Crystal structure of potassium hexabismuth enneaoxide iodide, $\text{KBi}_6\text{O}_9\text{I}$

U. Eggenweiler, E. Keller and V. Krämer

Albert-Ludwigs-Universität Freiburg, Kristallographisches Institut, Hebelstr. 25, D-79104 Freiburg, Germany

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Fig. 1. Oxygen atoms with $x, y, z > 0.5$ have been omitted for sake of clarity.

Source of material: Small single crystals of $\text{KBi}_6\text{O}_9\text{I}$ grew after drop by drop addition of a 0.005n solution of BiI_3 in 3n HI to 10n KOH.

The K, Bi and I atoms form a distorted bcc-like substructure. The K, I substructure consists of non-intersecting infinite linear chains parallel to $\langle 111 \rangle$. The coordination polyhedra of Bi are similar to those ones found in $\beta\text{-Bi}_5\text{O}_7\text{I}$ (see ref. 1).

Bi_6IKO_9 , cubic, $Ia\bar{3}d$ (No. 230), $a = 17.254(3) \text{ \AA}$, $V = 5136.5 \text{ \AA}^3$, $Z = 16$, $R(F) = 0.019$, $R_w(F^2) = 0.037$.

Table 1. Parameters used for the X-ray data collection

Crystal:	yellow, distorted rhomb-dodecahedron, size $0.057 \times 0.116 \times 0.135 \text{ mm}$
Wavelength:	Mo $K\alpha$ radiation ($0.71073 \text{ \AA}$)
μ :	806.50 cm^{-1}
Diffractometer:	Enraf-Nonius CAD4
Scan mode:	$\omega/2\theta$
$T_{\text{measurement}}$:	293 K
$2\theta_{\text{max}}$:	56°
$N(hkl)_{\text{unique}}$:	520
Criterion for I_o :	$I_o > 2 \sigma(I_o)$
$N(\text{param})_{\text{refined}}$:	30
Programs:	SHELXS-86, SHELXL-93

Table 2. Final atomic coordinates and displacement parameters (in $\text{\AA}^2$)

Atom	Site	x	y	z	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Bi(1)	48g	-0.10671(2)	7/8	0.14329(2)	0.0107(1)	0.0132(2)	U_{11}	-0.0008(1)	-0.0015(1)	$-U_{12}$
Bi(2)	48f	0.01194(2)	0	1/4	0.0092(2)	0.0092(2)	0.0116(2)	0	0	-0.0004(1)
K(1)	16a	0	0	0	0.0185(9)	U_{11}	U_{11}	0.004(1)	U_{12}	U_{12}
I(1)	16b	1/8	1/8	1/8	0.0177(3)	U_{11}	U_{11}	0.0042(3)	U_{12}	U_{12}
O(1)	96h	-0.0633(4)	0.0008(3)	0.1523(4)	0.010(3)	0.010(3)	0.015(3)	0.000(2)	-0.003(2)	-0.002(2)
O(2)	48g	-0.0216(3)	7/8	0.2284(3)	0.015(2)	0.003(3)	U_{11}	-0.001(2)	-0.008(3)	$-U_{12}$

References

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3. Sheldrick, G. M.: SHELXL-93, a program for refining crystal structures. University of Göttingen, Germany 1993.