg8	3*d*	0.5087(1)	0.4866(1)	–0.0629(2)	0.032(1)
Hg9	3*d*	0.3171(1)	0.2007(2)	0.6004(2)	0.040(1)
Hg10	3*d*	0.4761(1)	0.2153(1)	0.7418(2)	0.035(1)
Hg11	3*d*	0.2922(1)	0.4839(1)	0.5977(2)	0.039(1)
Hg12	3*d*	0.1586(2)	0.3120(2)	0.7268(2)	0.036(1)
O1	3*d*	0.284(2)	–0.241(2)	0.203(3)	0.036(7)
O2	3*d*	0.130(2)	0.076(3)	0.539(3)	0.041(8)
O3	3*d*	0.391(2)	–0.188(2)	0.460(3)	0.043(8)
O4	3*d*	0.534(3)	0.269(3)	0.126(3)	0.050(9)
O5	3*d*	0.090(2)	–0.047(2)	–0.223(3)	0.036(7)
O6	3*d*	0.628(2)	0.422(3)	–0.120(3)	0.047(8)
Cl1	3*d*	0.335(1)	0.2257(9)	0.3299(13)	0.057(3)
Cl2	3*d*	0.472(1)	–0.0058(11)	0.6738(13)	0.057(3)
Br1	1*c*	0.6667	0.3333	0.4678(9)	0.057(2)
Br2	1*a*	0	0	0.1594(13)	0.058(2)
Br3	1*b*	0.3333	0.6667	0.8165(10)	0.051(2)

Notes: $U_{eq} = 1/3(U_{11} + U_{22} + U_{33})$.

Three crystallographically independent antimony atoms are situated on threefold axes in the centers of octahedra of O atoms, with Sb-O distances of 1.96(3)–2.14(3) Å. The Sb and Br atoms alternate on the threefold axes at a distance of approximately *c*/2.

The O atoms have covalent bonds to the Hg and Sb atoms, and the structure may be represented as infinite chains with the ...Sb-O-Hg-Hg-O-Sb-... strong bonds going in different directions and intersecting in Sb atoms, followed by forming 3D-nets with Cl and Br atoms located in cavities (Figs. 1 and 2). An interesting feature of the kelyanite structure is the presence of the short contact between the $(Hg_2)^{2+}$ dumbbells [3.191(2) Å] (see Table

[1] Deposit item AM-08-048, Supplementary Table 1 (observed and calculated structure factors and anisotropic displacement parameters for kelyanite). Deposit items are available two ways: For a paper copy contact the Business Office of the Mineralogical Society of America (see inside front cover of recent issue) for price information. For an electronic copy visit the MSA web site at http://www.minsocam.org, go to the American Mineralogist Contents, find the table of contents for the specific volume/issue wanted, and then click on the deposit link there.

3), which was also observed in poyarkovite (3.109 Å) (Vasil'ev et al. 1999). This distance is close to the distance in metallic Hg (2.99 Å) (Barrett 1957). The other short distances Hg···Hg in kelyanite are in the range of 3.414(2)–3.450(3) Å.

Data obtained by chemical analysis of kelyanite samples (Vasil'ev et al. 1982) validate the Hg:Sb ratio, but differ noticeably for the Cl and Br relative content and the quantity of O as derived from the formula determined from the present X-ray study. The probable explanation would be partial isomorphous replacement of Br by Cl.

A distinctive feature of the kelyanite structure is the presence of trivalent Sb in octahedral coordination with six Sb-O bonds in the narrow range from 1.96(3) to 2.14(3) Å. The reason for this unusual coordination with non-stereoactive lone pair electrons on the Sb^{3+} cations can be seen in the "strong" covalent Hg-O bonds of 1.98(3)–2.33(3) Å. Thus the ($Sb^{3+}O_n$) groups in the structure of the kelyanite are not isolated as in other structures

TABLE 3. Interatomic distances (Å) and selected angles (°) for the kelyanite, $(Hg_2)_6(SbO_6)BrCl_2$

Hg1-Hg2	2.519(2)	Sb1-O2	1.97(3)
Hg3-Hg4	2.515(2)	Sb1-O2*	1.97(3)
Hg5-Hg6	2.487(2)	Sb1-O2†	1.97(3)
Hg7-Hg8	2.487(2)	Sb1-O5‡	1.99(3)
Hg9-Hg10	2.503(2)	Sb1-O5§	1.99(3)
Hg11-Hg12	2.482(3)	Sb1-O5‖	1.99(3)
Hg1-O1	2.09(3)	Sb2-O6**	1.96(3)
Hg2-O2	2.09(3)	Sb2-O6**	1.96(3)
Hg3-O3	2.07(3)	Sb2-O6§	1.96(3)
Hg4-O4	1.98(3)	Sb2-O4**	1.99(3)
Hg5-O4	2.33(3)	Sb2-O4**	1.99(3)
Hg6-O5	2.09(3)	Sb2-O4§	1.99(3)
Hg7-O1†	2.28(3)	Sb3-O1††	2.13(3)
Hg8-O6	2.26(3)	Sb3-O1†	2.13(3)
Hg9-O2	2.32(3)	Sb3-O1‡‡	2.13(3)
Hg10-O6**	2.01(3)	Sb3-O3††	2.14(3)
Hg11-O3‡‡	2.20(3)	Sb3-O3†	2.14(3)
Hg12-O5‡	2.14(3)	Sb3-O3‡‡	2.14(3)
Hg2-Br2	3.236(9)		
Hg3-Cl2	2.821(10)		
Hg4-Br1	2.996(6)	Hg7···O1	2.62(2)
Hg5-Cl1	2.689(13)	Hg1···Hg3	3.191(2)
Hg6-Br2	3.288(9)		
Hg7-Br3	3.349(8)		
Hg8-Cl2§§	2.680(13)		
Hg9-Cl1	2.723(13)		
Hg10-Br1	3.551(7)		
Hg11-Cl2‡‡	2.967(12)		
O1-Hg1-Hg2	166.58	O1†-Hg7-Hg8	167.56
O2-Hg2-Hg1	164.28	O6-Hg8-Hg7	162.17
O3-Hg3-Hg4	167.68	O2-Hg9-Hg10	142.38
O4-Hg4-Hg3	162.89	O6**-Hg10-Hg9	168.39
O4-Hg5-Hg6	140.37	O3‡‡-Hg11-Hg12	166.78
O5-Hg6-Hg5	166.37	O5‡-Hg12-Hg11	160.48
O2*-Sb1-O2	84.813	O6§-Sb2-O4**	88.712
O2*-Sb1-O2†	84.813	O4**-Sb2-O4**	85.114
O2-Sb1-O2†	84.813	O6**-Sb2-O4§	170.813
O2*-Sb1-O5‡	174.412	O6**-Sb2-O4§	88.712
O2-Sb1-O5‡	95.011	O6§-Sb2-O4§	101.211
O2†-Sb1-O5‡	89.611	O4**-Sb2-O4§	85.114
O2*-Sb1-O5§	95.011	O4**-Sb2-O4§	85.114
O2-Sb1-O5§	89.611	O1††-Sb3-O1†	87.010
O2†-Sb1-O5§	174.412	O1††-Sb3-O1‡‡	87.010
O5‡-Sb1-O5§	90.610	O1†-Sb3-O1‡‡	87.010
O2*-Sb1-O5‖	89.611	O1††-Sb3-O3††	84.19
O2-Sb1-O5‖	174.412	O1†-Sb3-O3††	166.69
O2†-Sb1-O5‖	95.011	O1‡‡-Sb3-O3††	102.59
O5‡-Sb1-O5‖	90.610	O1††-Sb3-O3†	102.59
O5§-Sb1-O5‖	90.610	O1†-Sb3-O3†	84.19
O6**-Sb2-O6**	85.814	O1‡‡-Sb3-O3†	166.69
O6**-Sb2-O6§	85.814	O3††-Sb3-O3†	88.012
O6**-Sb2-O6§	85.814	O1††-Sb3-O3‡‡	166.69
O6**-Sb2-O4**	88.712	O1†-Sb3-O3‡‡	102.59
O6**-Sb2-O4**	101.211	O1‡‡-Sb3-O3‡‡	84.19
O6§-Sb2-O4**	170.813	O3††-Sb3-O3‡‡	88.012
O6**-Sb2-O4**	101.211	O3†-Sb3-O3‡‡	88.012
O6**-Sb2-O4**	170.813		

Note: Symmetry transformations used to generate equivalent atoms:
* (–x + y, –x, z); † (–y, x – y, z); ‡ (–y, x – y, z + 1); § (x, y, z + 1); ‖ (–x + y, –x, z + 1); ** (–x + y + 1, –x + 1, z + 1); ** (–y + 1, x – y, z + 1); †† (x, y + 1, z); ‡‡ (–x + y + 1, –x + 1, z); §§ (–x + y + 1, –x + 1, z – 1).

TABLE 4. X-ray powder diffraction data for kelyanite, $(Hg_2)_6(SbO_6)BrCl_2$

I_{calc}† >1	I_{exp}*	d_{calc}	d_{exp}‡	hkl_{calc}
19	10	7.61	7.61	–1 1 1
9	5	5.61	5.76	1 1 1
13	5	5.06	5.06	0 2 1
5	5	4.60	4.57	0 1 2
4		4.44		–2 3 0
6	3	4.06	4.04	–3 2 1
23		4.02		1 1 2
27	30	3.91	3.90	0 3 0
59	60	3.81	3.80	–2 2 2
37	20	3.39	3.39	–2 4 0
13		3.33		0 0 3
100	100	3.32	3.31	1 2 2
46	45	3.26	3.25	–1 4 0
5		3.21		2 2 1
15	<5	3.10	3.06	1 3 1
2		2.99		–1 2 3
1		2.93		0 4 0
11	10	2.82	2.81	–4 4 1
22	30	2.81	2.76	2 2 2
68	60	2.73	2.72	–4 3 2
4		2.69		–3 5 0
17	20	2.60	2.60	–5 3 1
41	50	2.54	2.53	–3 3 3
8		2.48	2.44	–5 4 1
7	3	2.45		–1 1 4
3		2.38		–2 4 3
22	50	2.37	2.36	2 3 2
8		2.33		–4 3 3
24	40	2.30	2.29	0 2 4
3		2.28		–5 5 1
5		2.20		3 3 1
9		2.18		–3 2 4
6	>10	2.17	2.17	–6 4 1
5	5	2.11	2.10	–5 6 0
3		2.06		–5 6 1
6		2.05		3 3 2
15	20	2.03	2.03	–6 4 2
3		2.01		2 2 4
25	5	1.98	1.97	–4 3 4
18		1.96	1.95	0 6 0
7	40	1.93		–4 7 0
10		1.90	1.89	–4 4 4
18	20	1.89		–3 7 1
4		1.88		–2 7 0
6		1.85		–5 7 1
2		1.82		1 2 5
2	13	1.79	1.79	–6 7 0
9		1.78		1 5 3
11	10	1.76	1.76	1 6 1
4		1.76		2 5 2
15		1.70		–3 4 5
4	20	1.69	1.69	–4 8 0
4		1.69		–6 6 3
6		1.69		1 6 2
5		1.67		0 0 6
15		1.66		2 4 4
6		1.65		3 5 1
5		1.65		0 4 5
9	10	1.58	1.58	1 6 3
6	10	1.53	1.52	0 3 6

Notes: I_{exp}* are expressed on 100 scale; I_{calc}† = ΣI_{hkl} over all *hkl* with equal d_{hkl}.
‡ Data from Vasil'ev et al. (1982) (114.6 mm powder camera, Fe-filtered, Co-radiation, Si-internal standard).

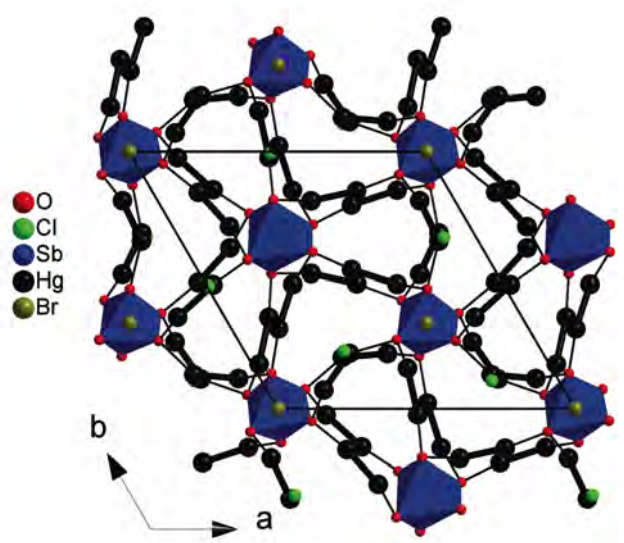

FIGURE 1. The projection of the structure of kelyanite, $(Hg_2)_6(SbO_6)BrCl_2$ along *c*.

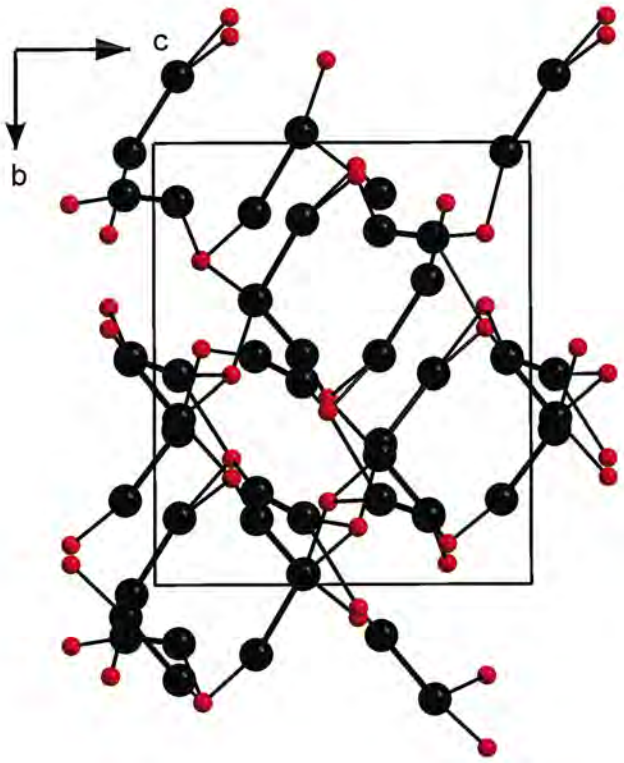

FIGURE 2. The projection of the structure of kelyanite, $(Hg_2)_6(SbO_6)BrCl_2$ along *a*. Only $(Hg_2)^{2+}$ dumbbells and covalently bonded O atoms are shown.

with trivalent Sb (Udovenko and Volkova 1981), but participate in a more complex fragment $(Hg_2)_6O_6Sb$ with six Hg-Hg-O-Sb bonds.

The structure of kelyanite is related to that of shakhovite, $(Hg_2)_2Sb(O,OH)_6$, where Hg atoms also form $(Hg_2)^{2+}$ dumbbells (Tillmanns et al. 1982) and the complex anion is a $[Sb^{5+}(O,OH)_6]^{4-}$ octahedron with pentavalent Sb. However, in shakhovite, the (Hg_2):Sb ratio is 2:1, whereas it is 6:1 in kelyanite. This requires complementary charge and volume compensation that is provided by the Br and Cl anions.

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