BPO_4 ($H0_7$) Structure: AB4C_tI12_82_c_g_a-001

This structure previously used the label(s) `AB4C_tI12_82_c_g_a`. Calls to these addresses will be redirected here.

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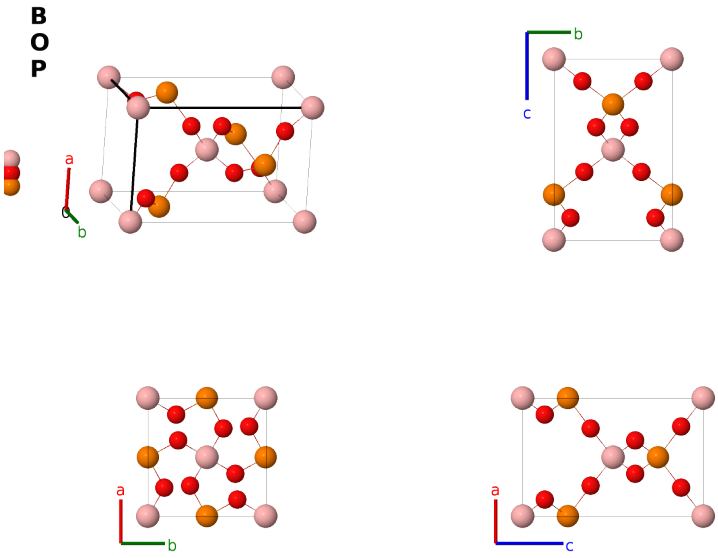
https://aflow.org/prototype-encyclopedia/C601

https://aflow.org/prototype-encyclopedia/AB4C_tI12_82_c_g_a-001

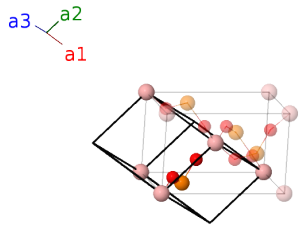


Prototype	BO_4P
AFLOW prototype label	AB4C_tI12_82_c_g_a-001
***Strukturbericht* designation**	$H0_7$
ICSD	55082
CCDC	1619417
Pearson symbol	tI12
Space group number	82
Space group symbol	$I\bar{4}$
AFLOW prototype command	`aflow --proto=AB4C_tI12_82_c_g_a-001 --params=`$a, c/a, x_3, y_3, z_3$

Other compounds with this structure
$AlAsO_4$, $BAsO_4$, $BLiF_4$, $BeSO_4$, NPO_4

Body-centered Tetragonal primitive vectors

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



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	0	=	0	(2a)	B I
$\mathbf{B_2}$	=	$\frac{3}{4}\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(2c)	P I
$\mathbf{B_3}$	=	$(y_3 + z_3)\,\mathbf{a}_1 + (x_3 + z_3)\,\mathbf{a}_2 + (x_3 + y_3)\,\mathbf{a}_3$	=	$ax_3\,\hat{\mathbf{x}} + ay_3\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$	(8g)	O I
$\mathbf{B_4}$	=	$-(y_3 - z_3)\,\mathbf{a}_1 - (x_3 - z_3)\,\mathbf{a}_2 - (x_3 + y_3)\,\mathbf{a}_3$	=	$-ax_3\,\hat{\mathbf{x}} - ay_3\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$	(8g)	O I
$\mathbf{B_5}$	=	$-(x_3 + z_3)\,\mathbf{a}_1 + (y_3 - z_3)\,\mathbf{a}_2 - (x_3 - y_3)\,\mathbf{a}_3$	=	$ay_3\,\hat{\mathbf{x}} - ax_3\,\hat{\mathbf{y}} - cz_3\,\hat{\mathbf{z}}$	(8g)	O I
$\mathbf{B_6}$	=	$(x_3 - z_3)\,\mathbf{a}_1 - (y_3 + z_3)\,\mathbf{a}_2 + (x_3 - y_3)\,\mathbf{a}_3$	=	$-ay_3\,\hat{\mathbf{x}} + ax_3\,\hat{\mathbf{y}} - cz_3\,\hat{\mathbf{z}}$	(8g)	O I

References

[1] M. Schmidt, B. Ewald, Y. Prots, R. Cardoso-Gil, M. Armbrüster, I. Loa, L. Zhang, Y.-X. Huang, U. Schwarz, and R. Kniep, *Growth and Characterization of BPO_4 Single Crystals*, Z. Anorganische und Allgemeine Chemie **630**, 655–662 (2004), doi:10.1002/zaac.200400002.

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