Hg_7Hg_5 Structure: A7B5_oP48_57_c3e_5d-001

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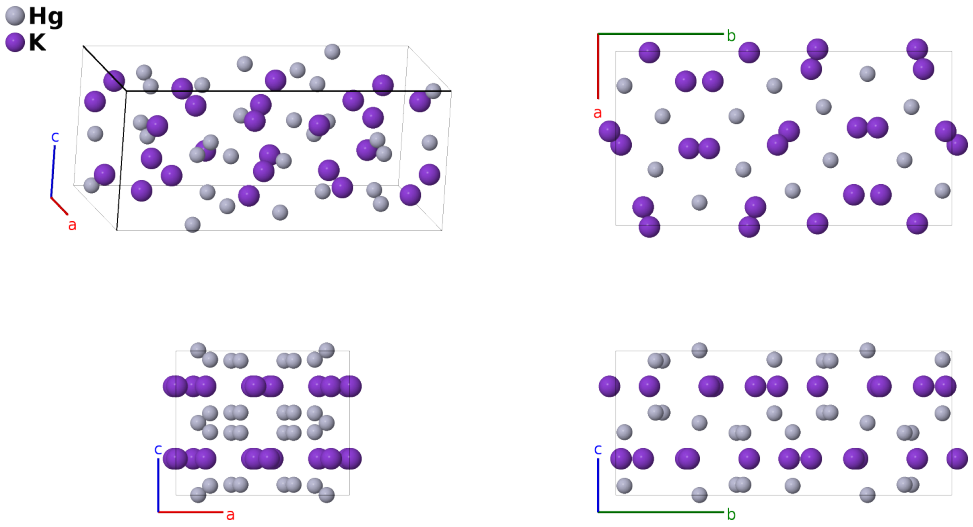
https://aflow.org/p/9PR5

https://aflow.org/p/A7B5_oP48_57_c3e_5d-001



Prototype	Hg_7K_5
AFLOW prototype label	A7B5_oP48_57_c3e_5d-001
ICSD	104304
Pearson symbol	oP48
Space group number	57
Space group symbol	*Pbcm*
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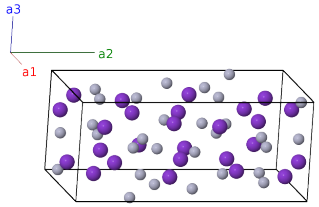
Simple Orthorhombic primitive vectors

$$\mathbf{a_1} = a\,\hat{\mathbf{x}}$$
$$\mathbf{a_2} = b\,\hat{\mathbf{y}}$$
$$\mathbf{a_3} = c\,\hat{\mathbf{z}}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$x_1\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2$	=	$ax_1\,\hat{\mathbf{x}} + \frac{1}{4}b\,\hat{\mathbf{y}}$	(4c)	Hg I
$\mathbf{B_2}$	=	$-x_1\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$-ax_1\,\hat{\mathbf{x}} + \frac{3}{4}b\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(4c)	Hg I
$\mathbf{B_3}$	=	$-x_1\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2$	=	$-ax_1\,\hat{\mathbf{x}} + \frac{3}{4}b\,\hat{\mathbf{y}}$	(4c)	Hg I
$\mathbf{B_4}$	=	$x_1\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$ax_1\,\hat{\mathbf{x}} + \frac{1}{4}b\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(4c)	Hg I
$\mathbf{B_5}$	=	$x_2\,\mathbf{a}_1 + y_2\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$ax_2\,\hat{\mathbf{x}} + by_2\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(4d)	K I
$\mathbf{B_6}$	=	$-x_2\,\mathbf{a}_1 - y_2\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$-ax_2\,\hat{\mathbf{x}} - by_2\,\hat{\mathbf{y}} + \frac{3}{4}c\,\hat{\mathbf{z}}$	(4d)	K I
$\mathbf{B_7}$	=	$-x_2\,\mathbf{a}_1 + \left(y_2 + \frac{1}{2}\right)\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$-ax_2\,\hat{\mathbf{x}} + b\left(y_2 + \frac{1}{2}\right)\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(4d)	K I
$\mathbf{B_8}$	=	$x_2\,\mathbf{a}_1 - \left(y_2 - \frac{1}{2}\right)\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$ax_2\,\hat{\mathbf{x}} - b\left(y_2 - \frac{1}{2}\right)\,\hat{\mathbf{y}} + \frac{3}{4}c\,\hat{\mathbf{z}}$	(4d)	K I
$\mathbf{B_9}$	=	$x_3\,\mathbf{a}_1 + y_3\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$ax_3\,\hat{\mathbf{x}} + by_3\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(4d)	K II
$\mathbf{B_{10}}$	=	$-x_3\,\mathbf{a}_1 - y_3\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$-ax_3\,\hat{\mathbf{x}} - by_3\,\hat{\mathbf{y}} + \frac{3}{4}c\,\hat{\mathbf{z}}$	(4d)	K II
$\mathbf{B_{11}}$	=	$-x_3\,\mathbf{a}_1 + \left(y_3 + \frac{1}{2}\right)\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$-ax_3\,\hat{\mathbf{x}} + b\left(y_3 + \frac{1}{2}\right)\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(4d)	K II
$\mathbf{B_{12}}$	=	$x_3\,\mathbf{a}_1 - \left(y_3 - \frac{1}{2}\right)\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$ax_3\,\hat{\mathbf{x}} - b\left(y_3 - \frac{1}{2}\right)\,\hat{\mathbf{y}} + \frac{3}{4}c\,\hat{\mathbf{z}}$	(4d)	K II
$\mathbf{B_{13}}$	=	$x_4\,\mathbf{a}_1 + y_4\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$ax_4\,\hat{\mathbf{x}} + by_4\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(4d)	K III
$\mathbf{B_{14}}$	=	$-x_4\,\mathbf{a}_1 - y_4\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$-ax_4\,\hat{\mathbf{x}} - by_4\,\hat{\mathbf{y}} + \frac{3}{4}c\,\hat{\mathbf{z}}$	(4d)	K III
$\mathbf{B_{15}}$	=	$-x_4\,\mathbf{a}_1 + \left(y_4 + \frac{1}{2}\right)\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$-ax_4\,\hat{\mathbf{x}} + b\left(y_4 + \frac{1}{2}\right)\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(4d)	K III
$\mathbf{B_{16}}$	=	$x_4\,\mathbf{a}_1 - \left(y_4 - \frac{1}{2}\right)\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$ax_4\,\hat{\mathbf{x}} - b\left(y_4 - \frac{1}{2}\right)\,\hat{\mathbf{y}} + \frac{3}{4}c\,\hat{\mathbf{z}}$	(4d)	K III
$\mathbf{B_{17}}$	=	$x_5\,\mathbf{a}_1 + y_5\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$ax_5\,\hat{\mathbf{x}} + by_5\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(4d)	K IV
$\mathbf{B_{18}}$	=	$-x_5\,\mathbf{a}_1 - y_5\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$-ax_5\,\hat{\mathbf{x}} - by_5\,\hat{\mathbf{y}} + \frac{3}{4}c\,\hat{\mathbf{z}}$	(4d)	K IV
$\mathbf{B_{19}}$	=	$-x_5\,\mathbf{a}_1 + \left(y_5 + \frac{1}{2}\right)\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$-ax_5\,\hat{\mathbf{x}} + b\left(y_5 + \frac{1}{2}\right)\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(4d)	K IV
$\mathbf{B_{20}}$	=	$x_5\,\mathbf{a}_1 - \left(y_5 - \frac{1}{2}\right)\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$ax_5\,\hat{\mathbf{x}} - b\left(y_5 - \frac{1}{2}\right)\,\hat{\mathbf{y}} + \frac{3}{4}c\,\hat{\mathbf{z}}$	(4d)	K IV
$\mathbf{B_{21}}$	=	$x_6\,\mathbf{a}_1 + y_6\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$ax_6\,\hat{\mathbf{x}} + by_6\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(4d)	K V
$\mathbf{B_{22}}$	=	$-x_6\,\mathbf{a}_1 - y_6\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$-ax_6\,\hat{\mathbf{x}} - by_6\,\hat{\mathbf{y}} + \frac{3}{4}c\,\hat{\mathbf{z}}$	(4d)	K V
$\mathbf{B_{23}}$	=	$-x_6\,\mathbf{a}_1 + \left(y_6 + \frac{1}{2}\right)\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$-ax_6\,\hat{\mathbf{x}} + b\left(y_6 + \frac{1}{2}\right)\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(4d)	K V
$\mathbf{B_{24}}$	=	$x_6\,\mathbf{a}_1 - \left(y_6 - \frac{1}{2}\right)\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$ax_6\,\hat{\mathbf{x}} - b\left(y_6 - \frac{1}{2}\right)\,\hat{\mathbf{y}} + \frac{3}{4}c\,\hat{\mathbf{z}}$	(4d)	K V
$\mathbf{B_{25}}$	=	$x_7\,\mathbf{a}_1 + y_7\,\mathbf{a}_2 + z_7\,\mathbf{a}_3$	=	$ax_7\,\hat{\mathbf{x}} + by_7\,\hat{\mathbf{y}} + cz_7\,\hat{\mathbf{z}}$	(8e)	Hg II
$\mathbf{B_{26}}$	=	$-x_7\,\mathbf{a}_1 - y_7\,\mathbf{a}_2 + \left(z_7 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ax_7\,\hat{\mathbf{x}} - by_7\,\hat{\mathbf{y}} + c\left(z_7 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8e)	Hg II
$\mathbf{B_{27}}$	=	$-x_7\,\mathbf{a}_1 + \left(y_7 + \frac{1}{2}\right)\,\mathbf{a}_2 - \left(z_7 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ax_7\,\hat{\mathbf{x}} + b\left(y_7 + \frac{1}{2}\right)\,\hat{\mathbf{y}} - c\left(z_7 - \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8e)	Hg II
$\mathbf{B_{28}}$	=	$x_7\,\mathbf{a}_1 - \left(y_7 - \frac{1}{2}\right)\,\mathbf{a}_2 - z_7\,\mathbf{a}_3$	=	$ax_7\,\hat{\mathbf{x}} - b\left(y_7 - \frac{1}{2}\right)\,\hat{\mathbf{y}} - cz_7\,\hat{\mathbf{z}}$	(8e)	Hg II
$\mathbf{B_{29}}$	=	$-x_7\,\mathbf{a}_1 - y_7\,\mathbf{a}_2 - z_7\,\mathbf{a}_3$	=	$-ax_7\,\hat{\mathbf{x}} - by_7\,\hat{\mathbf{y}} - cz_7\,\hat{\mathbf{z}}$	(8e)	Hg II
$\mathbf{B_{30}}$	=	$x_7\,\mathbf{a}_1 + y_7\,\mathbf{a}_2 - \left(z_7 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$ax_7\,\hat{\mathbf{x}} + by_7\,\hat{\mathbf{y}} - c\left(z_7 - \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8e)	Hg II
$\mathbf{B_{31}}$	=	$x_7\,\mathbf{a}_1 - \left(y_7 - \frac{1}{2}\right)\,\mathbf{a}_2 + \left(z_7 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$ax_7\,\hat{\mathbf{x}} - b\left(y_7 - \frac{1}{2}\right)\,\hat{\mathbf{y}} + c\left(z_7 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8e)	Hg II
$\mathbf{B_{32}}$	=	$-x_7\,\mathbf{a}_1 + \left(y_7 + \frac{1}{2}\right)\,\mathbf{a}_2 + z_7\,\mathbf{a}_3$	=	$-ax_7\,\hat{\mathbf{x}} + b\left(y_7 + \frac{1}{2}\right)\,\hat{\mathbf{y}} + cz_7\,\hat{\mathbf{z}}$	(8e)	Hg II
$\mathbf{B_{33}}$	=	$x_8\,\mathbf{a}_1 + y_8\,\mathbf{a}_2 + z_8\,\mathbf{a}_3$	=	$ax_8\,\hat{\mathbf{x}} + by_8\,\hat{\mathbf{y}} + cz_8\,\hat{\mathbf{z}}$	(8e)	Hg III
$\mathbf{B_{34}}$	=	$-x_8\,\mathbf{a}_1 - y_8\,\mathbf{a}_2 + \left(z_8 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ax_8\,\hat{\mathbf{x}} - by_8\,\hat{\mathbf{y}} + c\left(z_8 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8e)	Hg III
$\mathbf{B_{35}}$	=	$-x_8\,\mathbf{a}_1 + \left(y_8 + \frac{1}{2}\right)\,\mathbf{a}_2 - \left(z_8 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ax_8\,\hat{\mathbf{x}} + b\left(y_8 + \frac{1}{2}\right)\,\hat{\mathbf{y}} - c\left(z_8 - \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8e)	Hg III
$\mathbf{B_{36}}$	=	$x_8\,\mathbf{a}_1 - \left(y_8 - \frac{1}{2}\right)\,\mathbf{a}_2 - z_8\,\mathbf{a}_3$	=	$ax_8\,\hat{\mathbf{x}} - b\left(y_8 - \frac{1}{2}\right)\,\hat{\mathbf{y}} - cz_8\,\hat{\mathbf{z}}$	(8e)	Hg III
$\mathbf{B_{37}}$	=	$-x_8\,\mathbf{a}_1 - y_8\,\mathbf{a}_2 - z_8\,\mathbf{a}_3$	=	$-ax_8\,\hat{\mathbf{x}} - by_8\,\hat{\mathbf{y}} - cz_8\,\hat{\mathbf{z}}$	(8e)	Hg III
$\mathbf{B_{38}}$	=	$x_8\,\mathbf{a}_1 + y_8\,\mathbf{a}_2 - \left(z_8 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$ax_8\,\hat{\mathbf{x}} + by_8\,\hat{\mathbf{y}} - c\left(z_8 - \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8e)	Hg III

$\mathbf{B_{39}}$	=	$x_8\,\mathbf{a}_1-\left(y_8-\frac{1}{2}\right)\,\mathbf{a}_2+\left(z_8+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$ax_8\,\hat{\mathbf{x}}-b\left(y_8-\frac{1}{2}\right)\,\hat{\mathbf{y}}+c\left(z_8+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8e)	Hg III
$\mathbf{B_{40}}$	=	$-x_8\,\mathbf{a}_1+\left(y_8+\frac{1}{2}\right)\,\mathbf{a}_2+z_8\,\mathbf{a}_3$	=	$-ax_8\,\hat{\mathbf{x}}+b\left(y_8+\frac{1}{2}\right)\,\hat{\mathbf{y}}+cz_8\,\hat{\mathbf{z}}$	(8e)	Hg III
$\mathbf{B_{41}}$	=	$x_9\,\mathbf{a}_1+y_9\,\mathbf{a}_2+z_9\,\mathbf{a}_3$	=	$ax_9\,\hat{\mathbf{x}}+by_9\,\hat{\mathbf{y}}+cz_9\,\hat{\mathbf{z}}$	(8e)	Hg IV
$\mathbf{B_{42}}$	=	$-x_9\,\mathbf{a}_1-y_9\,\mathbf{a}_2+\left(z_9+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ax_9\,\hat{\mathbf{x}}-by_9\,\hat{\mathbf{y}}+c\left(z_9+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8e)	Hg IV
$\mathbf{B_{43}}$	=	$-x_9\,\mathbf{a}_1+\left(y_9+\frac{1}{2}\right)\,\mathbf{a}_2-\left(z_9-\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ax_9\,\hat{\mathbf{x}}+b\left(y_9+\frac{1}{2}\right)\,\hat{\mathbf{y}}-c\left(z_9-\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8e)	Hg IV
$\mathbf{B_{44}}$	=	$x_9\,\mathbf{a}_1-\left(y_9-\frac{1}{2}\right)\,\mathbf{a}_2-z_9\,\mathbf{a}_3$	=	$ax_9\,\hat{\mathbf{x}}-b\left(y_9-\frac{1}{2}\right)\,\hat{\mathbf{y}}-cz_9\,\hat{\mathbf{z}}$	(8e)	Hg IV
$\mathbf{B_{45}}$	=	$-x_9\,\mathbf{a}_1-y_9\,\mathbf{a}_2-z_9\,\mathbf{a}_3$	=	$-ax_9\,\hat{\mathbf{x}}-by_9\,\hat{\mathbf{y}}-cz_9\,\hat{\mathbf{z}}$	(8e)	Hg IV
$\mathbf{B_{46}}$	=	$x_9\,\mathbf{a}_1+y_9\,\mathbf{a}_2-\left(z_9-\frac{1}{2}\right)\,\mathbf{a}_3$	=	$ax_9\,\hat{\mathbf{x}}+by_9\,\hat{\mathbf{y}}-c\left(z_9-\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8e)	Hg IV
$\mathbf{B_{47}}$	=	$x_9\,\mathbf{a}_1-\left(y_9-\frac{1}{2}\right)\,\mathbf{a}_2+\left(z_9+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$ax_9\,\hat{\mathbf{x}}-b\left(y_9-\frac{1}{2}\right)\,\hat{\mathbf{y}}+c\left(z_9+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8e)	Hg IV
$\mathbf{B_{48}}$	=	$-x_9\,\mathbf{a}_1+\left(y_9+\frac{1}{2}\right)\,\mathbf{a}_2+z_9\,\mathbf{a}_3$	=	$-ax_9\,\hat{\mathbf{x}}+b\left(y_9+\frac{1}{2}\right)\,\hat{\mathbf{y}}+cz_9\,\hat{\mathbf{z}}$	(8e)	Hg IV

References

[1] E. J. Duwell and N. C. Baenziger, *The crystal structure of* K_5Hg_7, Acta Cryst. **13**, 476–479 (1960), doi:10.1107/S0365110X60001126.