

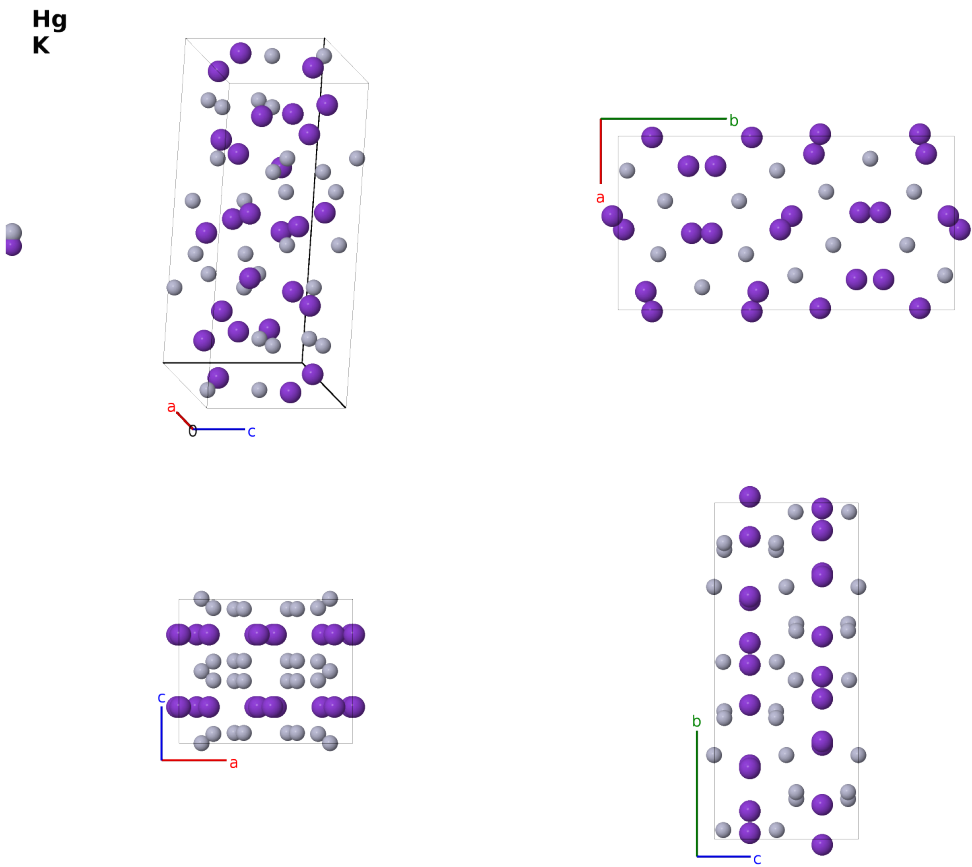
Hg₇Hg₅ Structure: A7B5_oP48_57_c3e_5d-001

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- D. Hicks, M. J. Mehl, M. Esters, C. Osos, O. Levy, G. L. W. Hart, C. Toher, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 3*, Comput. Mater. Sci. **199**, 110450 (2021), doi: 10.1016/j.commatsci.2021.110450.

<https://aflow.org/prototype-encyclopedia/9PR5>

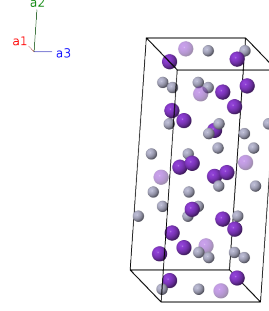
https://aflow.org/prototype-encyclopedia/A7B5_oP48_57_c3e_5d-001



Prototype	Hg ₇ K ₅
AFLOW prototype label	A7B5_oP48_57_c3e_5d-001
ICSD	104304
CCDC	1662220
Pearson symbol	oP48
Space group number	57
Space group symbol	<i>Pbcm</i>
AFLOW prototype command	<code>aflow --proto=A7B5_oP48_57_c3e_5d-001</code> <code>--params=a, b/a, c/a, x₁, x₂, y₂, x₃, y₃, x₄, y₄, x₅, y₅, x₆, y₆, x₇, y₇, z₇, x₈, y₈, z₈, x₉, y₉, z₉</code>

Simple Orthorhombic primitive vectors

$$\begin{aligned} \mathbf{a}_1 &= a \hat{\mathbf{x}} \\ \mathbf{a}_2 &= b \hat{\mathbf{y}} \\ \mathbf{a}_3 &= c \hat{\mathbf{z}} \end{aligned}$$



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$= x_1 \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2$	$=$	$ax_1 \hat{\mathbf{x}} + \frac{1}{4}b \hat{\mathbf{y}}$	(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
$\mathbf{B}_7$	$= -x_2 \mathbf{a}_1 + (y_2 + \frac{1}{2}) \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$-ax_2 \hat{\mathbf{x}} + b(y_2 + \frac{1}{2}) \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	(4d)	K I
$\mathbf{B}_8$	$= x_2 \mathbf{a}_1 - (y_2 - \frac{1}{2}) \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$ax_2 \hat{\mathbf{x}} - b(y_2 - \frac{1}{2}) \hat{\mathbf{y}} + \frac{3}{4}c \hat{\mathbf{z}}$	(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
$\mathbf{B}_{11}$	$= -x_3 \mathbf{a}_1 + (y_3 + \frac{1}{2}) \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$-ax_3 \hat{\mathbf{x}} + b(y_3 + \frac{1}{2}) \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	(4d)	K II
$\mathbf{B}_{12}$	$= x_3 \mathbf{a}_1 - (y_3 - \frac{1}{2}) \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$ax_3 \hat{\mathbf{x}} - b(y_3 - \frac{1}{2}) \hat{\mathbf{y}} + \frac{3}{4}c \hat{\mathbf{z}}$	(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
$\mathbf{B}_{15}$	$= -x_4 \mathbf{a}_1 + (y_4 + \frac{1}{2}) \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$-ax_4 \hat{\mathbf{x}} + b(y_4 + \frac{1}{2}) \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	(4d)	K III
$\mathbf{B}_{16}$	$= x_4 \mathbf{a}_1 - (y_4 - \frac{1}{2}) \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$ax_4 \hat{\mathbf{x}} - b(y_4 - \frac{1}{2}) \hat{\mathbf{y}} + \frac{3}{4}c \hat{\mathbf{z}}$	(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
$\mathbf{B}_{19}$	$= -x_5 \mathbf{a}_1 + (y_5 + \frac{1}{2}) \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$-ax_5 \hat{\mathbf{x}} + b(y_5 + \frac{1}{2}) \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	(4d)	K IV
$\mathbf{B}_{20}$	$= x_5 \mathbf{a}_1 - (y_5 - \frac{1}{2}) \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$ax_5 \hat{\mathbf{x}} - b(y_5 - \frac{1}{2}) \hat{\mathbf{y}} + \frac{3}{4}c \hat{\mathbf{z}}$	(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
$\mathbf{B}_{23}$	$= -x_6 \mathbf{a}_1 + (y_6 + \frac{1}{2}) \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$-ax_6 \hat{\mathbf{x}} + b(y_6 + \frac{1}{2}) \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	(4d)	K V
$\mathbf{B}_{24}$	$= x_6 \mathbf{a}_1 - (y_6 - \frac{1}{2}) \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$ax_6 \hat{\mathbf{x}} - b(y_6 - \frac{1}{2}) \hat{\mathbf{y}} + \frac{3}{4}c \hat{\mathbf{z}}$	(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
$\mathbf{B}_{26}$	$= -x_7 \mathbf{a}_1 - y_7 \mathbf{a}_2 + (z_7 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-ax_7 \hat{\mathbf{x}} - by_7 \hat{\mathbf{y}} + c(z_7 + \frac{1}{2}) \hat{\mathbf{z}}$	(8e)	Hg II
$\mathbf{B}_{27}$	$= -x_7 \mathbf{a}_1 + (y_7 + \frac{1}{2}) \mathbf{a}_2 - (z_7 - \frac{1}{2}) \mathbf{a}_3$	$=$	$-ax_7 \hat{\mathbf{x}} + b(y_7 + \frac{1}{2}) \hat{\mathbf{y}} - c(z_7 - \frac{1}{2}) \hat{\mathbf{z}}$	(8e)	Hg II

$\mathbf{B}_{28} =$	$x_7 \mathbf{a}_1 - (y_7 - \frac{1}{2}) \mathbf{a}_2 - z_7 \mathbf{a}_3$	$=$	$ax_7 \hat{\mathbf{x}} - b(y_7 - \frac{1}{2}) \hat{\mathbf{y}} - cz_7 \hat{\mathbf{z}}$	(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
$\mathbf{B}_{30} =$	$x_7 \mathbf{a}_1 + y_7 \mathbf{a}_2 - (z_7 - \frac{1}{2}) \mathbf{a}_3$	$=$	$ax_7 \hat{\mathbf{x}} + by_7 \hat{\mathbf{y}} - c(z_7 - \frac{1}{2}) \hat{\mathbf{z}}$	(8e)	Hg II
$\mathbf{B}_{31} =$	$x_7 \mathbf{a}_1 - (y_7 - \frac{1}{2}) \mathbf{a}_2 + (z_7 + \frac{1}{2}) \mathbf{a}_3$	$=$	$ax_7 \hat{\mathbf{x}} - b(y_7 - \frac{1}{2}) \hat{\mathbf{y}} + c(z_7 + \frac{1}{2}) \hat{\mathbf{z}}$	(8e)	Hg II
$\mathbf{B}_{32} =$	$-x_7 \mathbf{a}_1 + (y_7 + \frac{1}{2}) \mathbf{a}_2 + z_7 \mathbf{a}_3$	$=$	$-ax_7 \hat{\mathbf{x}} + b(y_7 + \frac{1}{2}) \hat{\mathbf{y}} + cz_7 \hat{\mathbf{z}}$	(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
$\mathbf{B}_{34} =$	$-x_8 \mathbf{a}_1 - y_8 \mathbf{a}_2 + (z_8 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-ax_8 \hat{\mathbf{x}} - by_8 \hat{\mathbf{y}} + c(z_8 + \frac{1}{2}) \hat{\mathbf{z}}$	(8e)	Hg III
$\mathbf{B}_{35} =$	$-x_8 \mathbf{a}_1 + (y_8 + \frac{1}{2}) \mathbf{a}_2 - (z_8 - \frac{1}{2}) \mathbf{a}_3$	$=$	$-ax_8 \hat{\mathbf{x}} + b(y_8 + \frac{1}{2}) \hat{\mathbf{y}} - c(z_8 - \frac{1}{2}) \hat{\mathbf{z}}$	(8e)	Hg III
$\mathbf{B}_{36} =$	$x_8 \mathbf{a}_1 - (y_8 - \frac{1}{2}) \mathbf{a}_2 - z_8 \mathbf{a}_3$	$=$	$ax_8 \hat{\mathbf{x}} - b(y_8 - \frac{1}{2}) \hat{\mathbf{y}} - cz_8 \hat{\mathbf{z}}$	(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
$\mathbf{B}_{38} =$	$x_8 \mathbf{a}_1 + y_8 \mathbf{a}_2 - (z_8 - \frac{1}{2}) \mathbf{a}_3$	$=$	$ax_8 \hat{\mathbf{x}} + by_8 \hat{\mathbf{y}} - c(z_8 - \frac{1}{2}) \hat{\mathbf{z}}$	(8e)	Hg III
$\mathbf{B}_{39} =$	$x_8 \mathbf{a}_1 - (y_8 - \frac{1}{2}) \mathbf{a}_2 + (z_8 + \frac{1}{2}) \mathbf{a}_3$	$=$	$ax_8 \hat{\mathbf{x}} - b(y_8 - \frac{1}{2}) \hat{\mathbf{y}} + c(z_8 + \frac{1}{2}) \hat{\mathbf{z}}$	(8e)	Hg III
$\mathbf{B}_{40} =$	$-x_8 \mathbf{a}_1 + (y_8 + \frac{1}{2}) \mathbf{a}_2 + z_8 \mathbf{a}_3$	$=$	$-ax_8 \hat{\mathbf{x}} + b(y_8 + \frac{1}{2}) \hat{\mathbf{y}} + cz_8 \hat{\mathbf{z}}$	(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
$\mathbf{B}_{42} =$	$-x_9 \mathbf{a}_1 - y_9 \mathbf{a}_2 + (z_9 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-ax_9 \hat{\mathbf{x}} - by_9 \hat{\mathbf{y}} + c(z_9 + \frac{1}{2}) \hat{\mathbf{z}}$	(8e)	Hg IV
$\mathbf{B}_{43} =$	$-x_9 \mathbf{a}_1 + (y_9 + \frac{1}{2}) \mathbf{a}_2 - (z_9 - \frac{1}{2}) \mathbf{a}_3$	$=$	$-ax_9 \hat{\mathbf{x}} + b(y_9 + \frac{1}{2}) \hat{\mathbf{y}} - c(z_9 - \frac{1}{2}) \hat{\mathbf{z}}$	(8e)	Hg IV
$\mathbf{B}_{44} =$	$x_9 \mathbf{a}_1 - (y_9 - \frac{1}{2}) \mathbf{a}_2 - z_9 \mathbf{a}_3$	$=$	$ax_9 \hat{\mathbf{x}} - b(y_9 - \frac{1}{2}) \hat{\mathbf{y}} - cz_9 \hat{\mathbf{z}}$	(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
$\mathbf{B}_{46} =$	$x_9 \mathbf{a}_1 + y_9 \mathbf{a}_2 - (z_9 - \frac{1}{2}) \mathbf{a}_3$	$=$	$ax_9 \hat{\mathbf{x}} + by_9 \hat{\mathbf{y}} - c(z_9 - \frac{1}{2}) \hat{\mathbf{z}}$	(8e)	Hg IV
$\mathbf{B}_{47} =$	$x_9 \mathbf{a}_1 - (y_9 - \frac{1}{2}) \mathbf{a}_2 + (z_9 + \frac{1}{2}) \mathbf{a}_3$	$=$	$ax_9 \hat{\mathbf{x}} - b(y_9 - \frac{1}{2}) \hat{\mathbf{y}} + c(z_9 + \frac{1}{2}) \hat{\mathbf{z}}$	(8e)	Hg IV
$\mathbf{B}_{48} =$	$-x_9 \mathbf{a}_1 + (y_9 + \frac{1}{2}) \mathbf{a}_2 + z_9 \mathbf{a}_3$	$=$	$-ax_9 \hat{\mathbf{x}} + b(y_9 + \frac{1}{2}) \hat{\mathbf{y}} + cz_9 \hat{\mathbf{z}}$	(8e)	Hg IV

References

- [1] E. J. Duwell and N. C. Baenziger, *The crystal structure of $K_5\text{Hg}_7$* , Acta Cryst. **13**, 476–479 (1960), doi:10.1107/S0365110X60001126.

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