$KBrO_3$ ($G0_7$) Structure: ABC3_hR5_160_a_a_b-001

This structure originally had the label `ABC3_hR5_160_a_a_b.KBrO3`. Calls to that address will be redirected here.

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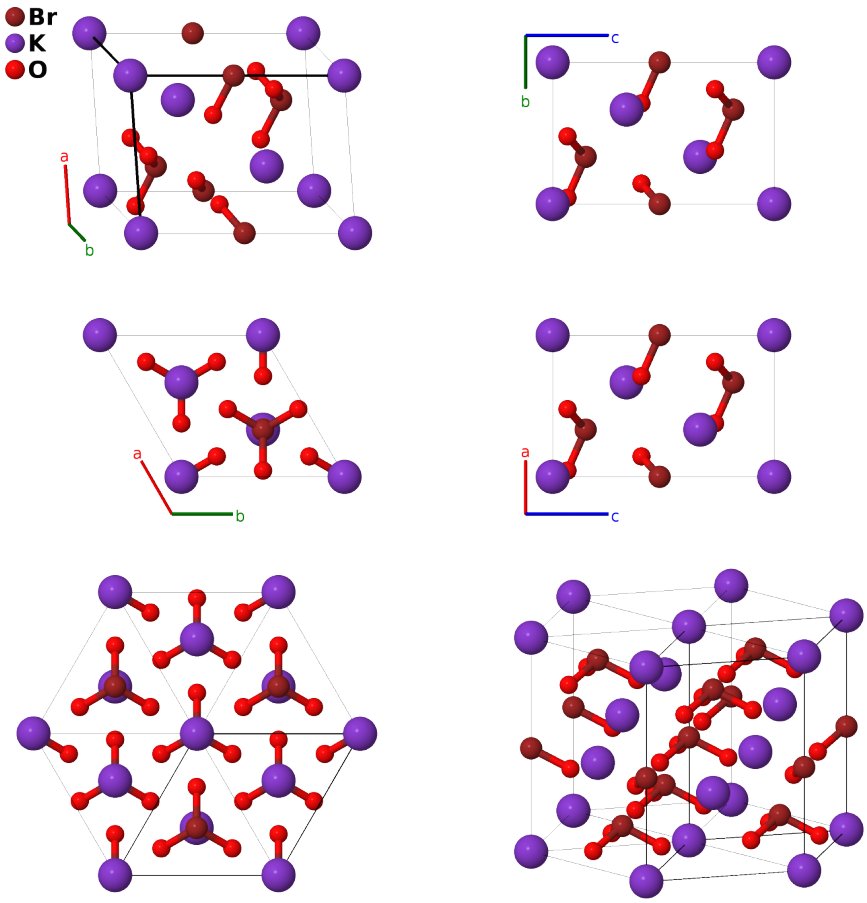
https://aflow.org/p/0ZSQ

https://aflow.org/p/ABC3_hR5_160_a_a_b-001



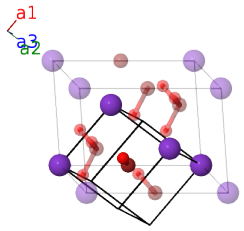
Prototype	$BrKO_3$
AFLOW prototype label	ABC3_hR5_160_a_a_b-001
***Strukturbericht* designation**	$G0_7$
ICSD	47173
Pearson symbol	hR5
Space group number	160
Space group symbol	$R3m$
AFLOW prototype command	`aflow --proto=ABC3_hR5_160_a_a_b-001 --params=`$a, c/a, x_1, x_2, x_3, z_3$

Other compounds with this structure
$FeBiO_3$, KNO_3, γ-KNO_3, $RbNO_3$

- γ-KNO_3 and $KBrO_3$ ($G0_7$) have the same AFLOW prototype label, ABC3_hR5_160_a_a_b. They are generated by the same symmetry operations with different sets of parameters (`--params`) specified in their corresponding CIF files.
- Hexagonal settings rhombohedral structures can be obtained with the option `--hex`.

Rhombohedral primitive vectors

$$\begin{aligned}
\mathbf{a_1} &= \tfrac{1}{2}a\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \tfrac{1}{3}c\,\hat{\mathbf{z}} \\
\mathbf{a_2} &= \tfrac{1}{\sqrt{3}}a\,\hat{\mathbf{y}} + \tfrac{1}{3}c\,\hat{\mathbf{z}} \\
\mathbf{a_3} &= -\tfrac{1}{2}a\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \tfrac{1}{3}c\,\hat{\mathbf{z}}
\end{aligned}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$x_1\,\mathbf{a}_1 + x_1\,\mathbf{a}_2 + x_1\,\mathbf{a}_3$	=	$cx_1\,\hat{\mathbf{z}}$	(1a)	Br I
$\mathbf{B_2}$	=	$x_2\,\mathbf{a}_1 + x_2\,\mathbf{a}_2 + x_2\,\mathbf{a}_3$	=	$cx_2\,\hat{\mathbf{z}}$	(1a)	K I
$\mathbf{B_3}$	=	$x_3\,\mathbf{a}_1 + x_3\,\mathbf{a}_2 + z_3\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_3 - z_3)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,(x_3 - z_3)\,\hat{\mathbf{y}} + \frac{1}{3}c\,(2x_3 + z_3)\,\hat{\mathbf{z}}$	(3b)	O I
$\mathbf{B_4}$	=	$z_3\,\mathbf{a}_1 + x_3\,\mathbf{a}_2 + x_3\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(x_3 - z_3)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,(x_3 - z_3)\,\hat{\mathbf{y}} + \frac{1}{3}c\,(2x_3 + z_3)\,\hat{\mathbf{z}}$	(3b)	O I
$\mathbf{B_5}$	=	$x_3\,\mathbf{a}_1 + z_3\,\mathbf{a}_2 + x_3\,\mathbf{a}_3$	=	$-\frac{1}{\sqrt{3}}a\,(x_3 - z_3)\,\hat{\mathbf{y}} + \frac{1}{3}c\,(2x_3 + z_3)\,\hat{\mathbf{z}}$	(3b)	O I

References

[1] D. H. Templeton and L. K. Templeton, *Tensor X-ray optical properties of the bromate ion*, Acta Crystallogr. Sect. A pp. 133–142 (1985), doi:10.1107/S0108767385000277.

Found in

[1] D. Santamaría-Pérez, R. Chulia-Jordan, P. Rodríguez-Hernández, and A. M. noz, *Crystal behavior of potassium bromate under compression*, Acta Crystallogr. Sect. B **71**, 798–804 (2015), doi:10.1107/S2052520615018156.