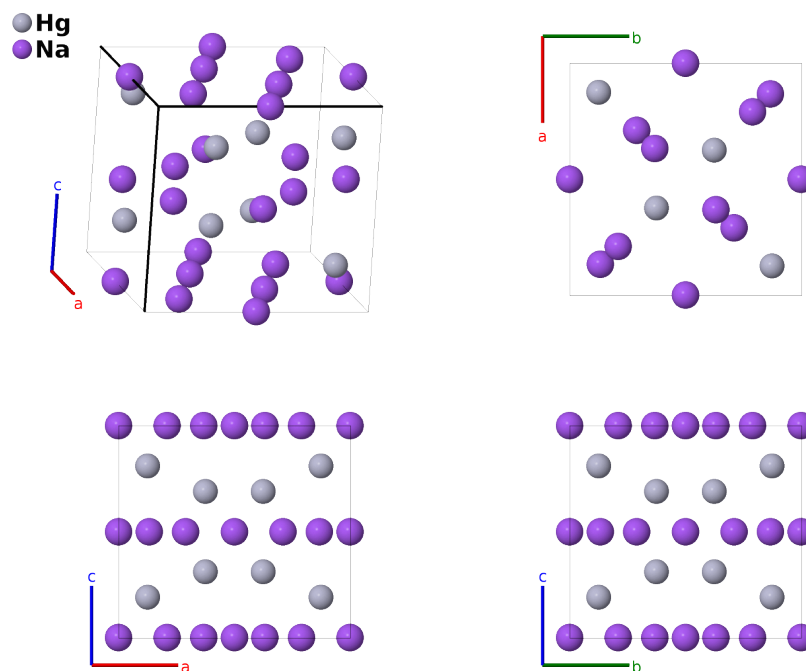


Na₃Hg₂ Structure: A2B3_tP20_136_j_cfg-001

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<https://aflow.org/p/T3N4>

https://aflow.org/p/A2B3_tP20_136_j_cfg-001



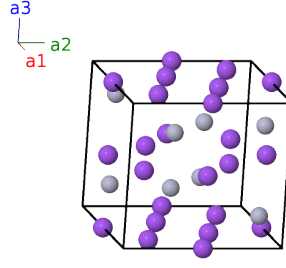
Prototype	Hg ₂ Na ₃
AFLOW prototype label	A2B3_tP20_136_j_cfg-001
ICSD	104328
Pearson symbol	tP20
Space group number	136
Space group symbol	$P4_2/mnm$
AFLOW prototype command	<code>aflow --proto=A2B3_tP20_136_j_cfg-001 --params=a, c/a, x₂, x₃, x₄, z₄</code>

Other compounds with this structure

Al₂Zr₃

Simple Tetragonal primitive vectors

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



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
\mathbf{B}_1	$= \frac{1}{2} \mathbf{a}_2$	$=$	$\frac{1}{2} a \hat{\mathbf{y}}$	(4c)	Na I
\mathbf{B}_2	$= \frac{1}{2} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(4c)	Na I
\mathbf{B}_3	$= \frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} c \hat{\mathbf{z}}$	(4c)	Na I
\mathbf{B}_4	$= \frac{1}{2} \mathbf{a}_1$	$=$	$\frac{1}{2} a \hat{\mathbf{x}}$	(4c)	Na I
\mathbf{B}_5	$= x_2 \mathbf{a}_1 + x_2 \mathbf{a}_2$	$=$	$a x_2 \hat{\mathbf{x}} + a x_2 \hat{\mathbf{y}}$	(4f)	Na II
\mathbf{B}_6	$= -x_2 \mathbf{a}_1 - x_2 \mathbf{a}_2$	$=$	$-a x_2 \hat{\mathbf{x}} - a x_2 \hat{\mathbf{y}}$	(4f)	Na II
\mathbf{B}_7	$= -(x_2 - \frac{1}{2}) \mathbf{a}_1 + (x_2 + \frac{1}{2}) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$-a (x_2 - \frac{1}{2}) \hat{\mathbf{x}} + a (x_2 + \frac{1}{2}) \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(4f)	Na II
\mathbf{B}_8	$= (x_2 + \frac{1}{2}) \mathbf{a}_1 - (x_2 - \frac{1}{2}) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$a (x_2 + \frac{1}{2}) \hat{\mathbf{x}} - a (x_2 - \frac{1}{2}) \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(4f)	Na II
\mathbf{B}_9	$= x_3 \mathbf{a}_1 - x_3 \mathbf{a}_2$	$=$	$a x_3 \hat{\mathbf{x}} - a x_3 \hat{\mathbf{y}}$	(4g)	Na III
\mathbf{B}_{10}	$= -x_3 \mathbf{a}_1 + x_3 \mathbf{a}_2$	$=$	$-a x_3 \hat{\mathbf{x}} + a x_3 \hat{\mathbf{y}}$	(4g)	Na III
\mathbf{B}_{11}	$= (x_3 + \frac{1}{2}) \mathbf{a}_1 + (x_3 + \frac{1}{2}) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$a (x_3 + \frac{1}{2}) \hat{\mathbf{x}} + a (x_3 + \frac{1}{2}) \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(4g)	Na III
\mathbf{B}_{12}	$= -(x_3 - \frac{1}{2}) \mathbf{a}_1 - (x_3 - \frac{1}{2}) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$-a (x_3 - \frac{1}{2}) \hat{\mathbf{x}} - a (x_3 - \frac{1}{2}) \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(4g)	Na III
\mathbf{B}_{13}	$= x_4 \mathbf{a}_1 + x_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$a x_4 \hat{\mathbf{x}} + a x_4 \hat{\mathbf{y}} + c z_4 \hat{\mathbf{z}}$	(8j)	Hg I
\mathbf{B}_{14}	$= -x_4 \mathbf{a}_1 - x_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$-a x_4 \hat{\mathbf{x}} - a x_4 \hat{\mathbf{y}} + c z_4 \hat{\mathbf{z}}$	(8j)	Hg I
\mathbf{B}_{15}	$= -(x_4 - \frac{1}{2}) \mathbf{a}_1 + (x_4 + \frac{1}{2}) \mathbf{a}_2 + (z_4 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-a (x_4 - \frac{1}{2}) \hat{\mathbf{x}} + a (x_4 + \frac{1}{2}) \hat{\mathbf{y}} + c (z_4 + \frac{1}{2}) \hat{\mathbf{z}}$	(8j)	Hg I
\mathbf{B}_{16}	$= (x_4 + \frac{1}{2}) \mathbf{a}_1 - (x_4 - \frac{1}{2}) \mathbf{a}_2 + (z_4 + \frac{1}{2}) \mathbf{a}_3$	$=$	$a (x_4 + \frac{1}{2}) \hat{\mathbf{x}} - a (x_4 - \frac{1}{2}) \hat{\mathbf{y}} + c (z_4 + \frac{1}{2}) \hat{\mathbf{z}}$	(8j)	Hg I
\mathbf{B}_{17}	$= -(x_4 - \frac{1}{2}) \mathbf{a}_1 + (x_4 + \frac{1}{2}) \mathbf{a}_2 - (z_4 - \frac{1}{2}) \mathbf{a}_3$	$=$	$-a (x_4 - \frac{1}{2}) \hat{\mathbf{x}} + a (x_4 + \frac{1}{2}) \hat{\mathbf{y}} - c (z_4 - \frac{1}{2}) \hat{\mathbf{z}}$	(8j)	Hg I
\mathbf{B}_{18}	$= (x_4 + \frac{1}{2}) \mathbf{a}_1 - (x_4 - \frac{1}{2}) \mathbf{a}_2 - (z_4 - \frac{1}{2}) \mathbf{a}_3$	$=$	$a (x_4 + \frac{1}{2}) \hat{\mathbf{x}} - a (x_4 - \frac{1}{2}) \hat{\mathbf{y}} - c (z_4 - \frac{1}{2}) \hat{\mathbf{z}}$	(8j)	Hg I
\mathbf{B}_{19}	$= x_4 \mathbf{a}_1 + x_4 \mathbf{a}_2 - z_4 \mathbf{a}_3$	$=$	$a x_4 \hat{\mathbf{x}} + a x_4 \hat{\mathbf{y}} - c z_4 \hat{\mathbf{z}}$	(8j)	Hg I
\mathbf{B}_{20}	$= -x_4 \mathbf{a}_1 - x_4 \mathbf{a}_2 - z_4 \mathbf{a}_3$	$=$	$-a x_4 \hat{\mathbf{x}} - a x_4 \hat{\mathbf{y}} - c z_4 \hat{\mathbf{z}}$	(8j)	Hg I

References

- [1] J. W. Nielsen and N. C. Baenziger, *The Crystal Structure of NaHg₃, NaHg and Na₃Hg*, Acta Cryst. **7**, 277–282 (1954), doi:10.1107/S0365110X54000783.