UB_{12} ($D2_f$) Structure: A12B_cF52_225_h_b-001

This structure originally had the label `A12B_cF52_225_i_a`. Calls to that address will be redirected here.

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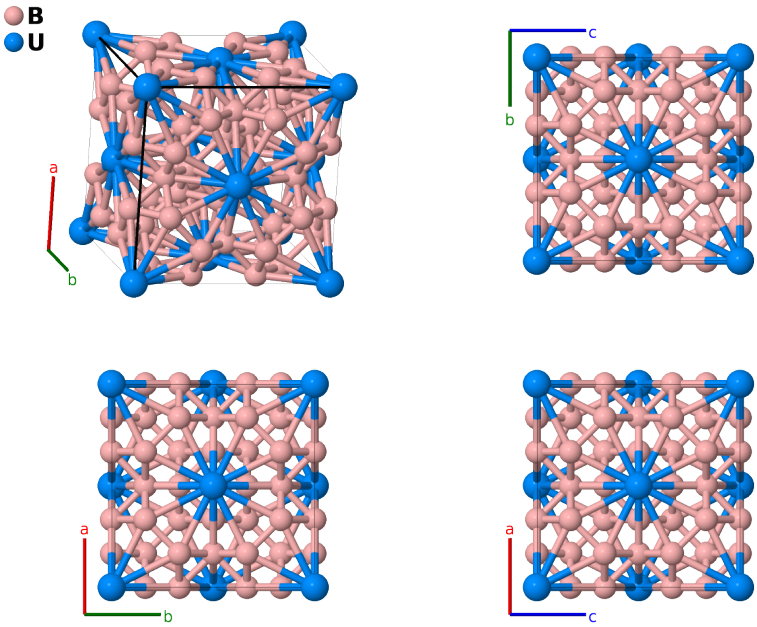
https://aflow.org/p/JTKK

https://aflow.org/p/A12B_cF52_225_h_b-001



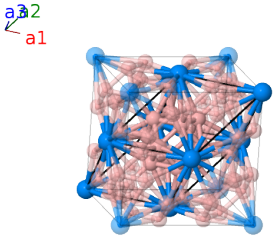
Prototype	$B_{12}U$
AFLOW prototype label	A12B_cF52_225_h_b-001
***Strukturbericht* designation**	$D2_f$
ICSD	24705
Pearson symbol	cF52
Space group number	225
Space group symbol	$Fm\bar{3}m$
AFLOW prototype command	`aflow --proto=A12B_cF52_225_h_b-001 --params=`a, y_2

Other compounds with this structure

DyB_{12}, ErB_{12}, LuB_{12}, ThB_{12}, TmB_{12}, YB_{12}, YbB_{12}, ZrB_{12}, $(Th_{0.93}Zr_{0.07})B_{12}$

Face-centered Cubic primitive vectors

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



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{y}} + \frac{1}{2}a\,\hat{\mathbf{z}}$	(4b)	U I
$\mathbf{B_2}$	=	$2y_2\,\mathbf{a}_1$	=	$ay_2\,\hat{\mathbf{y}} + ay_2\,\hat{\mathbf{z}}$	(48h)	B I
$\mathbf{B_3}$	=	$2y_2\,\mathbf{a}_2 - 2y_2\,\mathbf{a}_3$	=	$-ay_2\,\hat{\mathbf{y}} + ay_2\,\hat{\mathbf{z}}$	(48h)	B I
$\mathbf{B_4}$	=	$-2y_2\,\mathbf{a}_2 + 2y_2\,\mathbf{a}_3$	=	$ay_2\,\hat{\mathbf{y}} - ay_2\,\hat{\mathbf{z}}$	(48h)	B I
$\mathbf{B_5}$	=	$-2y_2\,\mathbf{a}_1$	=	$-ay_2\,\hat{\mathbf{y}} - ay_2\,\hat{\mathbf{z}}$	(48h)	B I
$\mathbf{B_6}$	=	$2y_2\,\mathbf{a}_2$	=	$ay_2\,\hat{\mathbf{x}} + ay_2\,\hat{\mathbf{z}}$	(48h)	B I
$\mathbf{B_7}$	=	$-2y_2\,\mathbf{a}_1 + 2y_2\,\mathbf{a}_3$	=	$ay_2\,\hat{\mathbf{x}} - ay_2\,\hat{\mathbf{z}}$	(48h)	B I
$\mathbf{B_8}$	=	$2y_2\,\mathbf{a}_1 - 2y_2\,\mathbf{a}_3$	=	$-ay_2\,\hat{\mathbf{x}} + ay_2\,\hat{\mathbf{z}}$	(48h)	B I
$\mathbf{B_9}$	=	$-2y_2\,\mathbf{a}_2$	=	$-ay_2\,\hat{\mathbf{x}} - ay_2\,\hat{\mathbf{z}}$	(48h)	B I
$\mathbf{B_{10}}$	=	$2y_2\,\mathbf{a}_3$	=	$ay_2\,\hat{\mathbf{x}} + ay_2\,\hat{\mathbf{y}}$	(48h)	B I
$\mathbf{B_{11}}$	=	$2y_2\,\mathbf{a}_1 - 2y_2\,\mathbf{a}_2$	=	$-ay_2\,\hat{\mathbf{x}} + ay_2\,\hat{\mathbf{y}}$	(48h)	B I
$\mathbf{B_{12}}$	=	$-2y_2\,\mathbf{a}_1 + 2y_2\,\mathbf{a}_2$	=	$ay_2\,\hat{\mathbf{x}} - ay_2\,\hat{\mathbf{y}}$	(48h)	B I
$\mathbf{B_{13}}$	=	$-2y_2\,\mathbf{a}_3$	=	$-ay_2\,\hat{\mathbf{x}} - ay_2\,\hat{\mathbf{y}}$	(48h)	B I

References

[1] P. Blum and F. Bertaut, *Contribution à l'Étude des Borures à Teneur Élevée en Bore*, Acta Cryst. **7**, 81–86 (1954), doi:10.1107/S0365110X54000151.

Found in

[1] W. B. Pearson, *The Crystal Chemistry and Physics of Metals and Alloys* (Wiley Interscience, New York, London, Sydney, Tornoto, 1972).