

PrOI Structure:

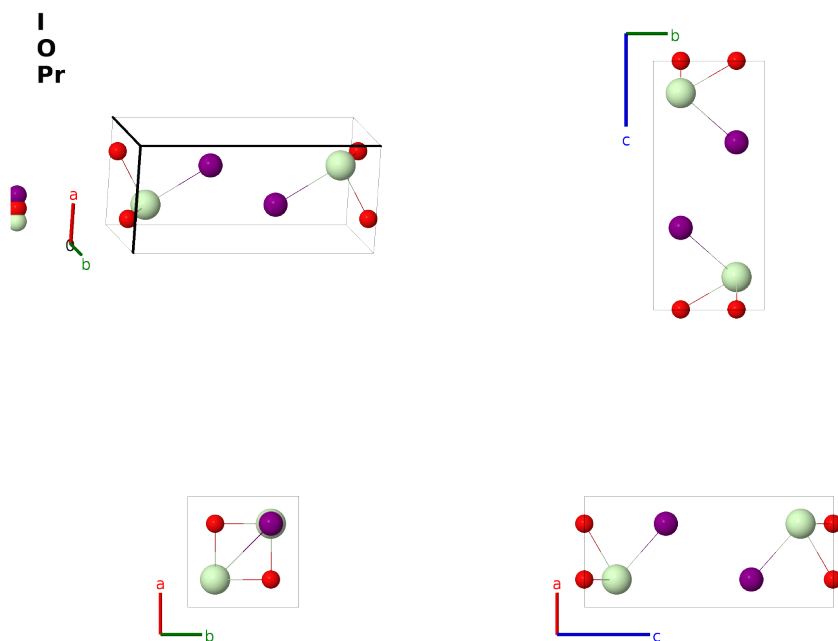
ABC_tP6_129_c_a_c-003

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- D. Hicks, M. J. Mehl, M. Esters, C. Oses, O. Levy, G. L. W. Hart, C. Toher, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 3*, Comput. Mater. Sci. **199**, 110450 (2021), doi: 10.1016/j.commatsci.2021.110450.

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

https://aflow.org/prototype-encyclopedia/ABC_tP6_129_c_a_c-003



Prototype	IOPr
AFLOW prototype label	ABC_tP6_129_c_a_c-003
ICSD	200047
CCDC	1705088
Pearson symbol	tP6
Space group number	129
Space group symbol	$P4/nmm$
AFLOW prototype command	<code>aflow --proto=ABC_tP6_129_c_a_c-003 --params=a, c/a, z₂, z₃</code>

Other compounds with this structure

AcOBr, AcOCl, AmOBr, AmOCl, AsCaRb, AsCdK, AsMnCs, AsMnK, AsMnRb, BaFBr, BaFI, BaHBr, BaHI, BaMnGe, BiMgK, BiMnCs, BiMnRb, BiOBr, BiOCl, BiOI, BrFEu, BrFPb, BrFSr, BrHCa, BrHEu, BrHSr, BrNTh, BrNU, BrOEu,

BrOLa, BrONd, BrOPr, BrOSm, BrOYb, CaCoSi, CaFCl, CaHCl, CaHI, CaMnGe, CaMnSi, CaMnSn, CaNiGe, CaRuSi, CeCoGe, CeCoSi, CeFS, CeFeSi, CeMnSi, CeOCl, CeOsSi, CeRuSi, CmOCl, CsMnP, CsMnSb, CsNaTe, EuOCl, EuOI, GdCoSi, GdFeSi, GdOGd, GdRuSi, HLiO, HoFeSi, HoOCl, KCdSb, KLiS, KMnP, KMnSb, LaClSi, LaCoGe, LaFS, LaFeSi, LaGeRu, LaOCl, LaOI, LaRuSi, MgMnGe, MnGeNd, NdClP, NdClSi, NdFeSi, NdOCl, NdOGe, NdRuSi, NpOI, NpOSe, PClPr, PClSm, PFeSm, PbFI, PrClSi, PrFeSi, PrOGe, PrRuFe, PrRuSi, RbCaSb, RbLiS, RbLiSe, RbMnP, RbMnSb, RbNaO, RuNdGe, SSuTl, SeCuTl, SeFeN, SiClTb, SiFeY, SiMnY, SmFeSi, SmOCl, SmRuGe, SmRuSi, SrMnGe, ThNCl, ThNI, ThOSe, ThOTe, TmOI, UNCl, UNI, UOSe, UOTe, YOCl, YbFeSi, YbHCl, ZrOS

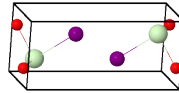
- Matlockite ($E0_1$) and PrOI have the same AFLOW prototype label, `ABC.tP6_c.a.c`. They are generated by the same symmetry operations with different sets of parameters (`--params`) specified in their corresponding CIF files.
- Indeed, (Potapova, 1977) state that PrOI is a Matlockite structure, but both AFLOW and the ICSD agree that they are different enough to warrant listing them as separate prototypes.
- In both cases we have $z_3 \approx -z_2$. We somewhat arbitrarily assign structures with the $\min(z_2, z_3) < 0.199$ to the PrOI structure and those with larger values to the Matlockite structure.
- Binary forms of Matlockite/PrOI occur when the species on the (2a) site is the same as one of the species on the (2c) sites. We assign these structures to the prototypes:
 - Cu_2Sb ($C38$) for structures with $c/a < 2$,
 - UP_2 for structures with $2 < c/a < 3$, and
 - $\text{LaSe}_{1.85}$ for structures with $c/a \approx 4$.
- (Potapova, 1977) give this structure in setting 1 of space group $P4/nmm$ #129. We shifted the origin to put it into our standard setting 2.

Simple Tetragonal primitive vectors

$$\mathbf{a}_1 = a \hat{\mathbf{x}}$$

$$\mathbf{a}_2 = a \hat{\mathbf{y}}$$

$$\mathbf{a}_3 = c \hat{\mathbf{z}}$$



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$= \frac{3}{4} \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2$	$=$	$\frac{3}{4} a \hat{\mathbf{x}} + \frac{1}{4} a \hat{\mathbf{y}}$	(2a)	O I
$\mathbf{B}_2$	$= \frac{1}{4} \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2$	$=$	$\frac{1}{4} a \hat{\mathbf{x}} + \frac{3}{4} a \hat{\mathbf{y}}$	(2a)	O I
$\mathbf{B}_3$	$= \frac{1}{4} \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_2 \mathbf{a}_3$	$=$	$\frac{1}{4} a \hat{\mathbf{x}} + \frac{1}{4} a \hat{\mathbf{y}} + cz_2 \hat{\mathbf{z}}$	(2c)	I I
$\mathbf{B}_4$	$= \frac{3}{4} \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_2 \mathbf{a}_3$	$=$	$\frac{3}{4} a \hat{\mathbf{x}} + \frac{3}{4} a \hat{\mathbf{y}} - cz_2 \hat{\mathbf{z}}$	(2c)	I I
$\mathbf{B}_5$	$= \frac{1}{4} \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$\frac{1}{4} a \hat{\mathbf{x}} + \frac{1}{4} a \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}}$	(2c)	Pr I
$\mathbf{B}_6$	$= \frac{3}{4} \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_3 \mathbf{a}_3$	$=$	$\frac{3}{4} a \hat{\mathbf{x}} + \frac{3}{4} a \hat{\mathbf{y}} - cz_3 \hat{\mathbf{z}}$	(2c)	Pr I

References

- [1] O. G. Potapova, I. G. Vasil'eva, and S. V. Borisov, *Crystal structure of praseodymium oxide iodide*, J. Struct. Chem. **18**, 459–462 (1977), doi:10.1007/BF00753092. Translated from Zhurnal Strukturnoi Khimii 18, 573 (1977).

Found in

[1] *Inorganic Crystal Structure Database*. Entry 200047 (PrOI).

First cited in

N. Anderson, M. J. Mehl, H. Eckert, S. Divilov, X. Campilongo, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 5*. Submitted to Computational Materials Science (2026).