Hexagonal ω ($C32$) Structure: AB2_hP3_191_a_d-001

This structure originally had the label `AB2_hP3_191_a_d`. Calls to that address will be redirected here.

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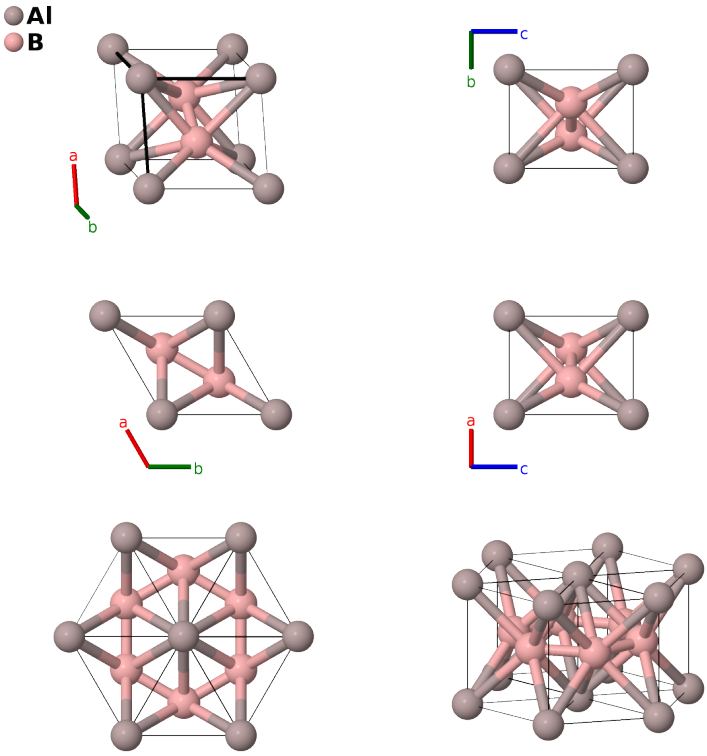
https://aflow.org/p/75K4

https://aflow.org/p/AB2_hP3_191_a_d-001



Prototype	AlB_2
AFLOW prototype label	AB2_hP3_191_a_d-001
***Strukturbericht* designation**	$C32$
Mineral name	ω-phase
ICSD	99639
Pearson symbol	hP3
Space group number	191
Space group symbol	$P6/mmm$
AFLOW prototype command	`aflow --proto=AB2_hP3_191_a_d-001 --params=`$a, c/a$

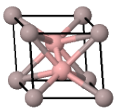
Other compounds with this structure

AgB_2, AuB_2, $BaGa_2$, $BaSi_2$, Be_2Hf, Be_2Zr, $CaGa_2$, CrB_2, $DyGa_2$, ErB_2, $ErGa_2$, $EuGa_2$, $GdGa_2$, HfB_2, $HgLa_2$, HoB_2, $HoGa_2$, $LaCu_2$, $LaGa_2$, LuB_2, MgB_2, MnB_2, MoB_2, $NaHg_2$, NbB_2, $NdGa_2$, OsB_2, $PrGa_2$, PuB_2, PuB_2, RuB_2, ScB_2, $SmGa_2$, $SrGa_2$, TaB_2, TbB_2, $TbGa_2$, $ThAg_2$, $ThAl_2$, $ThCd_2$, $ThCu_2$, $ThNi_2$, $ThZn_2$, $TiU2_2$, TlB_2, UB_2, β-UGa_2, UHg_2, USi_2, UZr_2, VB_2, YGa_2, ZrB_2

- This is the hexagonal ω phase. There is also a trigonal ω (C6) phase. For more details about the ω phase and materials which form in the ω phase see (Sikka, 1982).
- Many ω phase intermetallic alloys are disordered, we list some of the ordered structures here.
- In this structure the B-B distance is smaller than the Al-B distance for every c/a ratio.
- If c/a is small enough the structure looks like a set of inter-penetrating boron triangular planes and aluminium chains.
- If $c/a = 1/\sqrt{3}$ the Al-Al distance along (001) is the same as the B-B distance in the plane, and the B-B distance in the (001) direction. This value 0.577 is close to the value $\sqrt{3/8}\,(\approx 0.612)$ where the trigonal ω phase can transform to the body-centered cubic (A2) lattice, which probably explains the close connection between the ω and bcc phases.
- In the current sample (Burkhardt, 2004) the aluminum (1a) site has 10% vacancies.

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)	Al I
$\mathbf{B_2}$	=	$\frac{1}{3}\,\mathbf{a}_1 + \frac{2}{3}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(2d)	B I
$\mathbf{B_3}$	=	$\frac{2}{3}\,\mathbf{a}_1 + \frac{1}{3}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(2d)	B I

References

[1] U. Burkhardt, V. Gurin, F. Haarmann, H. Borrmann, and W. Schnelle, *On the electronic and structural properties of aluminum diboride $Al_{0.9}B_2$*, J. Solid State Chem. **177**, 389–394 (2004), doi:10.1016/j.jssc.2002.12.001.

Found in

[1] S. K. Sikka, Y. K. Vohra, and R. Chidambaram, *Omega Phase in Materials*, Prog. Mater. Sci. **27**, 245–310 (1982), doi:10.1016/0079-6425(82)90002-0.