

α -HgO₂ Structure:

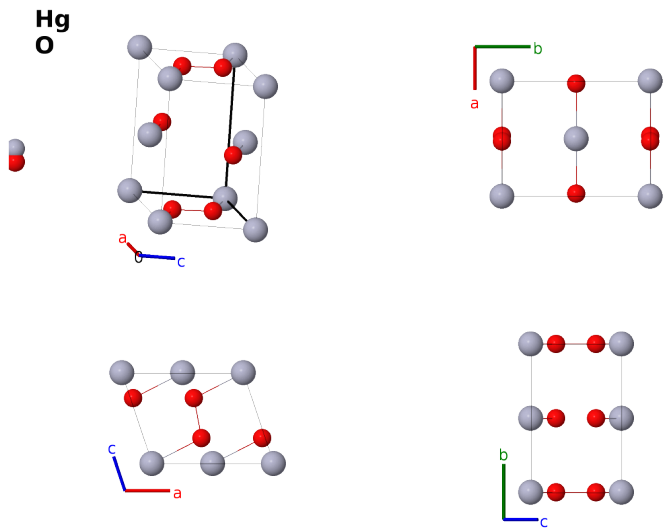
AB2_mC6_12_a_i-004

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

https://aflow.org/prototype-encyclopedia/AB2_mC6_12_a_i-004

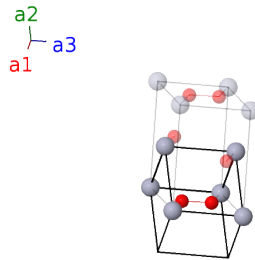


Prototype	HgO ₂
AFLOW prototype label	AB2_mC6_12_a_i-004
ICSD	655816
CCDC	1765892
Pearson symbol	mC6
Space group number	12
Space group symbol	$C2/m$
AFLOW prototype command	<code>aflow --proto=AB2_mC6_12_a_i-004</code> <code>--params=a, b/a, c/a, β, x_2, z_2</code>

- HgO₂ exists as
 - monoclinic α -HgO (this structure) and
 - orthorhombic β -HgO₂.
- C34 Calverite, α -HgO₂ (this structure), and NiO₂ have the same AFLOW prototype label, AB2_mC6_12_a.i. The structures are generated by the same symmetry operations with different sets of parameters (`--params`) specified in their corresponding CIF files.

Base-centered Monoclinic primitive vectors

$$\begin{aligned}\mathbf{a}_1 &= \frac{1}{2}a \hat{\mathbf{x}} - \frac{1}{2}b \hat{\mathbf{y}} \\ \mathbf{a}_2 &= \frac{1}{2}a \hat{\mathbf{x}} + \frac{1}{2}b \hat{\mathbf{y}} \\ \mathbf{a}_3 &= c \cos \beta \hat{\mathbf{x}} + c \sin \beta \hat{\mathbf{z}}\end{aligned}$$



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	=	0	=	0	(2a) Hg I
$\mathbf{B}_2$	=	$x_2 \mathbf{a}_1 + x_2 \mathbf{a}_2 + z_2 \mathbf{a}_3$	=	$(ax_2 + cz_2 \cos \beta) \hat{\mathbf{x}} + cz_2 \sin \beta \hat{\mathbf{z}}$	(4i) O I
$\mathbf{B}_3$	=	$-x_2 \mathbf{a}_1 - x_2 \mathbf{a}_2 - z_2 \mathbf{a}_3$	=	$-(ax_2 + cz_2 \cos \beta) \hat{\mathbf{x}} - cz_2 \sin \beta \hat{\mathbf{z}}$	(4i) O I

References

- [1] M. Pušelj, Z. Ban, E. Lukačević, and J. Morvaj, *On the Preparation of Mercuric Peroxides and Refinement of the α -HgO₂ Structure*, *Z. Anorganische und Allgemeine Chemie* **528**, 191–194 (1985).

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