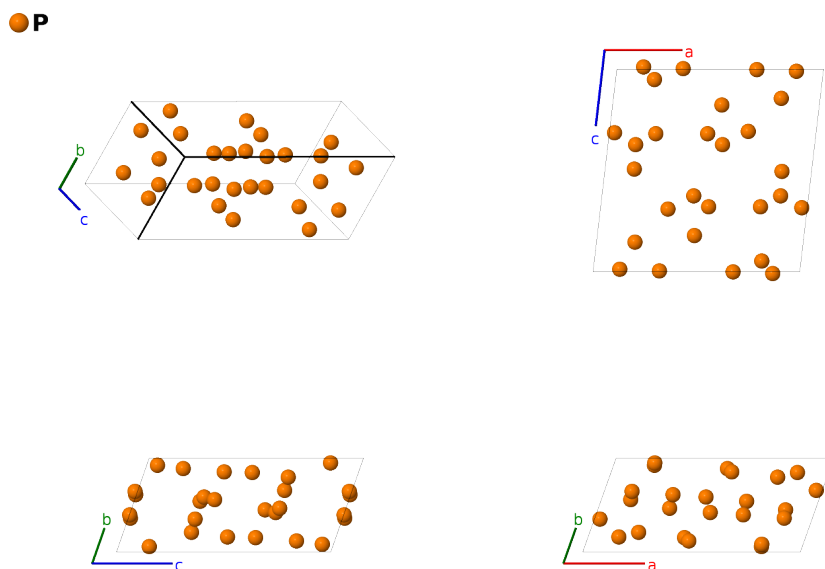


Low Temperature “White” Phosphorous Structure: A_aP24_2_12i-001

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<https://aflow.org/p/YLP3>

https://aflow.org/p/A_aP24_2_12i-001



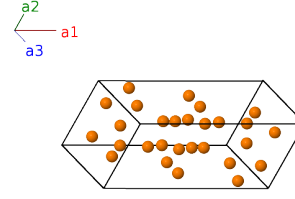
Prototype	P
AFLOW prototype label	A_aP24_2_12i-001
ICSD	68326
Pearson symbol	aP24
Space group number	2
Space group symbol	$P\bar{1}$
AFLOW prototype command	<pre>aflow --proto=A_aP24_2_12i-001 --params=a,b/a,c/a,α,β,γ,$x_1,y_1,z_1,x_2,y_2,z_2,x_3,y_3,z_3,x_4,y_4,z_4,x_5,y_5,z_5,x_6,y_6,z_6,x_7,y_7,z_7,x_8,y_8,z_8,x_9,y_9,z_9,x_{10},y_{10},z_{10},x_{11},y_{11},z_{11},x_{12},y_{12},z_{12}$</pre>

- Phosphorus is found in at least three forms:
 - Black phosphorus, *Strukturbericht* A17,
 - Monoclinic Hittorf’s phosphorus, and
 - Low temperature triclinic “white” phosphorus, stable below 197K. (this structure)
- We use the data taken at 162K.
- The P_4 molecules exhibit considerable rigid-body motion, both rotational and translational (Simon, 1987).

- There is considerable disagreement about the name of this structure. Most authors refer to it as β -white phosphorous, but (Donohue, 1982) refers to it as α -white phosphorous. Other authors refer to this as yellow phosphorous. Simply referring to this as low temperature phosphorous seems the easiest way to avoid confusion.

Triclinic primitive vectors

$$\begin{aligned}
 \mathbf{a}_1 &= a \hat{\mathbf{x}} \\
 \mathbf{a}_2 &= b \cos \gamma \hat{\mathbf{x}} + b \sin \gamma \hat{\mathbf{y}} \\
 \mathbf{a}_3 &= c_x \hat{\mathbf{x}} + c_y \hat{\mathbf{y}} + c_z \hat{\mathbf{z}} \\
 c_x &= c \cos \beta \\
 c_y &= c(\cos \alpha - \cos \beta \cos \gamma) / \sin \gamma \\
 c_z &= \sqrt{c^2 - c_x^2 - c_y^2}
 \end{aligned}$$



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
\mathbf{B}_1	$x_1 \mathbf{a}_1 + y_1 \mathbf{a}_2 + z_1 \mathbf{a}_3$	=	$(ax_1 + by_1 \cos \gamma + c_x z_1) \hat{\mathbf{x}} + (by_1 \sin \gamma + c_y z_1) \hat{\mathbf{y}} + c_z z_1 \hat{\mathbf{z}}$	(2i)	P I
\mathbf{B}_2	$-x_1 \mathbf{a}_1 - y_1 \mathbf{a}_2 - z_1 \mathbf{a}_3$	=	$-(ax_1 + by_1 \cos \gamma + c_x z_1) \hat{\mathbf{x}} - (by_1 \sin \gamma + c_y z_1) \hat{\mathbf{y}} - c_z z_1 \hat{\mathbf{z}}$	(2i)	P I
\mathbf{B}_3	$x_2 \mathbf{a}_1 + y_2 \mathbf{a}_2 + z_2 \mathbf{a}_3$	=	$(ax_2 + by_2 \cos \gamma + c_x z_2) \hat{\mathbf{x}} + (by_2 \sin \gamma + c_y z_2) \hat{\mathbf{y}} + c_z z_2 \hat{\mathbf{z}}$	(2i)	P II
\mathbf{B}_4	$-x_2 \mathbf{a}_1 - y_2 \mathbf{a}_2 - z_2 \mathbf{a}_3$	=	$-(ax_2 + by_2 \cos \gamma + c_x z_2) \hat{\mathbf{x}} - (by_2 \sin \gamma + c_y z_2) \hat{\mathbf{y}} - c_z z_2 \hat{\mathbf{z}}$	(2i)	P II
\mathbf{B}_5	$x_3 \mathbf{a}_1 + y_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$	=	$(ax_3 + by_3 \cos \gamma + c_x z_3) \hat{\mathbf{x}} + (by_3 \sin \gamma + c_y z_3) \hat{\mathbf{y}} + c_z z_3 \hat{\mathbf{z}}$	(2i)	P III
\mathbf{B}_6	$-x_3 \mathbf{a}_1 - y_3 \mathbf{a}_2 - z_3 \mathbf{a}_3$	=	$-(ax_3 + by_3 \cos \gamma + c_x z_3) \hat{\mathbf{x}} - (by_3 \sin \gamma + c_y z_3) \hat{\mathbf{y}} - c_z z_3 \hat{\mathbf{z}}$	(2i)	P III
\mathbf{B}_7	$x_4 \mathbf{a}_1 + y_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	=	$(ax_4 + by_4 \cos \gamma + c_x z_4) \hat{\mathbf{x}} + (by_4 \sin \gamma + c_y z_4) \hat{\mathbf{y}} + c_z z_4 \hat{\mathbf{z}}$	(2i)	P IV
\mathbf{B}_8	$-x_4 \mathbf{a}_1 - y_4 \mathbf{a}_2 - z_4 \mathbf{a}_3$	=	$-(ax_4 + by_4 \cos \gamma + c_x z_4) \hat{\mathbf{x}} - (by_4 \sin \gamma + c_y z_4) \hat{\mathbf{y}} - c_z z_4 \hat{\mathbf{z}}$	(2i)	P IV
\mathbf{B}_9	$x_5 \mathbf{a}_1 + y_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	=	$(ax_5 + by_5 \cos \gamma + c_x z_5) \hat{\mathbf{x}} + (by_5 \sin \gamma + c_y z_5) \hat{\mathbf{y}} + c_z z_5 \hat{\mathbf{z}}$	(2i)	P V
\mathbf{B}_{10}	$-x_5 \mathbf{a}_1 - y_5 \mathbf{a}_2 - z_5 \mathbf{a}_3$	=	$-(ax_5 + by_5 \cos \gamma + c_x z_5) \hat{\mathbf{x}} - (by_5 \sin \gamma + c_y z_5) \hat{\mathbf{y}} - c_z z_5 \hat{\mathbf{z}}$	(2i)	P V
\mathbf{B}_{11}	$x_6 \mathbf{a}_1 + y_6 \mathbf{a}_2 + z_6 \mathbf{a}_3$	=	$(ax_6 + by_6 \cos \gamma + c_x z_6) \hat{\mathbf{x}} + (by_6 \sin \gamma + c_y z_6) \hat{\mathbf{y}} + c_z z_6 \hat{\mathbf{z}}$	(2i)	P VI
\mathbf{B}_{12}	$-x_6 \mathbf{a}_1 - y_6 \mathbf{a}_2 - z_6 \mathbf{a}_3$	=	$-(ax_6 + by_6 \cos \gamma + c_x z_6) \hat{\mathbf{x}} - (by_6 \sin \gamma + c_y z_6) \hat{\mathbf{y}} - c_z z_6 \hat{\mathbf{z}}$	(2i)	P VI
\mathbf{B}_{13}	$x_7 \mathbf{a}_1 + y_7 \mathbf{a}_2 + z_7 \mathbf{a}_3$	=	$(ax_7 + by_7 \cos \gamma + c_x z_7) \hat{\mathbf{x}} + (by_7 \sin \gamma + c_y z_7) \hat{\mathbf{y}} + c_z z_7 \hat{\mathbf{z}}$	(2i)	P VII
\mathbf{B}_{14}	$-x_7 \mathbf{a}_1 - y_7 \mathbf{a}_2 - z_7 \mathbf{a}_3$	=	$-(ax_7 + by_7 \cos \gamma + c_x z_7) \hat{\mathbf{x}} - (by_7 \sin \gamma + c_y z_7) \hat{\mathbf{y}} - c_z z_7 \hat{\mathbf{z}}$	(2i)	P VII
\mathbf{B}_{15}	$x_8 \mathbf{a}_1 + y_8 \mathbf{a}_2 + z_8 \mathbf{a}_3$	=	$(ax_8 + by_8 \cos \gamma + c_x z_8) \hat{\mathbf{x}} + (by_8 \sin \gamma + c_y z_8) \hat{\mathbf{y}} + c_z z_8 \hat{\mathbf{z}}$	(2i)	P VIII

$$\begin{aligned}
\mathbf{B}_{16} &= -x_8 \mathbf{a}_1 - y_8 \mathbf{a}_2 - z_8 \mathbf{a}_3 &= & -(ax_8 + by_8 \cos \gamma + c_x z_8) \hat{\mathbf{x}} - & (2i) & \text{P VIII} \\
&&&& (by_8 \sin \gamma + c_y z_8) \hat{\mathbf{y}} - c_z z_8 \hat{\mathbf{z}} \\
\mathbf{B}_{17} &= x_9 \mathbf{a}_1 + y_9 \mathbf{a}_2 + z_9 \mathbf{a}_3 &= & (ax_9 + by_9 \cos \gamma + c_x z_9) \hat{\mathbf{x}} + & (2i) & \text{P IX} \\
&&&& (by_9 \sin \gamma + c_y z_9) \hat{\mathbf{y}} + c_z z_9 \hat{\mathbf{z}} \\
\mathbf{B}_{18} &= -x_9 \mathbf{a}_1 - y_9 \mathbf{a}_2 - z_9 \mathbf{a}_3 &= & -(ax_9 + by_9 \cos \gamma + c_x z_9) \hat{\mathbf{x}} - & (2i) & \text{P IX} \\
&&&& (by_9 \sin \gamma + c_y z_9) \hat{\mathbf{y}} - c_z z_9 \hat{\mathbf{z}} \\
\mathbf{B}_{19} &= x_{10} \mathbf{a}_1 + y_{10} \mathbf{a}_2 + z_{10} \mathbf{a}_3 &= & (ax_{10} + by_{10} \cos \gamma + c_x z_{10}) \hat{\mathbf{x}} + & (2i) & \text{P X} \\
&&&& (by_{10} \sin \gamma + c_y z_{10}) \hat{\mathbf{y}} + c_z z_{10} \hat{\mathbf{z}} \\
\mathbf{B}_{20} &= -x_{10} \mathbf{a}_1 - y_{10} \mathbf{a}_2 - z_{10} \mathbf{a}_3 &= & -(ax_{10} + by_{10} \cos \gamma + c_x z_{10}) \hat{\mathbf{x}} - & (2i) & \text{P X} \\
&&&& (by_{10} \sin \gamma + c_y z_{10}) \hat{\mathbf{y}} - c_z z_{10} \hat{\mathbf{z}} \\
\mathbf{B}_{21} &= x_{11} \mathbf{a}_1 + y_{11} \mathbf{a}_2 + z_{11} \mathbf{a}_3 &= & (ax_{11} + by_{11} \cos \gamma + c_x z_{11}) \hat{\mathbf{x}} + & (2i) & \text{P XI} \\
&&&& (by_{11} \sin \gamma + c_y z_{11}) \hat{\mathbf{y}} + c_z z_{11} \hat{\mathbf{z}} \\
\mathbf{B}_{22} &= -x_{11} \mathbf{a}_1 - y_{11} \mathbf{a}_2 - z_{11} \mathbf{a}_3 &= & -(ax_{11} + by_{11} \cos \gamma + c_x z_{11}) \hat{\mathbf{x}} - & (2i) & \text{P XI} \\
&&&& (by_{11} \sin \gamma + c_y z_{11}) \hat{\mathbf{y}} - c_z z_{11} \hat{\mathbf{z}} \\
\mathbf{B}_{23} &= x_{12} \mathbf{a}_1 + y_{12} \mathbf{a}_2 + z_{12} \mathbf{a}_3 &= & (ax_{12} + by_{12} \cos \gamma + c_x z_{12}) \hat{\mathbf{x}} + & (2i) & \text{P XII} \\
&&&& (by_{12} \sin \gamma + c_y z_{12}) \hat{\mathbf{y}} + c_z z_{12} \hat{\mathbf{z}} \\
\mathbf{B}_{24} &= -x_{12} \mathbf{a}_1 - y_{12} \mathbf{a}_2 - z_{12} \mathbf{a}_3 &= & -(ax_{12} + by_{12} \cos \gamma + c_x z_{12}) \hat{\mathbf{x}} - & (2i) & \text{P XII} \\
&&&& (by_{12} \sin \gamma + c_y z_{12}) \hat{\mathbf{y}} - c_z z_{12} \hat{\mathbf{z}}
\end{aligned}$$

References

- [1] A. Simon, H. Borrmann, and H. Craubner, *Crystal Structure of Ordered White Phosphorus (β -P)*, Phosphorus and Sulfur **30**, 507–510 (1987), doi:10.1080/03086648708080631.
- [2] J. Donohue, *The Structures of the Elements* (Robert E. Krieger Publishing Company, Malabar, Florida, 1982). Reprint of the 1974 John Wiley & Sons edition.