$CoGe_2$ Structure: AB2_oC24_64_d_ef-002

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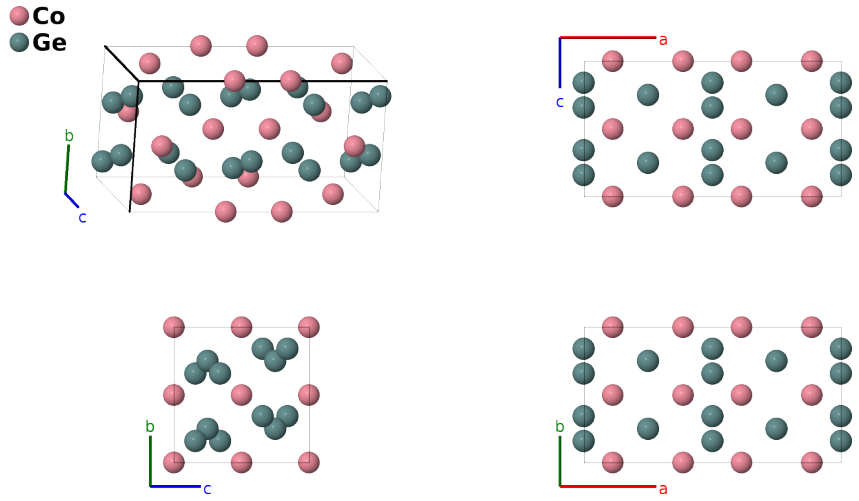
https://aflow.org/p/QB3A

https://aflow.org/p/AB2_oC24_64_d_ef-002

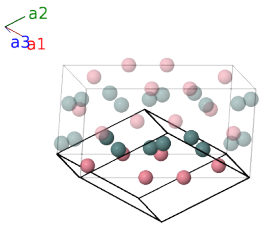


Prototype	$CoGe_2$
AFLOW prototype label	AB2_oC24_64_d_ef-002
ICSD	52964
Pearson symbol	oC24
Space group number	64
Space group symbol	*Cmce*
AFLOW prototype command	`aflow --proto=AB2_oC24_64_d_ef-002 --params=`$a, b/a, c/a, x_1, y_2, y_3, z_3$

- The actual stoichiometry is Co_7Ge_{16}, as the Co (8d) sites are 87.5% occupied.
- (Schubert, 1950) described this compound as being isotypic to $PdSn_2$ (C_e) in space group *Aba*2 #41.
- (Cenzual, 1991) showed that the given z coordinates for the cobalt atoms were consistent with space group *Cmca* #64.
- Although (Schubert, 1950) give the lattice parameters in Ångstroms, (Cenzual, 1991) asserts that they were actually in kX units and converts them to Ångstroms. We use the later values for the lattice parameters.

Base-centered Orthorhombic primitive vectors

$$
\begin{aligned}
\mathbf{a_1} &= \tfrac{1}{2}a\,\hat{\mathbf{x}} - \tfrac{1}{2}b\,\hat{\mathbf{y}} \\
\mathbf{a_2} &= \tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{1}{2}b\,\hat{\mathbf{y}} \\
\mathbf{a_3} &= c\,\hat{\mathbf{z}}
\end{aligned}
$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$x_1\,\mathbf{a}_1 + x_1\,\mathbf{a}_2$	=	$ax_1\,\hat{\mathbf{x}}$	(8d)	Co I
$\mathbf{B_2}$	=	$-\left(x_1 - \frac{1}{2}\right)\,\mathbf{a}_1 - \left(x_1 - \frac{1}{2}\right)\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$-a\left(x_1 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(8d)	Co I
$\mathbf{B_3}$	=	$-x_1\,\mathbf{a}_1 - x_1\,\mathbf{a}_2$	=	$-ax_1\,\hat{\mathbf{x}}$	(8d)	Co I
$\mathbf{B_4}$	=	$\left(x_1 + \frac{1}{2}\right)\,\mathbf{a}_1 + \left(x_1 + \frac{1}{2}\right)\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$a\left(x_1 + \frac{1}{2}\right)\,\hat{\mathbf{x}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(8d)	Co I
$\mathbf{B_5}$	=	$-\left(y_2 - \frac{1}{4}\right)\,\mathbf{a}_1 + \left(y_2 + \frac{1}{4}\right)\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + by_2\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(8e)	Ge I
$\mathbf{B_6}$	=	$\left(y_2 + \frac{1}{4}\right)\,\mathbf{a}_1 - \left(y_2 - \frac{1}{4}\right)\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} - by_2\,\hat{\mathbf{y}} + \frac{3}{4}c\,\hat{\mathbf{z}}$	(8e)	Ge I
$\mathbf{B_7}$	=	$\left(y_2 + \frac{3}{4}\right)\,\mathbf{a}_1 - \left(y_2 - \frac{3}{4}\right)\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$\frac{3}{4}a\,\hat{\mathbf{x}} - by_2\,\hat{\mathbf{y}} + \frac{3}{4}c\,\hat{\mathbf{z}}$	(8e)	Ge I
$\mathbf{B_8}$	=	$-\left(y_2 - \frac{3}{4}\right)\,\mathbf{a}_1 + \left(y_2 + \frac{3}{4}\right)\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$\frac{3}{4}a\,\hat{\mathbf{x}} + by_2\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(8e)	Ge I
$\mathbf{B_9}$	=	$-y_3\,\mathbf{a}_1 + y_3\,\mathbf{a}_2 + z_3\,\mathbf{a}_3$	=	$by_3\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$	(8f)	Ge II
$\mathbf{B_{10}}$	=	$\left(y_3 + \frac{1}{2}\right)\,\mathbf{a}_1 - \left(y_3 - \frac{1}{2}\right)\,\mathbf{a}_2 + \left(z_3 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - by_3\,\hat{\mathbf{y}} + c\left(z_3 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8f)	Ge II
$\mathbf{B_{11}}$	=	$-\left(y_3 - \frac{1}{2}\right)\,\mathbf{a}_1 + \left(y_3 + \frac{1}{2}\right)\,\mathbf{a}_2 - \left(z_3 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + by_3\,\hat{\mathbf{y}} - c\left(z_3 - \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8f)	Ge II
$\mathbf{B_{12}}$	=	$y_3\,\mathbf{a}_1 - y_3\,\mathbf{a}_2 - z_3\,\mathbf{a}_3$	=	$-by_3\,\hat{\mathbf{y}} - cz_3\,\hat{\mathbf{z}}$	(8f)	Ge II

References

[1] K. Schubert and H. Pfisterer, *Zur Kristallchemie der B-Metall-reichsten Phasen in Legierungen von Ü"bergangsmetallen der Eisen- und Platintriaden mit Elementen der vierten Nebengruppe*, Zeitschrift für Metallkunde **41**, 433–441 (1950).

Found in

[1] K. Cenzual, L. M. Gelato, M. Penzo, and E. Parthé, *Inorganic structure types with revised space groups. I*, Acta Crystallogr. Sect. B **47**, 433–439 (1991), doi:10.1107/S0108768191000903.