Tungsten Carbide (WC, B_h) Structure: AB_hP2_187_a_d-001

This structure previously used the label(s) `AB_hP2_187_d_a`. Calls to these addresses will be redirected here.

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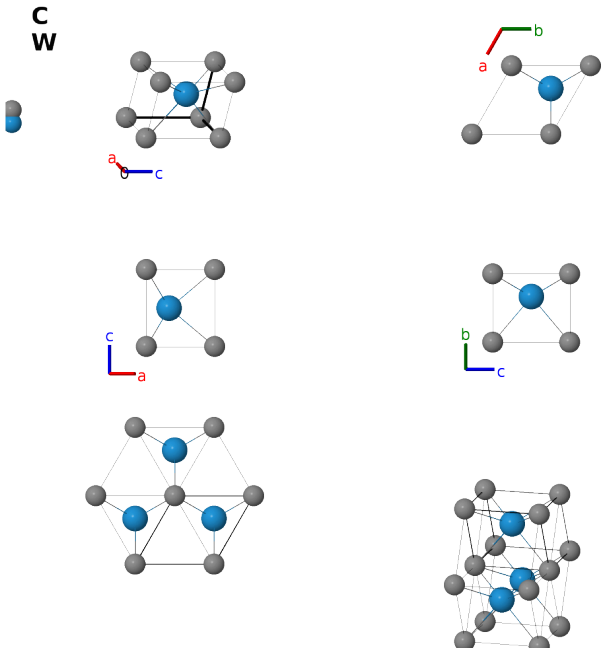
https://aflow.org/prototype-encyclopedia/X4K0

https://aflow.org/prototype-encyclopedia/AB_hP2_187_a_d-001



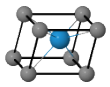
Prototype	CW
AFLOW prototype label	AB_hP2_187_a_d-001
***Strukturbericht* designation**	B_h
ICSD	15406
CCDC	1596158
Pearson symbol	hP2
Space group number	187
Space group symbol	$P\bar{6}m2$
AFLOW prototype command	`aflow --proto=AB_hP2_187_a_d-001 --params=`$a, c/a$

Other compounds with this structure

AgN, AlSn, AuC, BIr, CdN, CrAs, CrC, CrN, HfC, HfS, HfSe, HfTe, IrB, IrC, IrN, LaC, MoC, MoN, MoP, NbC, NbN, NbS, OsB, OsC, PbS, PdN, PrN, PtC, ReB, ReC, ReN, RhN, RuC, RuN, TaAs, TaC, TaN, TaS, TcB, TcN, TeZr, TiO, TiS, TiSe, TiTe, VN, WC, WN, YN, ZrN, ZrS, ZrSe, ZrTe

Hexagonal primitive vectors

$$\mathbf{a_1} = \frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a\,\hat{\mathbf{y}}$$
$$\mathbf{a_2} = \frac{1}{2}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a\,\hat{\mathbf{y}}$$
$$\mathbf{a_3} = c\,\hat{\mathbf{z}}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	0	=	0	(1a)	C I
$\mathbf{B_2}$	=	$\frac{1}{3}\,\mathbf{a}_1 + \frac{2}{3}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(1d)	W I

References

[1] J. Leciejewicz, *A note on the structure of tungsten carbide*, Acta Cryst. **14**, 200 (1961), doi:10.1107/S0365110X6100067X.

Found in

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

First cited in

M. J. Mehl, D. Hicks, C. Toher, O. Levy, R. M. Hanson, G. L. W. Hart, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 1*, Comput. Mater. Sci. **136**, S1-828 (2017). doi: 10.1016/j.commatsci.2017.01.017