α-Hg (A10) Structure: A_hR1_166_a-002

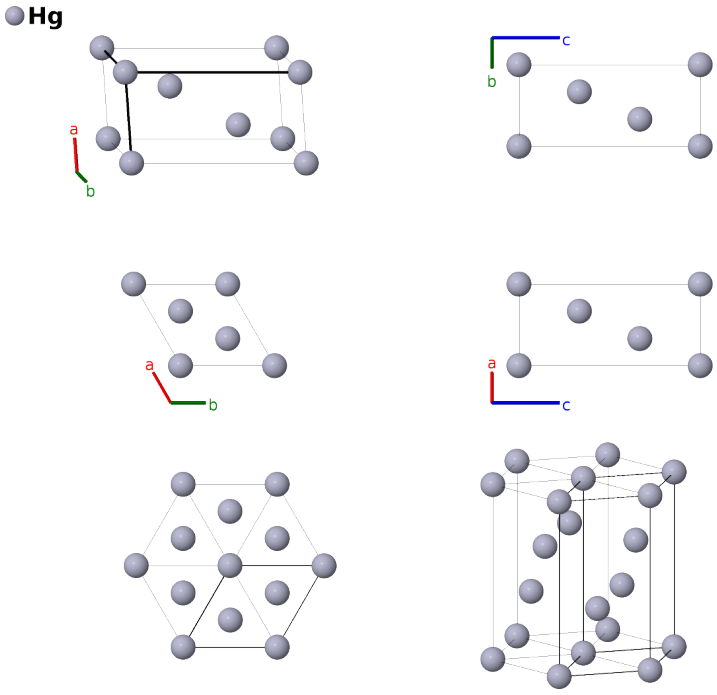
This structure originally had the label `A_hR1_166_a.alpha-Hg`. Calls to that address will be redirected here.

Cite this page as: M. J. Mehl, D. Hicks, C. Toher, O. Levy, R. M. Hanson, G. Hart, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 1*, Comput. Mater. Sci. **136**, S1-828 (2017). doi: 10.1016/j.commatsci.2017.01.017

---

https://aflow.org/p/8ZQP

https://aflow.org/p/A_hR1_166_a-002



Prototype	Hg
AFLOW prototype label	A_hR1_166_a-002
***Strukturbericht* designation**	$A10$
ICSD	174006
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=`$a, c/a$

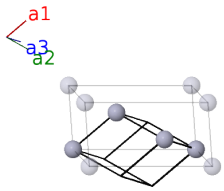
- This rhombohedral structure becomes cubic at various values of c/a (or α) to wit,

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 (A_hR1_166_a and α-Hg (A_hR1_166_a) have the same AFLOW prototype label. 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

$$\begin{aligned}
\mathbf{a_1} &= \tfrac{1}{2}a\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \tfrac{1}{3}c\,\hat{\mathbf{z}} \\
\mathbf{a_2} &= \tfrac{1}{\sqrt{3}}a\,\hat{\mathbf{y}} + \tfrac{1}{3}c\,\hat{\mathbf{z}} \\
\mathbf{a_3} &= -\tfrac{1}{2}a\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \tfrac{1}{3}c\,\hat{\mathbf{z}}
\end{aligned}$$



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).