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

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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