KHg_2 Structure: A2B_oI12_74_h_e-001

This structure originally had the label `A2B_oI12_74_h_e`. Calls to that address will be redirected here.

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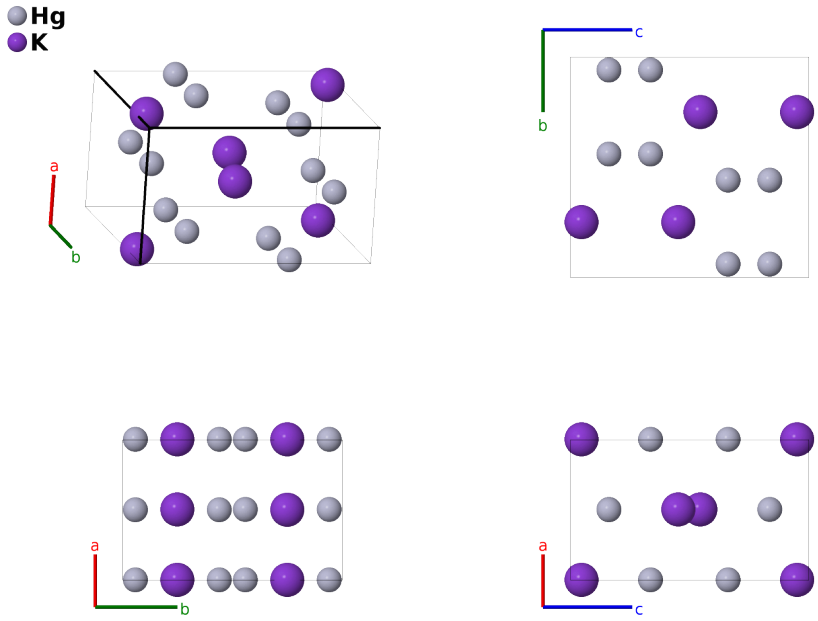
https://aflow.org/p/TWQQ

https://aflow.org/p/A2B_oI12_74_h_e-001

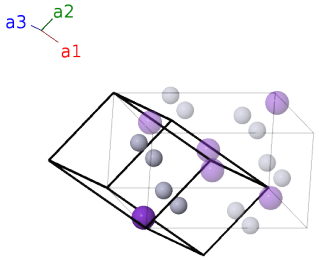


Prototype	Hg_2K
AFLOW prototype label	A2B_oI12_74_h_e-001
ICSD	104303
Pearson symbol	oI12
Space group number	74
Space group symbol	*Imma*
AFLOW prototype command	`aflow --proto=A2B_oI12_74_h_e-001 --params=`$a, b/a, c/a, z_1, y_2, z_2$

Other compounds with this structure
$BaZn_2$, $CaAg_2$, $SrZn_2$

Body-centered Orthorhombic primitive vectors

$$\mathbf{a_1} = -\tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{1}{2}b\,\hat{\mathbf{y}} + \tfrac{1}{2}c\,\hat{\mathbf{z}}$$
$$\mathbf{a_2} = \tfrac{1}{2}a\,\hat{\mathbf{x}} - \tfrac{1}{2}b\,\hat{\mathbf{y}} + \tfrac{1}{2}c\,\hat{\mathbf{z}}$$
$$\mathbf{a_3} = \tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{1}{2}b\,\hat{\mathbf{y}} - \tfrac{1}{2}c\,\hat{\mathbf{z}}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$\left(z_1 + \frac{1}{4}\right)\,\mathbf{a}_1 + z_1\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$\frac{1}{4}b\,\hat{\mathbf{y}} + cz_1\,\hat{\mathbf{z}}$	(4e)	K I
$\mathbf{B_2}$	=	$-\left(z_1 - \frac{3}{4}\right)\,\mathbf{a}_1 - z_1\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$\frac{3}{4}b\,\hat{\mathbf{y}} - cz_1\,\hat{\mathbf{z}}$	(4e)	K I
$\mathbf{B_3}$	=	$(y_2 + z_2)\,\mathbf{a}_1 + z_2\,\mathbf{a}_2 + y_2\,\mathbf{a}_3$	=	$by_2\,\hat{\mathbf{y}} + cz_2\,\hat{\mathbf{z}}$	(8h)	Hg I
$\mathbf{B_4}$	=	$\left(-y_2 + z_2 + \frac{1}{2}\right)\,\mathbf{a}_1 + z_2\,\mathbf{a}_2 - \left(y_2 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-b\left(y_2 - \frac{1}{2}\right)\,\hat{\mathbf{y}} + cz_2\,\hat{\mathbf{z}}$	(8h)	Hg I
$\mathbf{B_5}$	=	$\left(y_2 - z_2 + \frac{1}{2}\right)\,\mathbf{a}_1 - z_2\,\mathbf{a}_2 + \left(y_2 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$b\left(y_2 + \frac{1}{2}\right)\,\hat{\mathbf{y}} - cz_2\,\hat{\mathbf{z}}$	(8h)	Hg I
$\mathbf{B_6}$	=	$-\left(y_2 + z_2\right)\,\mathbf{a}_1 - z_2\,\mathbf{a}_2 - y_2\,\mathbf{a}_3$	=	$-by_2\,\hat{\mathbf{y}} - cz_2\,\hat{\mathbf{z}}$	(8h)	Hg I

References

[1] E. J. Duwell and N. C. Baenziger, *The Crystal Structure of KHg and KHg_2*, Acta Cryst. **8**, 705–710 (1955), doi:10.1107/S0365110X55002168.

Found in

[1] P. Villars and K. Cenzual, *Pearson's Crystal Data – Crystal Structure Database for Inorganic Compounds* (2013). ASM International.