

Y₂Ga₉Co₃ Structure:

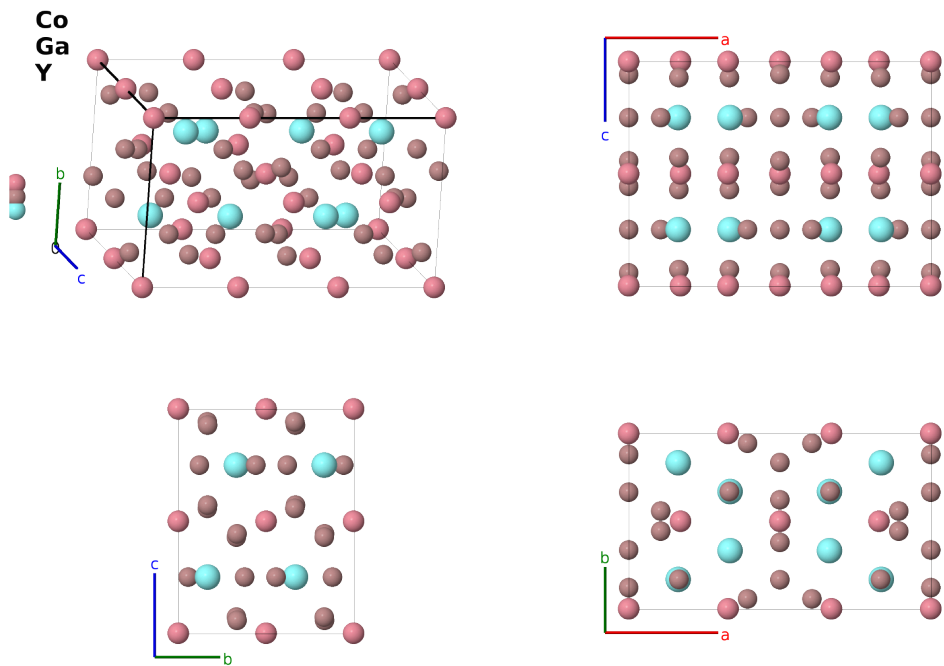
A3B9C2_oC56_63_ae_cfgh_g-001

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<https://aflow.org/prototype-encyclopedia/1YQJ>

https://aflow.org/prototype-encyclopedia/A3B9C2_oC56_63_ae_cfgh_g-001



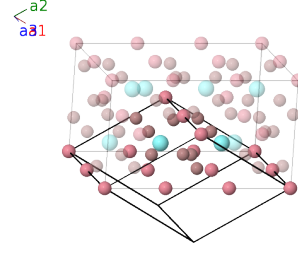
Prototype	Co ₃ Ga ₉ Y ₂
AFLOW prototype label	A3B9C2_oC56_63_ae_cfgh_g-001
ICSD	623242
CCDC	1750303
Pearson symbol	oC56
Space group number	63
Space group symbol	<i>Cmcm</i>
AFLOW prototype command	<code>aflow --proto=A3B9C2_oC56_63_ae_cfgh_g-001</code> <code>--params=a, b/a, c/a, y₂, x₃, y₄, z₄, x₅, 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

$$\begin{aligned}
\mathbf{B}_{25} &= - (x_7 - y_7) \mathbf{a}_1 - (x_7 + y_7) \mathbf{a}_2 - z_7 \mathbf{a}_3 = -ax_7 \hat{\mathbf{x}} - by_7 \hat{\mathbf{y}} - cz_7 \hat{\mathbf{z}} & (16h) & \text{Ga IV} \\
\mathbf{B}_{26} &= (x_7 - y_7) \mathbf{a}_1 + (x_7 + y_7) \mathbf{a}_2 - \left(z_7 - \frac{1}{2}\right) \mathbf{a}_3 = ax_7 \hat{\mathbf{x}} + by_7 \hat{\mathbf{y}} - c \left(z_7 - \frac{1}{2}\right) \hat{\mathbf{z}} & (16h) & \text{Ga IV} \\
\mathbf{B}_{27} &= (x_7 + y_7) \mathbf{a}_1 + (x_7 - y_7) \mathbf{a}_2 + \left(z_7 + \frac{1}{2}\right) \mathbf{a}_3 = ax_7 \hat{\mathbf{x}} - by_7 \hat{\mathbf{y}} + c \left(z_7 + \frac{1}{2}\right) \hat{\mathbf{z}} & (16h) & \text{Ga IV} \\
\mathbf{B}_{28} &= - (x_7 + y_7) \mathbf{a}_1 - (x_7 - y_7) \mathbf{a}_2 + z_7 \mathbf{a}_3 = -ax_7 \hat{\mathbf{x}} + by_7 \hat{\mathbf{y}} + cz_7 \hat{\mathbf{z}} & (16h) & \text{Ga IV}
\end{aligned}$$

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. Cenxual, 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.

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