

Gd₃Al₂ Structure:

A2B3_tP20_102_2c_b2c-001

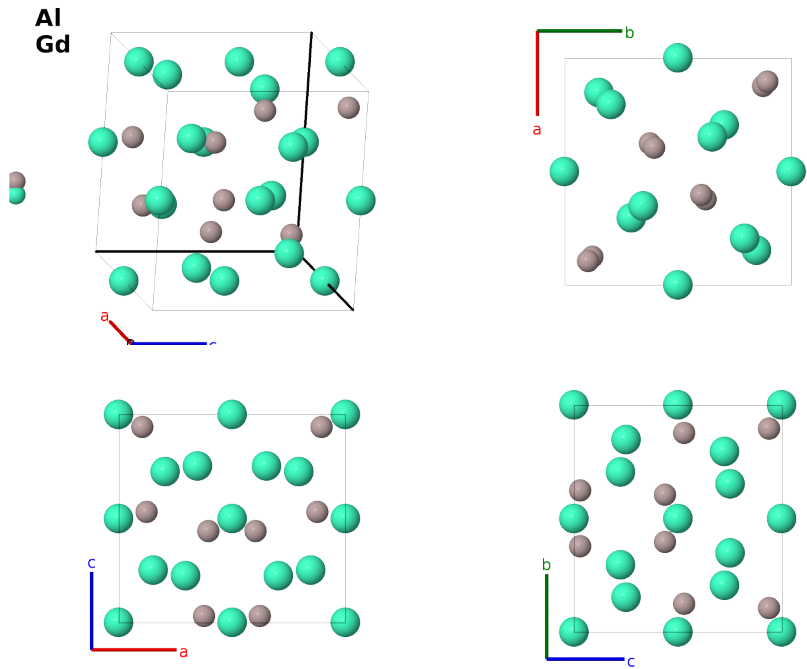
This structure previously used the label(s) **A2B3_tP20_102_2c.b2c**. Calls to these addresses will be redirected here.

Cite this page as:

- H. Eckert, S. Divilov, M. J. Mehl, D. Hicks, A. C. Zettel, M. Esters, X. Campilongo, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 4*, Comput. Mater. Sci. **240**, 112988 (2024), doi: 10.1016/j.commatsci.2024.112988.
- D. Hicks, M. J. Mehl, M. Esters, C. Oses, O. Levy, G. L. W. Hart, C. Toher, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 3*, Comput. Mater. Sci. **199**, 110450 (2021), doi: 10.1016/j.commatsci.2021.110450.

<https://aflow.org/prototype-encyclopedia/AY9W>

https://aflow.org/prototype-encyclopedia/A2B3_tP20_102_2c_b2c-001



Prototype	Al ₂ Gd ₃
AFLOW prototype label	A2B3_tP20_102_2c.b2c-001
ICSD	57869
CCDC	1621909
Pearson symbol	tP20
Space group number	102
Space group symbol	$P4_2nm$
AFLOW prototype command	<code>aflow --proto=A2B3_tP20_102_2c_b2c-001</code> <code>--params=a, c/a, z₁, x₂, z₂, x₃, z₃, x₄, z₄, x₅, z₅</code>

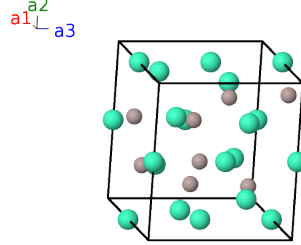
Other compounds with this structure

Dy₃Al₂, Er₃Al₂, Ho₃Al₂, Tb₃Al₂, Y₃Al₂, Zr₃Al₂

- 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 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

$$\mathbf{B}_{19} = -\left(x_5 - \frac{1}{2}\right) \mathbf{a}_1 + \left(x_5 + \frac{1}{2}\right) \mathbf{a}_2 + \left(z_5 + \frac{1}{2}\right) \mathbf{a}_3 = -a\left(x_5 - \frac{1}{2}\right) \hat{\mathbf{x}} + a\left(x_5 + \frac{1}{2}\right) \hat{\mathbf{y}} + c\left(z_5 + \frac{1}{2}\right) \hat{\mathbf{z}} \quad (4c) \quad \text{Gd III}$$

$$\mathbf{B}_{20} = \left(x_5 + \frac{1}{2}\right) \mathbf{a}_1 - \left(x_5 - \frac{1}{2}\right) \mathbf{a}_2 + \left(z_5 + \frac{1}{2}\right) \mathbf{a}_3 = a\left(x_5 + \frac{1}{2}\right) \hat{\mathbf{x}} - a\left(x_5 - \frac{1}{2}\right) \hat{\mathbf{y}} + c\left(z_5 + \frac{1}{2}\right) \hat{\mathbf{z}} \quad (4c) \quad \text{Gd III}$$

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.

First cited in

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