

# Gd<sub>3</sub>Al<sub>2</sub> Structure:

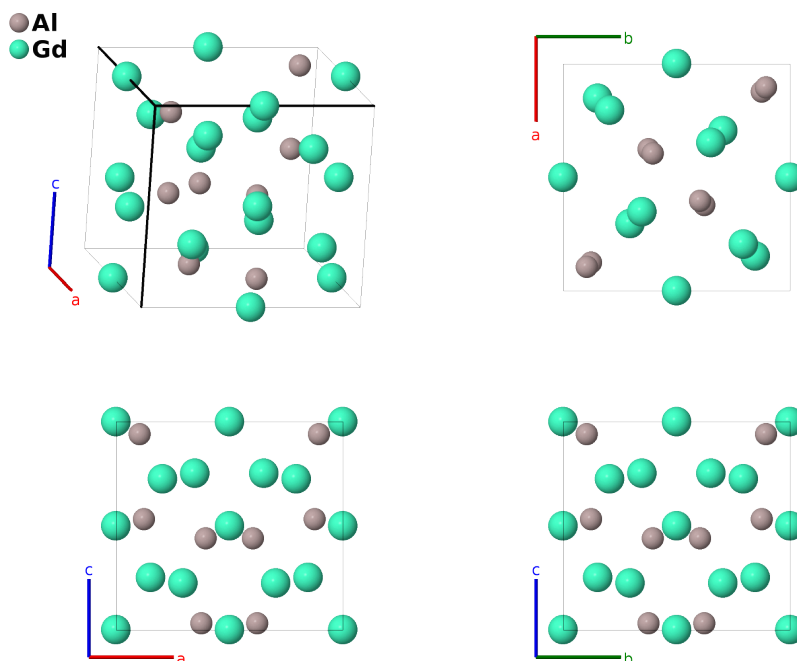
## A2B3\_tP20\_102\_2c\_b2c-001

This structure originally had the label **A2B3\_tP20\_102.2c.b2c**. Calls to that address will be redirected here.

Cite this page as: D. Hicks, M. J. Mehl, E. Gossett, C. Toher, O. Levy, R. M. Hanson, G. Hart, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 2*, Comput. Mater. Sci. **161**, S1 (2019). doi: 10.1016/j.commatsci.2018.10.043

<https://aflow.org/p/AY9W>

[https://aflow.org/p/A2B3\\_tP20\\_102\\_2c\\_b2c-001](https://aflow.org/p/A2B3_tP20_102_2c_b2c-001)



Prototype	Al <sub>2</sub> Gd <sub>3</sub>
AFLOW prototype label	A2B3_tP20_102.2c.b2c-001
ICSD	57869
Pearson symbol	tP20
Space group number	102
Space group symbol	$P4_2nm$
AFLOW prototype command	<code>aflow --proto=A2B3_tP20_102_2c_b2c-001 --params=a, c/a, z<sub>1</sub>, x<sub>2</sub>, z<sub>2</sub>, x<sub>3</sub>, z<sub>3</sub>, x<sub>4</sub>, z<sub>4</sub>, x<sub>5</sub>, z<sub>5</sub></code>

### Other compounds with this structure

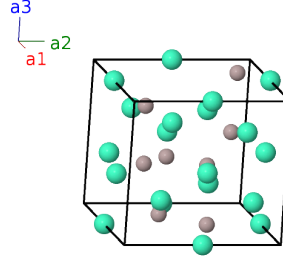
Dy<sub>3</sub>Al<sub>2</sub>, Er<sub>3</sub>Al<sub>2</sub>, Ho<sub>3</sub>Al<sub>2</sub>, Tb<sub>3</sub>Al<sub>2</sub>, Y<sub>3</sub>Al<sub>2</sub>, Zr<sub>3</sub>Al<sub>2</sub>

- We have added the reference to (Baenziger, 1964), which has the description of this structure.
- Space group  $P4_2nm$  #102 allows an arbitrary placement of the origin of the  $z$ -axis. We choose this so that  $z_1 = 1/2$  for the Gd-I atom. This represents a shift of  $0.017c$  from the origin of (Baenziger, 1964).

- (Buschow, 1965) says that the prototype for this structure is  $Zr_3Al_2$ , but note that there is a competing  $Zr_3Al_2$  structure in in the centrosymmetric space group  $P4_2/mnm$  #136.

### Simple Tetragonal primitive vectors

$$\begin{aligned} \mathbf{a}_1 &= a \hat{\mathbf{x}} \\ \mathbf{a}_2 &= a \hat{\mathbf{y}} \\ \mathbf{a}_3 &= c \hat{\mathbf{z}} \end{aligned}$$



### Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$= \frac{1}{2} \mathbf{a}_2 + z_1 \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{y}} + cz_1 \hat{\mathbf{z}}$	(4b)	Gd I
$\mathbf{B}_2$	$= \frac{1}{2} \mathbf{a}_2 + (z_1 + \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{y}} + c(z_1 + \frac{1}{2}) \hat{\mathbf{z}}$	(4b)	Gd I
$\mathbf{B}_3$	$= \frac{1}{2} \mathbf{a}_1 + (z_1 + \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + c(z_1 + \frac{1}{2}) \hat{\mathbf{z}}$	(4b)	Gd I
$\mathbf{B}_4$	$= \frac{1}{2} \mathbf{a}_1 + z_1 \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + cz_1 \hat{\mathbf{z}}$	(4b)	Gd I
$\mathbf{B}_5$	$= x_2 \mathbf{a}_1 + x_2 \mathbf{a}_2 + z_2 \mathbf{a}_3$	$=$	$ax_2 \hat{\mathbf{x}} + ax_2 \hat{\mathbf{y}} + cz_2 \hat{\mathbf{z}}$	(4c)	Al I
$\mathbf{B}_6$	$= -x_2 \mathbf{a}_1 - x_2 \mathbf{a}_2 + z_2 \mathbf{a}_3$	$=$	$-ax_2 \hat{\mathbf{x}} - ax_2 \hat{\mathbf{y}} + cz_2 \hat{\mathbf{z}}$	(4c)	Al I
$\mathbf{B}_7$	$= -(x_2 - \frac{1}{2}) \mathbf{a}_1 + (x_2 + \frac{1}{2}) \mathbf{a}_2 + (z_2 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-a(x_2 - \frac{1}{2}) \hat{\mathbf{x}} + a(x_2 + \frac{1}{2}) \hat{\mathbf{y}} + c(z_2 + \frac{1}{2}) \hat{\mathbf{z}}$	(4c)	Al I
$\mathbf{B}_8$	$= (x_2 + \frac{1}{2}) \mathbf{a}_1 - (x_2 - \frac{1}{2}) \mathbf{a}_2 + (z_2 + \frac{1}{2}) \mathbf{a}_3$	$=$	$a(x_2 + \frac{1}{2}) \hat{\mathbf{x}} - a(x_2 - \frac{1}{2}) \hat{\mathbf{y}} + c(z_2 + \frac{1}{2}) \hat{\mathbf{z}}$	(4c)	Al I
$\mathbf{B}_9$	$= x_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$ax_3 \hat{\mathbf{x}} + ax_3 \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}}$	(4c)	Al II
$\mathbf{B}_{10}$	$= -x_3 \mathbf{a}_1 - x_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$-ax_3 \hat{\mathbf{x}} - ax_3 \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}}$	(4c)	Al II
$\mathbf{B}_{11}$	$= -(x_3 - \frac{1}{2}) \mathbf{a}_1 + (x_3 + \frac{1}{2}) \mathbf{a}_2 + (z_3 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-a(x_3 - \frac{1}{2}) \hat{\mathbf{x}} + a(x_3 + \frac{1}{2}) \hat{\mathbf{y}} + c(z_3 + \frac{1}{2}) \hat{\mathbf{z}}$	(4c)	Al II
$\mathbf{B}_{12}$	$= (x_3 + \frac{1}{2}) \mathbf{a}_1 - (x_3 - \frac{1}{2}) \mathbf{a}_2 + (z_3 + \frac{1}{2}) \mathbf{a}_3$	$=$	$a(x_3 + \frac{1}{2}) \hat{\mathbf{x}} - a(x_3 - \frac{1}{2}) \hat{\mathbf{y}} + c(z_3 + \frac{1}{2}) \hat{\mathbf{z}}$	(4c)	Al II
$\mathbf{B}_{13}$	$= x_4 \mathbf{a}_1 + x_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$ax_4 \hat{\mathbf{x}} + ax_4 \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}}$	(4c)	Gd II
$\mathbf{B}_{14}$	$= -x_4 \mathbf{a}_1 - x_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$-ax_4 \hat{\mathbf{x}} - ax_4 \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}}$	(4c)	Gd II
$\mathbf{B}_{15}$	$= -(x_4 - \frac{1}{2}) \mathbf{a}_1 + (x_4 + \frac{1}{2}) \mathbf{a}_2 + (z_4 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-a(x_4 - \frac{1}{2}) \hat{\mathbf{x}} + a(x_4 + \frac{1}{2}) \hat{\mathbf{y}} + c(z_4 + \frac{1}{2}) \hat{\mathbf{z}}$	(4c)	Gd II
$\mathbf{B}_{16}$	$= (x_4 + \frac{1}{2}) \mathbf{a}_1 - (x_4 - \frac{1}{2}) \mathbf{a}_2 + (z_4 + \frac{1}{2}) \mathbf{a}_3$	$=$	$a(x_4 + \frac{1}{2}) \hat{\mathbf{x}} - a(x_4 - \frac{1}{2}) \hat{\mathbf{y}} + c(z_4 + \frac{1}{2}) \hat{\mathbf{z}}$	(4c)	Gd II
$\mathbf{B}_{17}$	$= x_5 \mathbf{a}_1 + x_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$ax_5 \hat{\mathbf{x}} + ax_5 \hat{\mathbf{y}} + cz_5 \hat{\mathbf{z}}$	(4c)	Gd III
$\mathbf{B}_{18}$	$= -x_5 \mathbf{a}_1 - x_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$-ax_5 \hat{\mathbf{x}} - ax_5 \hat{\mathbf{y}} + cz_5 \hat{\mathbf{z}}$	(4c)	Gd III
$\mathbf{B}_{19}$	$= -(x_5 - \frac{1}{2}) \mathbf{a}_1 + (x_5 + \frac{1}{2}) \mathbf{a}_2 + (z_5 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-a(x_5 - \frac{1}{2}) \hat{\mathbf{x}} + a(x_5 + \frac{1}{2}) \hat{\mathbf{y}} + c(z_5 + \frac{1}{2}) \hat{\mathbf{z}}$	(4c)	Gd III
$\mathbf{B}_{20}$	$= (x_5 + \frac{1}{2}) \mathbf{a}_1 - (x_5 - \frac{1}{2}) \mathbf{a}_2 + (z_5 + \frac{1}{2}) \mathbf{a}_3$	$=$	$a(x_5 + \frac{1}{2}) \hat{\mathbf{x}} - a(x_5 - \frac{1}{2}) \hat{\mathbf{y}} + c(z_5 + \frac{1}{2}) \hat{\mathbf{z}}$	(4c)	Gd III

## References

- [1] N. C. Baenziger and J. J. Hegenbarth, *Gadolinium and dysprosium intermetallic phases. III. The structures of  $Gd_3Al_2$ ,  $Dy_3Al_2$ ,  $Gd_5Ge_3$ ,  $Dy_5Ge_3$  and  $DyAl_3$* , Acta Cryst. **17**, 620–621 (1964), doi:10.1107/S0365110X64001499.

## Found in

- [1] K. H. J. Buschow, *Rare earth-aluminium intermetallic compounds of the form  $RAl$  and  $R_3Al_2$* , J. Less-Common Met. **8**, 209–212 (1965), doi:10.1016/0022-5088(65)90047-0.
- [2] P. Villars and K. Cenzual, *Pearson's Crystal Data – Crystal Structure Database for Inorganic Compounds* (2013). ASM International.