

A19 Po Structure (*Obsolete*): A_mC12_5_3c-001

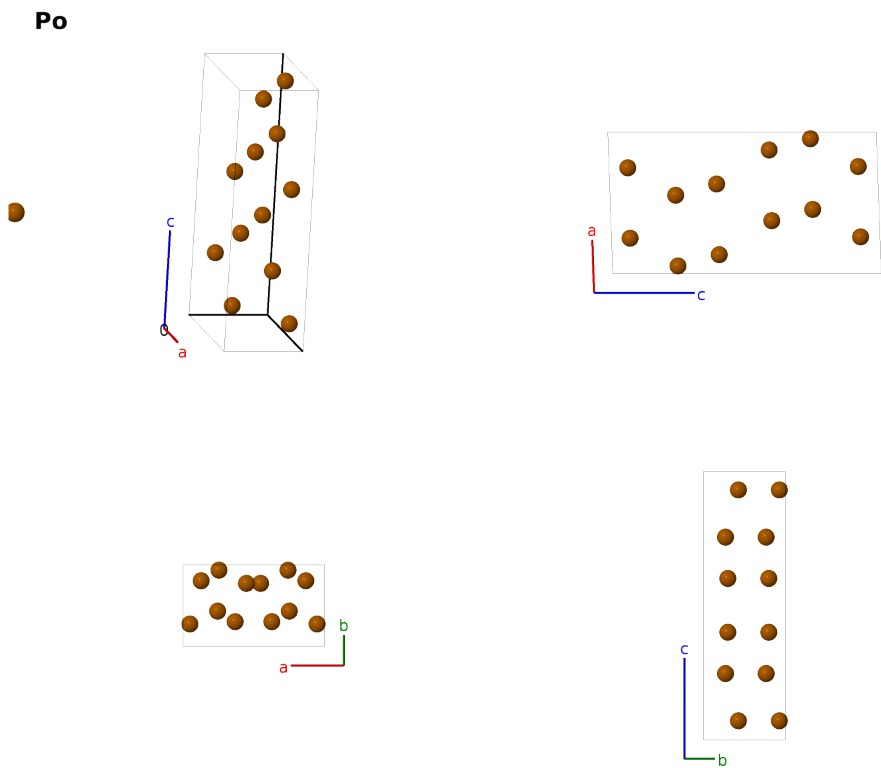
This structure previously used the label(s) **A_mC12_5_3c**. Calls to these addresses will be redirected here.

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

https://aflow.org/prototype-encyclopedia/A_mC12_5_3c-001

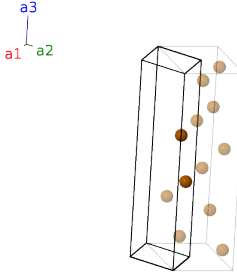


Prototype	Po
AFLOW prototype label	A_mC12_5_3c-001
<i>Strukturbericht</i> designation	A19
ICSD	31684
CCDC	1605682
Pearson symbol	mC12
Space group number	5
Space group symbol	<i>C</i> 2

AFLOW prototype command `aflow --proto=A_mC12_5_3c-001`
 `--params=a, b/a, c/a,  $\beta$ ,  $x_1$ ,  $y_1$ ,  $z_1$ ,  $x_2$ ,  $y_2$ ,  $z_2$ ,  $x_3$ ,  $y_3$ ,  $z_3$`

- This was the original determination of the structure of Po, given the *Strukturbericht* designation A19 by (Gottfried, 1938, 4-5). Eventually it was found that the sample used here was a mixture of α -Po (A_h) and β -Po (A_i) (Donohue, 1982, 390). We retain the A19 page for historical interest.
- The ICSD entry uses polonium coordinates that are slightly different from the ones we use. Both sets are published in (Rollier, 1936).

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
$\mathbf{B}_1$	$(x_1 - y_1) \mathbf{a}_1 + (x_1 + y_1) \mathbf{a}_2 + z_1 \mathbf{a}_3$	$=$	$(ax_1 + cz_1 \cos \beta) \hat{\mathbf{x}} + by_1 \hat{\mathbf{y}} + cz_1 \sin \beta \hat{\mathbf{z}}$	(4c)	Po I
$\mathbf{B}_2$	$-(x_1 + y_1) \mathbf{a}_1 - (x_1 - y_1) \mathbf{a}_2 - z_1 \mathbf{a}_3$	$=$	$-(ax_1 + cz_1 \cos \beta) \hat{\mathbf{x}} + by_1 \hat{\mathbf{y}} - cz_1 \sin \beta \hat{\mathbf{z}}$	(4c)	Po I
$\mathbf{B}_3$	$(x_2 - y_2) \mathbf{a}_1 + (x_2 + y_2) \mathbf{a}_2 + z_2 \mathbf{a}_3$	$=$	$(ax_2 + cz_2 \cos \beta) \hat{\mathbf{x}} + by_2 \hat{\mathbf{y}} + cz_2 \sin \beta \hat{\mathbf{z}}$	(4c)	Po II
$\mathbf{B}_4$	$-(x_2 + y_2) \mathbf{a}_1 - (x_2 - y_2) \mathbf{a}_2 - z_2 \mathbf{a}_3$	$=$	$-(ax_2 + cz_2 \cos \beta) \hat{\mathbf{x}} + by_2 \hat{\mathbf{y}} - cz_2 \sin \beta \hat{\mathbf{z}}$	(4c)	Po II
$\mathbf{B}_5$	$(x_3 - y_3) \mathbf{a}_1 + (x_3 + y_3) \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$(ax_3 + cz_3 \cos \beta) \hat{\mathbf{x}} + by_3 \hat{\mathbf{y}} + cz_3 \sin \beta \hat{\mathbf{z}}$	(4c)	Po III
$\mathbf{B}_6$	$-(x_3 + y_3) \mathbf{a}_1 - (x_3 - y_3) \mathbf{a}_2 - z_3 \mathbf{a}_3$	$=$	$-(ax_3 + cz_3 \cos \beta) \hat{\mathbf{x}} + by_3 \hat{\mathbf{y}} - cz_3 \sin \beta \hat{\mathbf{z}}$	(4c)	Po III

References

- [1] M. A. Rollier, S. B. Hendricks, and L. R. Maxwell, *The Crystal Structure of Polonium by Electron Diffraction*, J. Chem. Phys. **4**, 648–652 (1936), doi:10.1063/1.1749762.
- [2] C. Gottfried and F. Schossberger, eds., *Strukturbericht Band III 1933-1935* (Akademische Verlagsgesellschaft M. B. H., Leipzig, 1937).
- [3] J. Donohue, *The Structures of the Elements* (Robert E. Krieger Publishing Company, New York, 1974).

Found in

- [1] R. T. Downs and M. Hall-Wallace, *The American Mineralogist Crystal Structure Database*, Am. Mineral. **88**, 247–250 (2003).

First cited in

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