Black Phosphorus ($A17$) Structure: A_oC8_64_f-002

This structure originally had the label `A_oC8_64_f.P`. Calls to that address will be redirected here.

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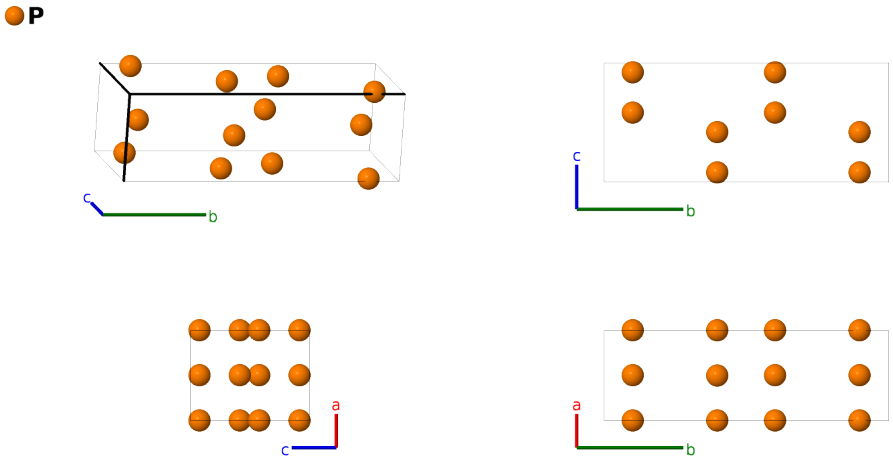
https://aflow.org/p/7VYH

https://aflow.org/p/A_oC8_64_f-002

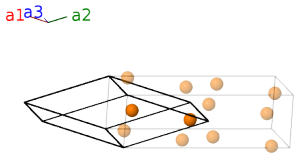


Prototype	P
AFLOW prototype label	A_oC8_64_f-002
***Strukturbericht* designation**	$A17$
ICSD	23836
Pearson symbol	oC8
Space group number	64
Space group symbol	$Cmce$
AFLOW prototype command	`aflow --proto=A_oC8_64_f-002 --params=`$a, b/a, c/a, y_1, z_1$

- 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

$$\mathbf{a_1} = \frac{1}{2}a\,\hat{\mathbf{x}} - \frac{1}{2}b\,\hat{\mathbf{y}}$$
$$\mathbf{a_2} = \frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}b\,\hat{\mathbf{y}}$$
$$\mathbf{a_3} = c\,\hat{\mathbf{z}}$$



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
$\mathbf{B_2}$	=	$\left(y_1+\frac{1}{2}\right)\,\mathbf{a}_1 - \left(y_1-\frac{1}{2}\right)\,\mathbf{a}_2 + \left(z_1+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - by_1\,\hat{\mathbf{y}} + c\left(z_1+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8f)	P I
$\mathbf{B_3}$	=	$-\left(y_1-\frac{1}{2}\right)\,\mathbf{a}_1 + \left(y_1+\frac{1}{2}\right)\,\mathbf{a}_2 - \left(z_1-\frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + by_1\,\hat{\mathbf{y}} - c\left(z_1-\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(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.