

NaHg Structure:

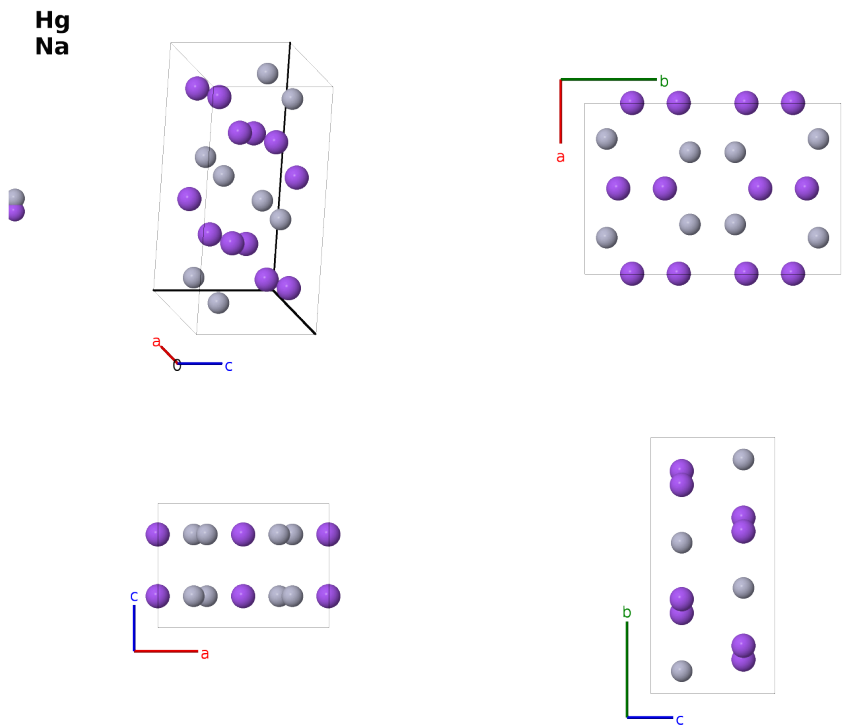
AB_oC16_63_g_2c-001

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

https://aflow.org/prototype-encyclopedia/AB_oC16_63_g_2c-001

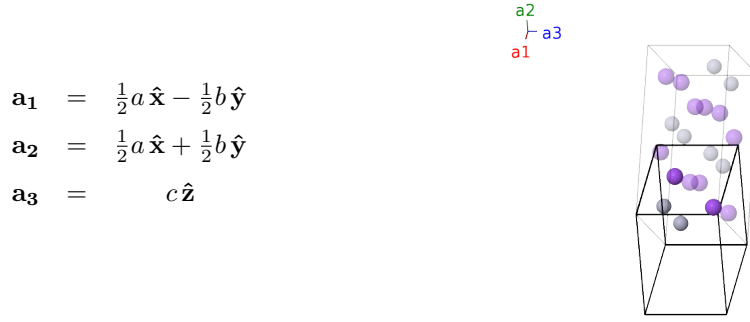


Prototype	HgNa
AFLOW prototype label	AB_oC16_63_g_2c-001
ICSD	104326
CCDC	1662242
Pearson symbol	oC16
Space group number	63
Space group symbol	$Cmcm$
AFLOW prototype command	<code>aflow --proto=AB_oC16_63_g_2c-001</code> <code>--params=$a, b/a, c/a, y_1, y_2, x_3, y_3$</code>

- (Nielsen, 1954) give the coordinates of the (4c) Na atoms as (0 y 3/4), but this gives Na-Hg distances which are too small. Using (0 y 1/4) with the given values of y gives reasonable distances in agreement with those reported in the reference.

- The ICSD entry has the correct coordinates.

Base-centered Orthorhombic primitive vectors



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$= -y_1 \mathbf{a}_1 + y_1 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$by_1 \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	(4c)	Na I
$\mathbf{B}_2$	$= y_1 \mathbf{a}_1 - y_1 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$-by_1 \hat{\mathbf{y}} + \frac{3}{4}c \hat{\mathbf{z}}$	(4c)	Na I
$\mathbf{B}_3$	$= -y_2 \mathbf{a}_1 + y_2 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$by_2 \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	(4c)	Na II
$\mathbf{B}_4$	$= y_2 \mathbf{a}_1 - y_2 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$-by_2 \hat{\mathbf{y}} + \frac{3}{4}c \hat{\mathbf{z}}$	(4c)	Na II
$\mathbf{B}_5$	$= (x_3 - y_3) \mathbf{a}_1 + (x_3 + y_3) \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$ax_3 \hat{\mathbf{x}} + by_3 \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	(8g)	Hg I
$\mathbf{B}_6$	$= -(x_3 - y_3) \mathbf{a}_1 - (x_3 + y_3) \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$-ax_3 \hat{\mathbf{x}} - by_3 \hat{\mathbf{y}} + \frac{3}{4}c \hat{\mathbf{z}}$	(8g)	Hg I
$\mathbf{B}_7$	$= -(x_3 + y_3) \mathbf{a}_1 - (x_3 - y_3) \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$-ax_3 \hat{\mathbf{x}} + by_3 \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	(8g)	Hg I
$\mathbf{B}_8$	$= (x_3 + y_3) \mathbf{a}_1 + (x_3 - y_3) \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$ax_3 \hat{\mathbf{x}} - by_3 \hat{\mathbf{y}} + \frac{3}{4}c \hat{\mathbf{z}}$	(8g)	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.

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