

α -UB₂C Structure:

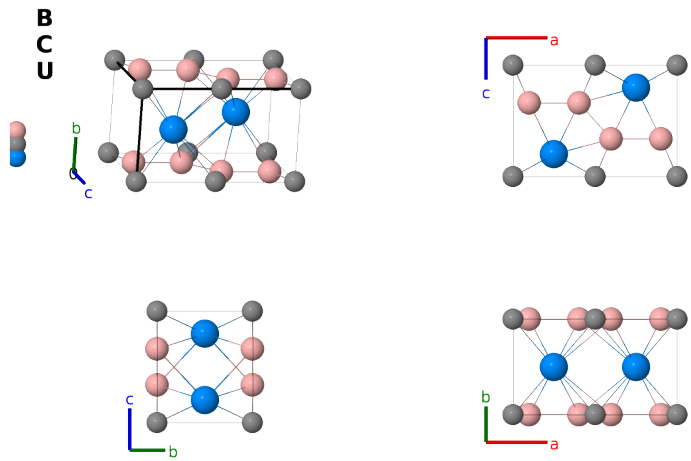
A2BC_oP8_51_i_a_f-001

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<https://aflow.org/prototype-encyclopedia/DRSV>

https://aflow.org/prototype-encyclopedia/A2BC_oP8_51_i_a_f-001



Prototype	BCU ₂
AFLOW prototype label	A2BC_oP8_51_i_a_f-001
ICSD	69767
CCDC	1631617
Pearson symbol	oP8
Space group number	51
Space group symbol	<i>Pmma</i>
AFLOW prototype command	<code>aflow --proto=A2BC_oP8_51_i_a_f-001</code> <code>--params=a, b/a, c/a, z₂, x₃, z₃</code>

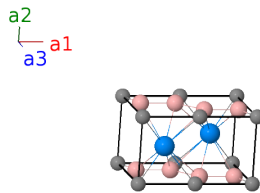
- This is the ground state of UB₂C, stable up to 1675°C. Above that temperature it transforms to rhombohedral β -UB₂C with the ThB₂C structure. (Rogl, 1991)
- We use the data taken at 29K.
- The origin has been shifted to put the carbon atoms on the (2a) site.

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
$\mathbf{B}_6$	$=$	$-(x_3 - \frac{1}{2}) \mathbf{a}_1 + z_3 \mathbf{a}_3$	$=$	$-a(x_3 - \frac{1}{2}) \hat{\mathbf{x}} + cz_3 \hat{\mathbf{z}}$	$(4i)$ 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
$\mathbf{B}_8$	$=$	$(x_3 + \frac{1}{2}) \mathbf{a}_1 - z_3 \mathbf{a}_3$	$=$	$a(x_3 + \frac{1}{2}) \hat{\mathbf{x}} - cz_3 \hat{\mathbf{z}}$	$(4i)$ B I

References

- [1] P. Rogl and P. Fischer, *Powder neutron diffraction of αUB_2C (αUB_2C -type)*, J. Solid State Chem. **90**, 285–290 (1991), doi:10.1016/0022-4596(91)90144-7.

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