

KHg₂ Structure: A2B_oI12_74_h_e-001

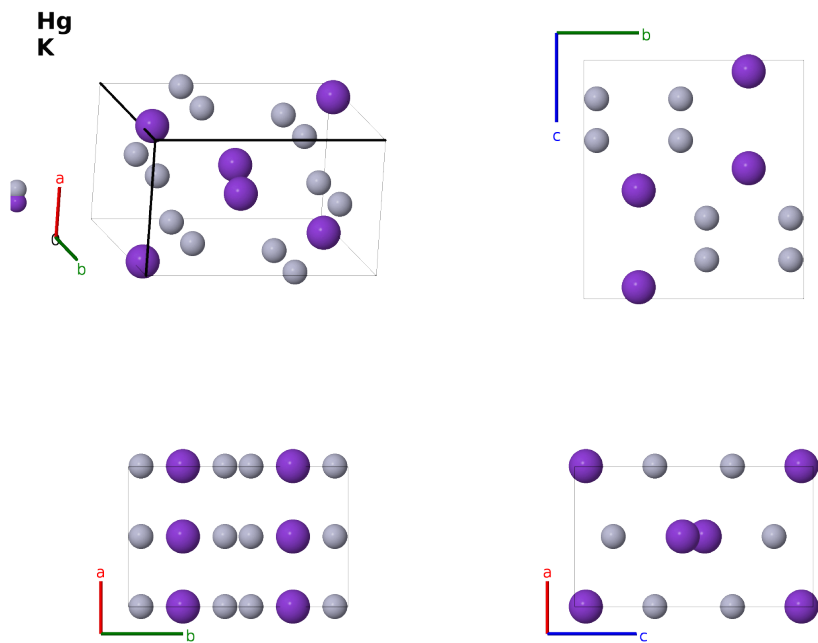
This structure previously used the label(s) **A2B_oI12_74_h_e**. Calls to these addresses will be redirected here.

Cite this page as:

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<https://aflow.org/prototype-encyclopedia/TWQQ>

https://aflow.org/prototype-encyclopedia/A2B_oI12_74_h_e-001



Prototype	Hg ₂ K
AFLOW prototype label	A2B_oI12_74_h_e-001
ICSD	104303
CCDC	1662219
Pearson symbol	oI12
Space group number	74
Space group symbol	<i>Imma</i>
AFLOW prototype command	<code>aflow --proto=A2B_oI12_74_h_e-001 --params=a, b/a, c/a, z₁, y₂, z₂</code>

Other compounds with this structure

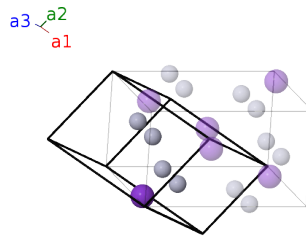
BaZn₂, CaAg₂, SrZn₂

Body-centered Orthorhombic primitive vectors

$$\mathbf{a}_1 = -\frac{1}{2}a \hat{\mathbf{x}} + \frac{1}{2}b \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}}$$

$$\mathbf{a}_2 = \frac{1}{2}a \hat{\mathbf{x}} - \frac{1}{2}b \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}}$$

$$\mathbf{a}_3 = \frac{1}{2}a \hat{\mathbf{x}} + \frac{1}{2}b \hat{\mathbf{y}} - \frac{1}{2}c \hat{\mathbf{z}}$$



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
$\mathbf{B}_6$	$= -(y_2 + z_2) \mathbf{a}_1 - z_2 \mathbf{a}_2 - y_2 \mathbf{a}_3$	$=$	$-by_2 \hat{\mathbf{y}} - cz_2 \hat{\mathbf{z}}$	(8h)	Hg I

References

- [1] E. J. Duwell and N. C. Baenziger, *The Crystal Structure of KHg and KHg₂*, 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.

First cited in

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