

Black Phosphorus (A17) Structure: A_oC8_64_f-002

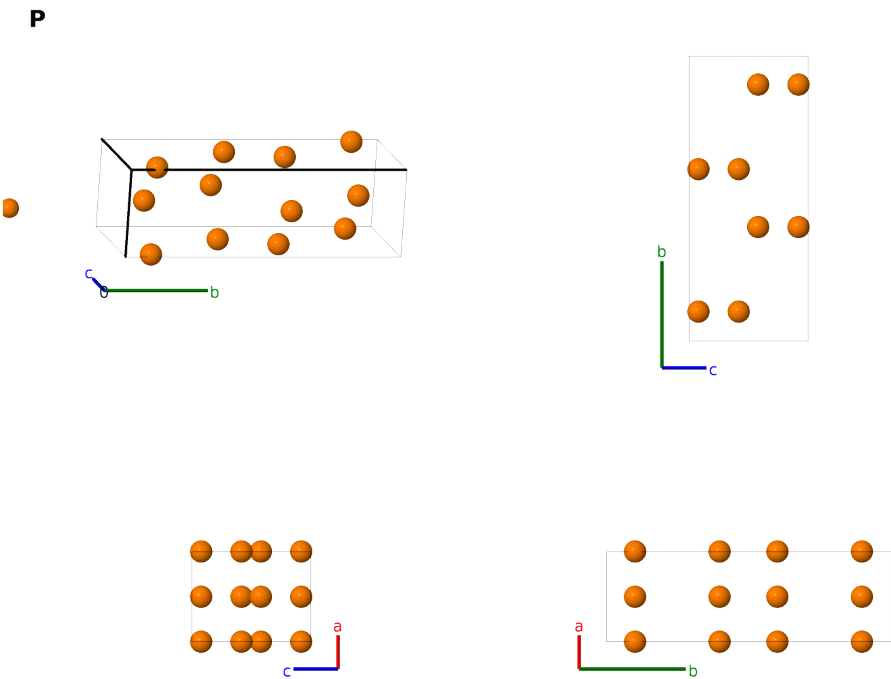
This structure previously used the label(s) **A_oC8_64_f.P**. Calls to these addresses will be redirected here.

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<https://aflow.org/prototype-encyclopedia/7VYH>

https://aflow.org/prototype-encyclopedia/A_oC8_64_f-002



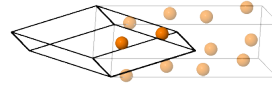
Prototype	P
AFLOW prototype label	A_oC8_64_f-002
<i>Strukturbericht</i> designation	A17
ICSD	23836
CCDC	1599907
Pearson symbol	oC8
Space group number	64
Space group symbol	<i>Cmce</i>
AFLOW prototype command	<code>aflow --proto=A_oC8_64_f-002 --params=a, b/a, c/a, y₁, z₁</code>

- Phosphorus is found in at least three forms:
 - Black phosphorus, *Strukturbericht* A17, (this structure)
 - Monoclinic Hittorf’s phosphorus, and
 - Low temperature triclinic “white” phosphorus, stable below 197K.
- α -gallium (A11), molecular iodine (A14), and black phosphorous (A17) all share the same AFLOW label, A_oC8_64_f. The structures are generated by the same symmetry operations with different sets of parameters (`--params`) specified in their corresponding CIF files.

Base-centered Orthorhombic primitive vectors

$$\begin{aligned}
 \mathbf{a}_1 &= \frac{1}{2}a \hat{\mathbf{x}} - \frac{1}{2}b \hat{\mathbf{y}} \\
 \mathbf{a}_2 &= \frac{1}{2}a \hat{\mathbf{x}} + \frac{1}{2}b \hat{\mathbf{y}} \\
 \mathbf{a}_3 &= c \hat{\mathbf{z}}
 \end{aligned}$$

a#3 - a2



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$= -y_1 \mathbf{a}_1 + y_1 \mathbf{a}_2 + z_1 \mathbf{a}_3$	$=$	$by_1 \hat{\mathbf{y}} + cz_1 \hat{\mathbf{z}}$	(8f)	P I
$\mathbf{B}_2$	$= (y_1 + \frac{1}{2}) \mathbf{a}_1 - (y_1 - \frac{1}{2}) \mathbf{a}_2 + (z_1 + \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} - by_1 \hat{\mathbf{y}} + c(z_1 + \frac{1}{2}) \hat{\mathbf{z}}$	(8f)	P I
$\mathbf{B}_3$	$= -(y_1 - \frac{1}{2}) \mathbf{a}_1 + (y_1 + \frac{1}{2}) \mathbf{a}_2 - (z_1 - \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} + by_1 \hat{\mathbf{y}} - c(z_1 - \frac{1}{2}) \hat{\mathbf{z}}$	(8f)	P I
$\mathbf{B}_4$	$= y_1 \mathbf{a}_1 - y_1 \mathbf{a}_2 - z_1 \mathbf{a}_3$	$=$	$-by_1 \hat{\mathbf{y}} - cz_1 \hat{\mathbf{z}}$	(8f)	P I

References

- [1] A. Brown and S. Rundqvist, *Refinement of the crystal structure of black phosphorus*, Acta Cryst. **19**, 684–685 (1965), doi:10.1107/S0365110X65004140.

First cited in

M. J. Mehl, D. Hicks, C. Toher, O. Levy, R. M. Hanson, G. L. W. 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