

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

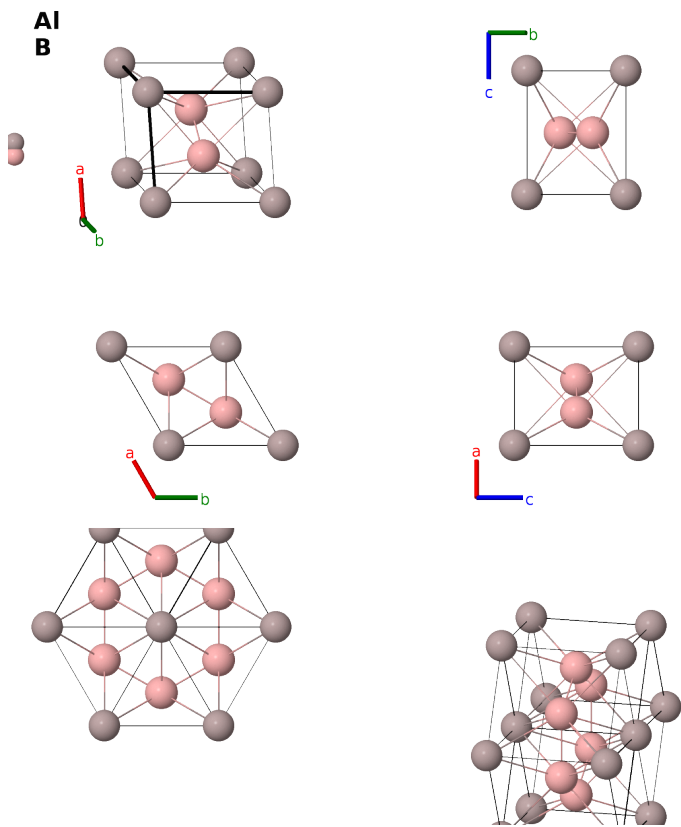
This structure previously used the label(s) **AB2_hP3_191_a_d**. Calls to these addresses will be redirected here.

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<https://aflow.org/prototype-encyclopedia/75K4>

https://aflow.org/prototype-encyclopedia/AB2_hP3_191_a_d-001



Prototype	AlB ₂
AFLOW prototype label	AB2_hP3_191_a_d-001
<i>Strukturbericht</i> designation	C32
Mineral name	ω -phase
ICSD	99639
CCDC	1658856
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

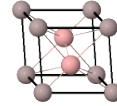
AgB₂, AuB₂, BaGa₂, BaSi₂, Be₂Hf, Be₂Zr, CaGa₂, CrB₂, DyGa₂, ErB₂, ErGa₂, EuGa₂, GdGa₂, HfB₂, HgLa₂, HoB₂, HoGa₂, LaCu₂, LaGa₂, LuB₂, MgB₂, MnB₂, MoB₂, NaHg₂, NbB₂, NdGa₂, OsB₂, PrGa₂, PuB₂, PuB₂, RuB₂, ScB₂, SmGa₂, SrGa₂, TaB₂, TbB₂, TbGa₂, ThAg₂, ThAl₂, ThCd₂, ThCu₂, ThNi₂, ThZn₂, TiU₂, TlB₂, UB₂, β -UGa₂, UHg₂, USi₂, UZr₂, VB₂, YGa₂, ZrB₂

- 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

$$\begin{aligned}\mathbf{a}_1 &= \frac{1}{2}a\hat{x} - \frac{\sqrt{3}}{2}a\hat{y} \\ \mathbf{a}_2 &= \frac{1}{2}a\hat{x} + \frac{\sqrt{3}}{2}a\hat{y} \\ \mathbf{a}_3 &= c\hat{z}\end{aligned}$$

$\mathbf{a}_1$
 $\mathbf{a}_2$
 $\mathbf{a}_3$



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	=	0	=	0	(1a) Al I
$\mathbf{B}_2$	=	$\frac{1}{3}\mathbf{a}_1 + \frac{2}{3}\mathbf{a}_2 + \frac{1}{2}\mathbf{a}_3$	=	$\frac{1}{2}a\hat{x} + \frac{\sqrt{3}}{6}a\hat{y} + \frac{1}{2}c\hat{z}$	(2d) B I
$\mathbf{B}_3$	=	$\frac{2}{3}\mathbf{a}_1 + \frac{1}{3}\mathbf{a}_2 + \frac{1}{2}\mathbf{a}_3$	=	$\frac{1}{2}a\hat{x} - \frac{\sqrt{3}}{6}a\hat{y} + \frac{1}{2}c\hat{z}$	(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}B₂*, 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.

First cited in

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