α-HgO_2 Structure: AB2_mC6_12_a_i-004

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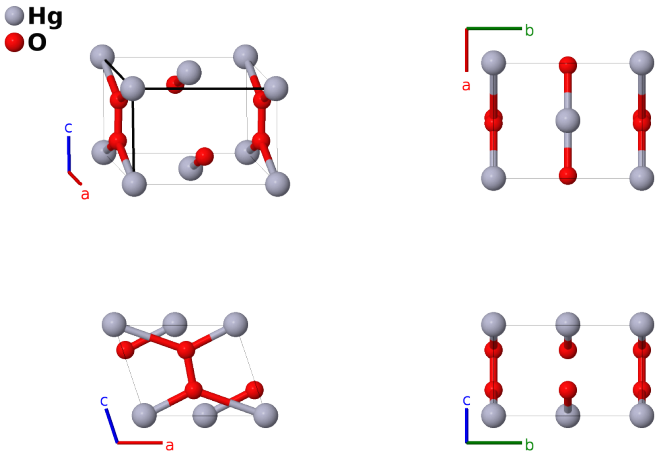
https://aflow.org/p/RMCX

https://aflow.org/p/AB2_mC6_12_a_i-004

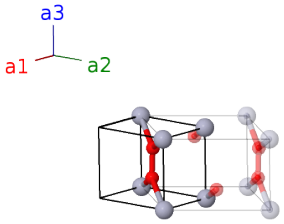


Prototype	HgO_2
AFLOW prototype label	AB2_mC6_12_a_i-004
ICSD	655816
Pearson symbol	mC6
Space group number	12
Space group symbol	$C2/m$
AFLOW prototype command	`aflow --proto=AB2_mC6_12_a_i-004 --params=`$a, b/a, c/a, \beta, x_2, z_2$

- HgO_2 exists as
  - monoclinic α-HgO (this structure) and
  - orthorhombic β-HgO_2.
- $C34$ Calverite, α-HgO2 (this structure), and NiO_2 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

$$\mathbf{a_1} = \tfrac{1}{2}a\,\hat{\mathbf{x}} - \tfrac{1}{2}b\,\hat{\mathbf{y}}$$
$$\mathbf{a_2} = \tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{1}{2}b\,\hat{\mathbf{y}}$$
$$\mathbf{a_3} = c\cos\beta\,\hat{\mathbf{x}} + c\sin\beta\,\hat{\mathbf{z}}$$



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-HgO_2 Structure*, Z. Anorganische und Allgemeine Chemie **528**, 191–194 (1985).