β-Po (A_i) Structure: A_hR1_166_a-001

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

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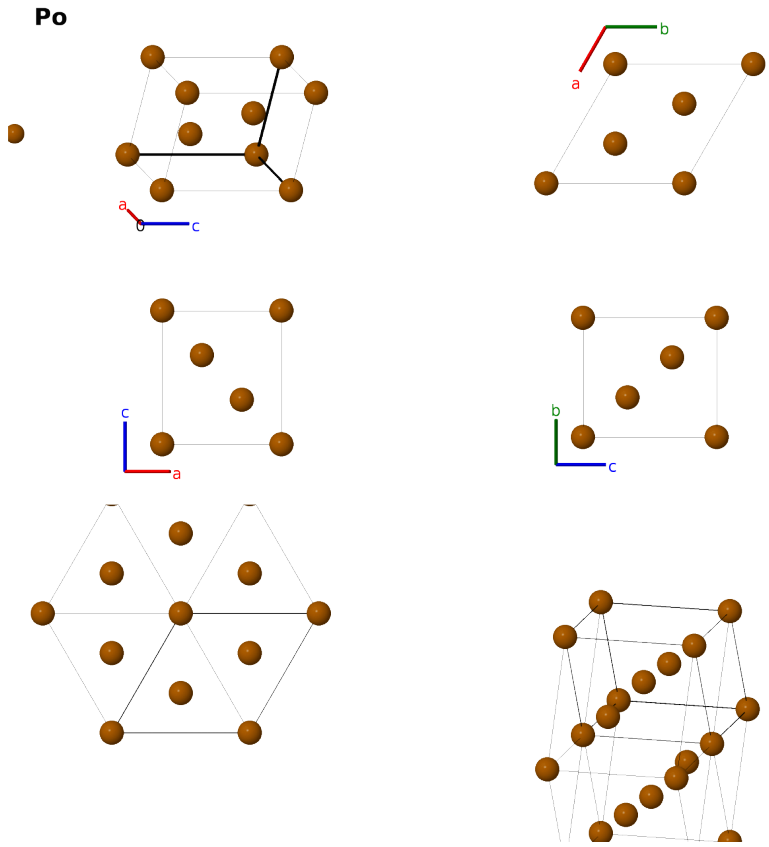
https://aflow.org/prototype-encyclopedia/RUSN

https://aflow.org/prototype-encyclopedia/A_hR1_166_a-001



Prototype	Po
AFLOW prototype label	A_hR1_166_a-001
***Strukturbericht* designation**	A_i
ICSD	649161
CCDC	1763583
Pearson symbol	hR1
Space group number	166
Space group symbol	$R\bar{3}m$

AFLOW prototype command `aflow --proto=A_hR1_166_a-001 --params=`$a, c/a$

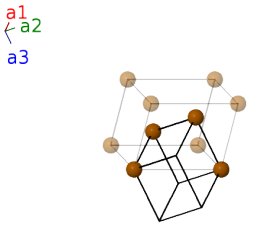
- Originally, Po was assigned Strukturbericht designation $A19$, which is now considered to be incorrect. (Donohue, 1982, 390).
- Solid polonium actually exists in two phases: cubic α-Po (A_h) is the ground state and rhombohedral β-Po (A_l) (this structure) (Donohue, 1974). There is a large amount of hysteresis observed in the transition, which occurs at 54°C for $\alpha \rightarrow \beta$ and 18° for $\beta \rightarrow \alpha$.
- This rhombohedral structure becomes cubic at various values of c/a (or α)

c/a	α	**Cubic Lattice**
$\sqrt{7}$	60°	Face-Centered Cubic
$\sqrt{\frac{3}{2}}$	90°	Simple Cubic
$\sqrt{\frac{3}{8}}$	109.47°	Body-Centered Cubic

- Note that 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)	Po I

References

[1] W. H. Beamer and C. L. Maxwell, *Physical Properties of Polonium. II. X-Ray Studies and Crystal Structure*, J. Chem. Phys. **17**, 1293–1298 (1949), doi:10.1063/1.1747155.

Found in

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

First cited in

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