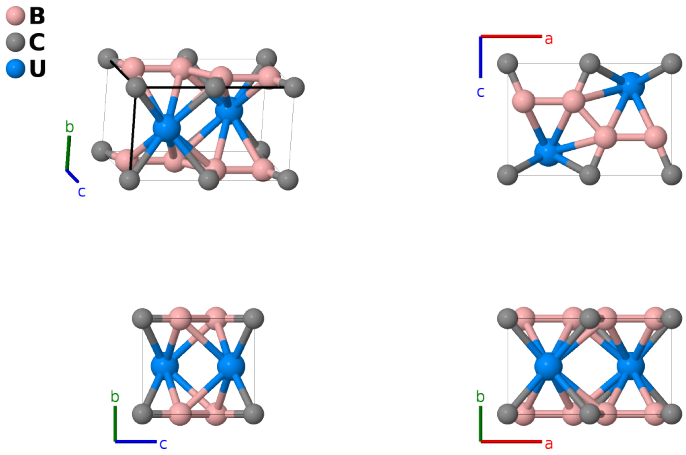
α-UB_2C Structure: A2BC_oP8_51_i_a_f-001

Cite this page as: H. Eckert, S. Divilov, A. Zettel, M. J. Mehl, D. Hicks, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 4*. In preparation.

https://aflow.org/p/DRSV

https://aflow.org/p/A2BC_oP8_51_i_a_f-001

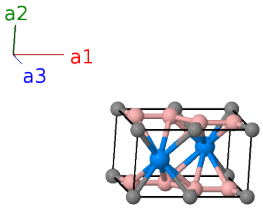


Prototype	BCU_2
AFLOW prototype label	A2BC_oP8_51_i_a_f-001
ICSD	69767
Pearson symbol	oP8
Space group number	51
Space group symbol	*Pmma*
AFLOW prototype command	`aflow --proto=A2BC_oP8_51_i_a_f-001 --params=`$a, b/a, c/a, z_2, x_3, z_3$

- This is the ground state of UB_2C, stable up to 1675°C. Above that temperature it transforms to rhombohedral β-UB_2C with the ThB_2C structure. (Rogl, 1991)
- We use the data taken at 29K.
- The origin has been shifted to put the carbon atoms on the (2a) site.

Simple Orthorhombic primitive vectors

$$\mathbf{a_1} = a\,\hat{\mathbf{x}}$$
$$\mathbf{a_2} = b\,\hat{\mathbf{y}}$$
$$\mathbf{a_3} = c\,\hat{\mathbf{z}}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	0	=	0	(2a)	C I
$\mathbf{B_2}$	=	$\frac{1}{2}\,\mathbf{a}_1$	=	$\frac{1}{2}a\,\hat{\mathbf{x}}$	(2a)	C I
$\mathbf{B_3}$	=	$\frac{1}{4}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 + z_2\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + \frac{1}{2}b\,\hat{\mathbf{y}} + cz_2\,\hat{\mathbf{z}}$	(2f)	U I
$\mathbf{B_4}$	=	$\frac{3}{4}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 - z_2\,\mathbf{a}_3$	=	$\frac{3}{4}a\,\hat{\mathbf{x}} + \frac{1}{2}b\,\hat{\mathbf{y}} - cz_2\,\hat{\mathbf{z}}$	(2f)	U I
$\mathbf{B_5}$	=	$x_3\,\mathbf{a}_1 + z_3\,\mathbf{a}_3$	=	$ax_3\,\hat{\mathbf{x}} + cz_3\,\hat{\mathbf{z}}$	(4i)	B I
$\mathbf{B_6}$	=	$-\left(x_3 - \frac{1}{2}\right)\,\mathbf{a}_1 + z_3\,\mathbf{a}_3$	=	$-a\left(x_3 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + cz_3\,\hat{\mathbf{z}}$	(4i)	B I
$\mathbf{B_7}$	=	$-x_3\,\mathbf{a}_1 - z_3\,\mathbf{a}_3$	=	$-ax_3\,\hat{\mathbf{x}} - cz_3\,\hat{\mathbf{z}}$	(4i)	B I
$\mathbf{B_8}$	=	$\left(x_3 + \frac{1}{2}\right)\,\mathbf{a}_1 - z_3\,\mathbf{a}_3$	=	$a\left(x_3 + \frac{1}{2}\right)\,\hat{\mathbf{x}} - cz_3\,\hat{\mathbf{z}}$	(4i)	B I

References

[1] P. Rogl and P. Fischer, *Powder neutron diffraction of $\alpha\,UB_2C$ ($\alpha\,UB_2C$-type)*, J. Solid State Chem. **90**, 285–290 (1991), doi:10.1016/0022-4596(91)90144-7.