α-Hg (A10) Structure: A_hR1_166_a-002

This structure previously used the label(s) `A_hR1_166_a.alpha-Hg`. Calls to these addresses will be redirected here.

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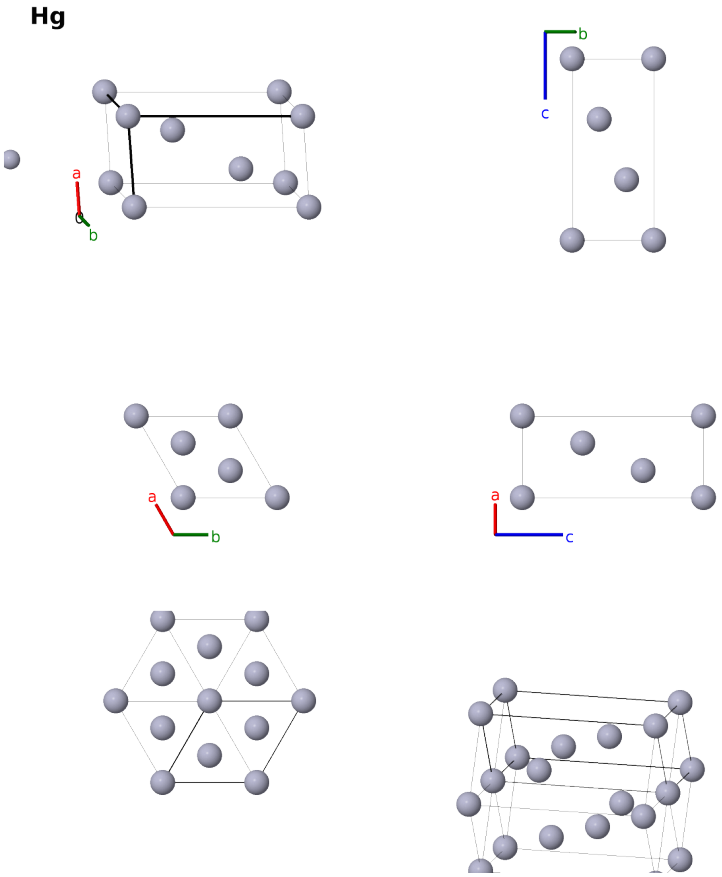
https://aflow.org/prototype-encyclopedia/8ZQP

https://aflow.org/prototype-encyclopedia/A_hR1_166_a-002



Prototype	Hg
AFLOW prototype label	A_hR1_166_a-002
***Strukturbericht* designation**	*A*10
ICSD	174006
CCDC	1688899
Pearson symbol	hR1
Space group number	166

Space group symbol $R\bar{3}m$

AFLOW prototype command `aflow --proto=A_hR1_166_a-002 --params=`$a, c/a$

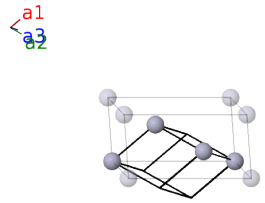
- This rhombohedral structure becomes cubic at various values of c/a (or α) to wit,

c/a	α	Cubic Lattice
$\sqrt{6}$	60°	Face-Centered Cubic
$\sqrt{\frac{3}{2}}$	90°	Simple Cubic
$\sqrt{\frac{3}{8}}$	109.47°	Body-Centered Cubic

- β-Po and α-Hg have the same AFLOW prototype label, A_hR1_166_a. They are generated by the same symmetry operations with different sets of parameters (`--params`) specified in their corresponding CIF files. Experimentally, β-Po (A_i) has c/a near 1, or $\alpha > 90°$, while α-Hg (A10) has c/a near 2, or $\alpha < 90°$.
- Hexagonal settings of rhombohedral structures can be obtained with the option `--hex`.

Rhombohedral primitive vectors

$$\mathbf{a_1} = \frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \frac{1}{3}c\,\hat{\mathbf{z}}$$
$$\mathbf{a_2} = \frac{1}{\sqrt{3}}a\,\hat{\mathbf{y}} + \frac{1}{3}c\,\hat{\mathbf{z}}$$
$$\mathbf{a_3} = -\frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \frac{1}{3}c\,\hat{\mathbf{z}}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	0	=	0	(1a)	Hg I

References

[1] C. S. Barrett, *The structure of mercury at low temperatures*, Acta Cryst. **10**, 58–60 (1957), doi:10.1107/S0365110X57000134.

Found in

[1] J. Donohue, *The Structures of the Elements* (Robert E. Krieger Publishing Company, New York, 1974).

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