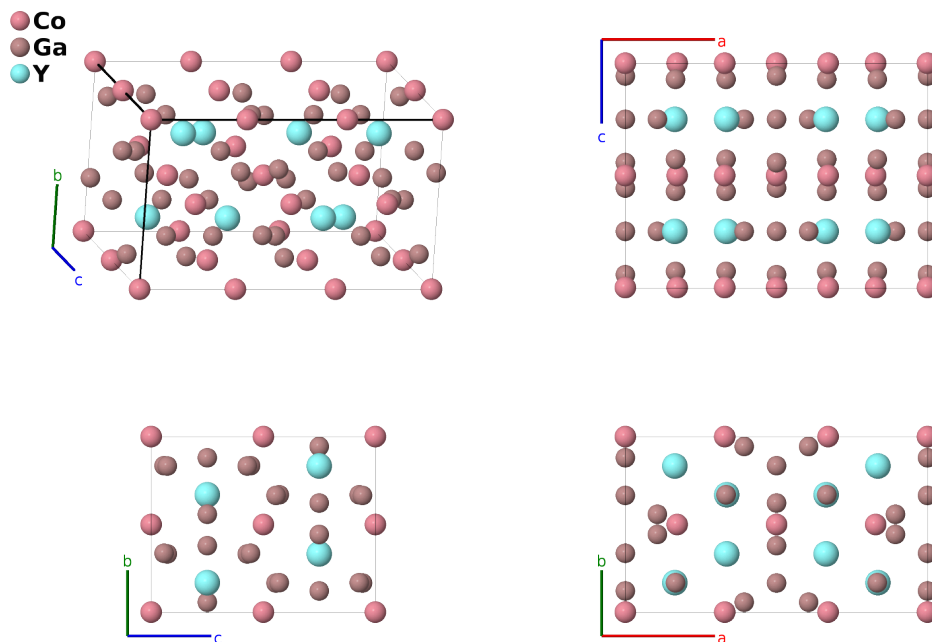


Y₂Ga₉Co₃ Structure: A3B9C2_oC56_63_ae_cfgh_g-001

Cite this page as: H. Eckert, S. Divilov, A. Zettel, M. J. Mehl, D. Hicks, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 4*. In preparation.

<https://afLOW.org/p/1YQJ>

https://afLOW.org/p/A3B9C2_oC56_63_ae_cfgh_g-001



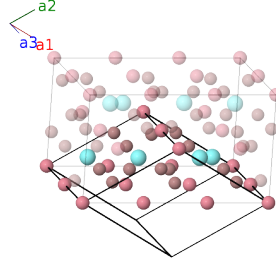
Prototype	Co ₃ Ga ₉ Y ₂
AFLOW prototype label	A3B9C2_oC56_63_ae_cfgh_g-001
ICSD	623242
Pearson symbol	oC56
Space group number	63
Space group symbol	<i>Cmcm</i>
AFLOW prototype command	<code>afLOW --proto=A3B9C2_oC56_63_ae_cfgh_g-001 --params=a, b/a, c/a, y₂, x₃, y₄, z₄, x₅, y₅, x₆, y₆, x₇, y₇, z₇</code>

Other compounds with this structure

Dy₂Ga₉Co₃, Er₂Ga₉Co₃, Gd₂Ga₉Co₃, Lu₂Ga₉Co₃, Nd₂Ga₉Co₃, Sm₂Ga₉Co₃, Tb₂Ga₉Co₃, Tm₂Ga₉Co₃, Yb₂Ga₉Co₃

Base-centered Orthorhombic primitive vectors

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



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
\mathbf{B}_1	0	$=$	0	(4a)	Co I
\mathbf{B}_2	$\frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2}c \hat{\mathbf{z}}$	(4a)	Co I
\mathbf{B}_3	$-y_2 \mathbf{a}_1 + y_2 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$by_2 \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	(4c)	Ga I
\mathbf{B}_4	$y_2 \mathbf{a}_1 - y_2 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$-by_2 \hat{\mathbf{y}} + \frac{3}{4}c \hat{\mathbf{z}}$	(4c)	Ga I
\mathbf{B}_5	$x_3 \mathbf{a}_1 + x_3 \mathbf{a}_2$	$=$	$ax_3 \hat{\mathbf{x}}$	(8e)	Co II
\mathbf{B}_6	$-x_3 \mathbf{a}_1 - x_3 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$-ax_3 \hat{\mathbf{x}} + \frac{1}{2}c \hat{\mathbf{z}}$	(8e)	Co II
\mathbf{B}_7	$-x_3 \mathbf{a}_1 - x_3 \mathbf{a}_2$	$=$	$-ax_3 \hat{\mathbf{x}}$	(8e)	Co II
\mathbf{B}_8	$x_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$ax_3 \hat{\mathbf{x}} + \frac{1}{2}c \hat{\mathbf{z}}$	(8e)	Co II
\mathbf{B}_9	$-y_4 \mathbf{a}_1 + y_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$by_4 \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}}$	(8f)	Ga II
\mathbf{B}_{10}	$y_4 \mathbf{a}_1 - y_4 \mathbf{a}_2 + (z_4 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-by_4 \hat{\mathbf{y}} + c(z_4 + \frac{1}{2}) \hat{\mathbf{z}}$	(8f)	Ga II
\mathbf{B}_{11}	$-y_4 \mathbf{a}_1 + y_4 \mathbf{a}_2 - (z_4 - \frac{1}{2}) \mathbf{a}_3$	$=$	$by_4 \hat{\mathbf{y}} - c(z_4 - \frac{1}{2}) \hat{\mathbf{z}}$	(8f)	Ga II
\mathbf{B}_{12}	$y_4 \mathbf{a}_1 - y_4 \mathbf{a}_2 - z_4 \mathbf{a}_3$	$=$	$-by_4 \hat{\mathbf{y}} - cz_4 \hat{\mathbf{z}}$	(8f)	Ga II
\mathbf{B}_{13}	$(x_5 - y_5) \mathbf{a}_1 + (x_5 + y_5) \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$ax_5 \hat{\mathbf{x}} + by_5 \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	(8g)	Ga III
\mathbf{B}_{14}	$-(x_5 - y_5) \mathbf{a}_1 - (x_5 + y_5) \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$-ax_5 \hat{\mathbf{x}} - by_5 \hat{\mathbf{y}} + \frac{3}{4}c \hat{\mathbf{z}}$	(8g)	Ga III
\mathbf{B}_{15}	$-(x_5 + y_5) \mathbf{a}_1 - (x_5 - y_5) \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$-ax_5 \hat{\mathbf{x}} + by_5 \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	(8g)	Ga III
\mathbf{B}_{16}	$(x_5 + y_5) \mathbf{a}_1 + (x_5 - y_5) \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$ax_5 \hat{\mathbf{x}} - by_5 \hat{\mathbf{y}} + \frac{3}{4}c \hat{\mathbf{z}}$	(8g)	Ga III
\mathbf{B}_{17}	$(x_6 - y_6) \mathbf{a}_1 + (x_6 + y_6) \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$ax_6 \hat{\mathbf{x}} + by_6 \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	(8g)	Y I
\mathbf{B}_{18}	$-(x_6 - y_6) \mathbf{a}_1 - (x_6 + y_6) \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$-ax_6 \hat{\mathbf{x}} - by_6 \hat{\mathbf{y}} + \frac{3}{4}c \hat{\mathbf{z}}$	(8g)	Y I
\mathbf{B}_{19}	$-(x_6 + y_6) \mathbf{a}_1 - (x_6 - y_6) \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$-ax_6 \hat{\mathbf{x}} + by_6 \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	(8g)	Y I
\mathbf{B}_{20}	$(x_6 + y_6) \mathbf{a}_1 + (x_6 - y_6) \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$ax_6 \hat{\mathbf{x}} - by_6 \hat{\mathbf{y}} + \frac{3}{4}c \hat{\mathbf{z}}$	(8g)	Y I
\mathbf{B}_{21}	$(x_7 - y_7) \mathbf{a}_1 + (x_7 + y_7) \mathbf{a}_2 + z_7 \mathbf{a}_3$	$=$	$ax_7 \hat{\mathbf{x}} + by_7 \hat{\mathbf{y}} + cz_7 \hat{\mathbf{z}}$	(16h)	Ga IV
\mathbf{B}_{22}	$-(x_7 - y_7) \mathbf{a}_1 - (x_7 + y_7) \mathbf{a}_2 + (z_7 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-ax_7 \hat{\mathbf{x}} - by_7 \hat{\mathbf{y}} + c(z_7 + \frac{1}{2}) \hat{\mathbf{z}}$	(16h)	Ga IV
\mathbf{B}_{23}	$-(x_7 + y_7) \mathbf{a}_1 - (x_7 - y_7) \mathbf{a}_2 - (z_7 - \frac{1}{2}) \mathbf{a}_3$	$=$	$-ax_7 \hat{\mathbf{x}} + by_7 \hat{\mathbf{y}} - c(z_7 - \frac{1}{2}) \hat{\mathbf{z}}$	(16h)	Ga IV
\mathbf{B}_{24}	$(x_7 + y_7) \mathbf{a}_1 + (x_7 - y_7) \mathbf{a}_2 - z_7 \mathbf{a}_3$	$=$	$ax_7 \hat{\mathbf{x}} - by_7 \hat{\mathbf{y}} - cz_7 \hat{\mathbf{z}}$	(16h)	Ga IV

$$\mathbf{B}_{25} = \begin{matrix} -(x_7 - y_7) \mathbf{a}_1 - (x_7 + y_7) \mathbf{a}_2 - \\ z_7 \mathbf{a}_3 \end{matrix} = -ax_7 \hat{\mathbf{x}} - by_7 \hat{\mathbf{y}} - cz_7 \hat{\mathbf{z}} \quad (16h) \quad \text{Ga IV}$$

$$\mathbf{B}_{26} = \begin{matrix} (x_7 - y_7) \mathbf{a}_1 + (x_7 + y_7) \mathbf{a}_2 - \\ (z_7 - \frac{1}{2}) \mathbf{a}_3 \end{matrix} = ax_7 \hat{\mathbf{x}} + by_7 \hat{\mathbf{y}} - c(z_7 - \frac{1}{2}) \hat{\mathbf{z}} \quad (16h) \quad \text{Ga IV}$$

$$\mathbf{B}_{27} = \begin{matrix} (x_7 + y_7) \mathbf{a}_1 + (x_7 - y_7) \mathbf{a}_2 + \\ (z_7 + \frac{1}{2}) \mathbf{a}_3 \end{matrix} = ax_7 \hat{\mathbf{x}} - by_7 \hat{\mathbf{y}} + c(z_7 + \frac{1}{2}) \hat{\mathbf{z}} \quad (16h) \quad \text{Ga IV}$$

$$\mathbf{B}_{28} = \begin{matrix} -(x_7 + y_7) \mathbf{a}_1 - (x_7 - y_7) \mathbf{a}_2 + \\ z_7 \mathbf{a}_3 \end{matrix} = -ax_7 \hat{\mathbf{x}} + by_7 \hat{\mathbf{y}} + cz_7 \hat{\mathbf{z}} \quad (16h) \quad \text{Ga IV}$$

References

- [1] Y. N. Grin', R. E. Gladyshevskii, O. M. Sichevich, V. E. Zavodnik, Y. P. Yarmolyuk, and I. V. Rozhdestvenskaya, *Crystal structure of $R_2Ga_9Co_3$ compounds ($R = Nd, Sm, Gd, Y, Tb, Dy, Ho, Er, Tm, Yb, Lu$)*, Sov. Phys. Crystallogr. **29**, 528–530 (1984).

Found in

- [1] R. E. Gladyshevskii, K. Cenzual, and E. Parthé, *$Y_2Co_3Al_9$ with $Y_2Co_3Ga_9$ type structure: an intergrowth of CsCl- and Th_3Pd_5 -type slabs*, J. Alloys Compd. **182**, 165–170 (1992), doi:10.1016/0925-8388(92)90584-V.