UBC Structure: ABC_oC12_63_c_c_c-004

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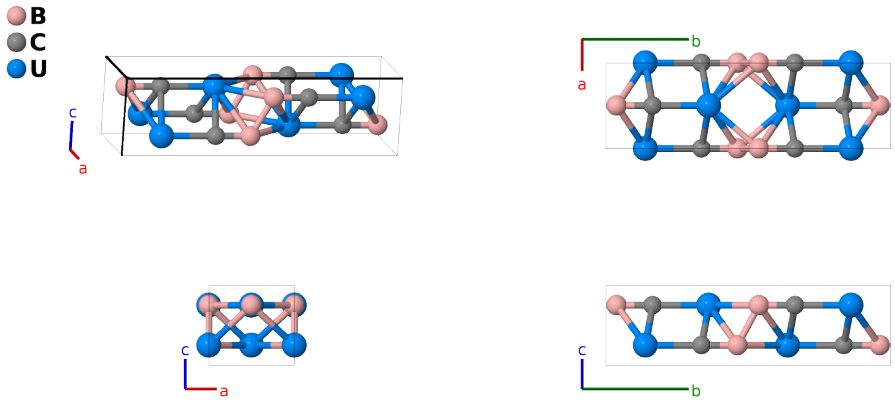
https://aflow.org/p/NQGP

https://aflow.org/p/ABC_oC12_63_c_c_c-004

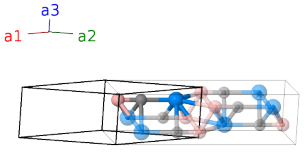


Prototype	BCU
AFLOW prototype label	ABC_oC12_63_c_c_c-004
ICSD	73828
Pearson symbol	oC12
Space group number	63
Space group symbol	$Cmcm$
AFLOW prototype command	`aflow --proto=ABC_oC12_63_c_c_c-004 --params=`$a, b/a, c/a, y_1, y_2, y_3$

- (Rogl, 1993) found that excess carbon could replace boron, and that some uranium atoms could be replaced by scandium, lutetium, or thorium.
- See the note on the MoAlB structure page concerning the relationship between this structure and other structures with the ABC_oC12_63_c_c_c label.

Base-centered Orthorhombic primitive vectors

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



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$-y_1\,\mathbf{a}_1 + y_1\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$by_1\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(4c)	B I
$\mathbf{B_2}$	=	$y_1\,\mathbf{a}_1 - y_1\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$-by_1\,\hat{\mathbf{y}} + \frac{3}{4}c\,\hat{\mathbf{z}}$	(4c)	B I
$\mathbf{B_3}$	=	$-y_2\,\mathbf{a}_1 + y_2\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$by_2\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(4c)	C I
$\mathbf{B_4}$	=	$y_2\,\mathbf{a}_1 - y_2\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$-by_2\,\hat{\mathbf{y}} + \frac{3}{4}c\,\hat{\mathbf{z}}$	(4c)	C I
$\mathbf{B_5}$	=	$-y_3\,\mathbf{a}_1 + y_3\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$by_3\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(4c)	U I
$\mathbf{B_6}$	=	$y_3\,\mathbf{a}_1 - y_3\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$-by_3\,\hat{\mathbf{y}} + \frac{3}{4}c\,\hat{\mathbf{z}}$	(4c)	U I

References

[1] P. Rogl, B. Rupp, I. Felner, and P. Fischer, *Crystal Chemistry and Magnetism of Ternary Actinoid Boron Carbides $UB_{1-x}C_{1+x}$ and $U_{1-x}M_xB_2C$ with M = Sc, Lu, and Th*, J. Solid State Chem. **104**, 377–390 (1993), doi:10.1006/jssc.1993.1173.

Found in

[1] ICSD, *Inorganic Crystal Structure Database*. ID 73828.