Pr$_5$Co$_2$Ge$_4$ Structure: A2B3C5_mC40_12_2i_3i_5i-001

https://aflow.org/p/422U

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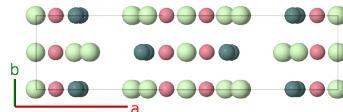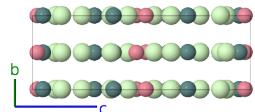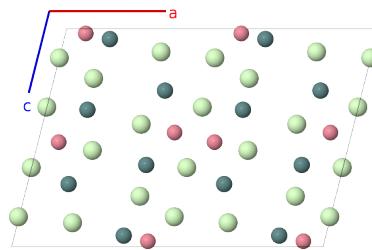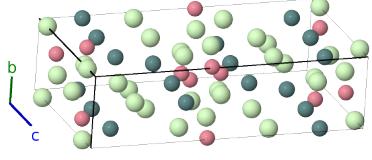
Prototype	Co$_2$Ge$_4$Pr$_5$
AFLOW prototype label	A2B3C5_mC40_12_2i_3i_5i-001
CCDC	1882993
Pearson symbol	mC40
Space group number	12
Space group symbol	$C2/m$
AFLOW prototype command	aflow --proto=A2B3C5_mC40_12_2i_3i_5i-001 --params=$a, b/a, c/a, \beta, x_1, z_1, x_2, z_2, x_3, z_3, x_4, z_4, x_5, z_5, x_6, z_6, x_7, z_7, x_8, z_8, x_9, z_9, x_{10},$ z_{10}

Other compounds with this structure

Ce$_5$Co$_2$Ge$_4$, La$_5$Co$_2$Ge$_4$, Nd$_5$Co$_2$Ge$_4$, Pm$_5$Co$_2$Ge$_4$, Sm$_5$Co$_2$Ge$_4$

Base-centered Monoclinic primitive vectors

$$\mathbf{a_1} = \tfrac{1}{2}a\,\hat{\mathbf{x}} - \tfrac{1}{2}b\,\hat{\mathbf{y}}$$

$$\mathbf{a_2} = \tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{1}{2}b\,\hat{\mathbf{y}}$$

$$\mathbf{a_3} = c\cos\beta\,\hat{\mathbf{x}} + c\sin\beta\,\hat{\mathbf{z}}$$
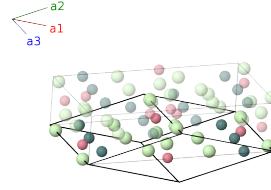
Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$x_1\,\mathbf{a_1} + x_1\,\mathbf{a_2} + z_1\,\mathbf{a_3}$	=	$(ax_1 + cz_1\cos\beta)\,\hat{\mathbf{x}} + cz_1\sin\beta\,\hat{\mathbf{z}}$	(4i)	Co I
$\mathbf{B_2}$	=	$-x_1\,\mathbf{a_1} - x_1\,\mathbf{a_2} - z_1\,\mathbf{a_3}$	=	$-(ax_1 + cz_1\cos\beta)\,\hat{\mathbf{x}} - cz_1\sin\beta\,\hat{\mathbf{z}}$	(4i)	Co I
$\mathbf{B_3}$	=	$x_2\,\mathbf{a_1} + x_2\,\mathbf{a_2} + z_2\,\mathbf{a_3}$	=	$(ax_2 + cz_2\cos\beta)\,\hat{\mathbf{x}} + cz_2\sin\beta\,\hat{\mathbf{z}}$	(4i)	Co II
$\mathbf{B_4}$	=	$-x_2\,\mathbf{a_1} - x_2\,\mathbf{a_2} - z_2\,\mathbf{a_3}$	=	$-(ax_2 + cz_2\cos\beta)\,\hat{\mathbf{x}} - cz_2\sin\beta\,\hat{\mathbf{z}}$	(4i)	Co II
$\mathbf{B_5}$	=	$x_3\,\mathbf{a_1} + x_3\,\mathbf{a_2} + z_3\,\mathbf{a_3}$	=	$(ax_3 + cz_3\cos\beta)\,\hat{\mathbf{x}} + cz_3\sin\beta\,\hat{\mathbf{z}}$	(4i)	Ge I
$\mathbf{B_6}$	=	$-x_3\,\mathbf{a_1} - x_3\,\mathbf{a_2} - z_3\,\mathbf{a_3}$	=	$-(ax_3 + cz_3\cos\beta)\,\hat{\mathbf{x}} - cz_3\sin\beta\,\hat{\mathbf{z}}$	(4i)	Ge I
$\mathbf{B_7}$	=	$x_4\,\mathbf{a_1} + x_4\,\mathbf{a_2} + z_4\,\mathbf{a_3}$	=	$(ax_4 + cz_4\cos\beta)\,\hat{\mathbf{x}} + cz_4\sin\beta\,\hat{\mathbf{z}}$	(4i)	Ge II
$\mathbf{B_8}$	=	$-x_4\,\mathbf{a_1} - x_4\,\mathbf{a_2} - z_4\,\mathbf{a_3}$	=	$-(ax_4 + cz_4\cos\beta)\,\hat{\mathbf{x}} - cz_4\sin\beta\,\hat{\mathbf{z}}$	(4i)	Ge II
$\mathbf{B_9}$	=	$x_5\,\mathbf{a_1} + x_5\,\mathbf{a_2} + z_5\,\mathbf{a_3}$	=	$(ax_5 + cz_5\cos\beta)\,\hat{\mathbf{x}} + cz_5\sin\beta\,\hat{\mathbf{z}}$	(4i)	Ge III
$\mathbf{B_{10}}$	=	$-x_5\,\mathbf{a_1} - x_5\,\mathbf{a_2} - z_5\,\mathbf{a_3}$	=	$-(ax_5 + cz_5\cos\beta)\,\hat{\mathbf{x}} - cz_5\sin\beta\,\hat{\mathbf{z}}$	(4i)	Ge III
$\mathbf{B_{11}}$	=	$x_6\,\mathbf{a_1} + x_6\,\mathbf{a_2} + z_6\,\mathbf{a_3}$	=	$(ax_6 + cz_6\cos\beta)\,\hat{\mathbf{x}} + cz_6\sin\beta\,\hat{\mathbf{z}}$	(4i)	Pr I
$\mathbf{B_{12}}$	=	$-x_6\,\mathbf{a_1} - x_6\,\mathbf{a_2} - z_6\,\mathbf{a_3}$	=	$-(ax_6 + cz_6\cos\beta)\,\hat{\mathbf{x}} - cz_6\sin\beta\,\hat{\mathbf{z}}$	(4i)	Pr I
$\mathbf{B_{13}}$	=	$x_7\,\mathbf{a_1} + x_7\,\mathbf{a_2} + z_7\,\mathbf{a_3}$	=	$(ax_7 + cz_7\cos\beta)\,\hat{\mathbf{x}} + cz_7\sin\beta\,\hat{\mathbf{z}}$	(4i)	Pr II
$\mathbf{B_{14}}$	=	$-x_7\,\mathbf{a_1} - x_7\,\mathbf{a_2} - z_7\,\mathbf{a_3}$	=	$-(ax_7 + cz_7\cos\beta)\,\hat{\mathbf{x}} - cz_7\sin\beta\,\hat{\mathbf{z}}$	(4i)	Pr II
$\mathbf{B_{15}}$	=	$x_8\,\mathbf{a_1} + x_8\,\mathbf{a_2} + z_8\,\mathbf{a_3}$	=	$(ax_8 + cz_8\cos\beta)\,\hat{\mathbf{x}} + cz_8\sin\beta\,\hat{\mathbf{z}}$	(4i)	Pr III
$\mathbf{B_{16}}$	=	$-x_8\,\mathbf{a_1} - x_8\,\mathbf{a_2} - z_8\,\mathbf{a_3}$	=	$-(ax_8 + cz_8\cos\beta)\,\hat{\mathbf{x}} - cz_8\sin\beta\,\hat{\mathbf{z}}$	(4i)	Pr III
$\mathbf{B_{17}}$	=	$x_9\,\mathbf{a_1} + x_9\,\mathbf{a_2} + z_9\,\mathbf{a_3}$	=	$(ax_9 + cz_9\cos\beta)\,\hat{\mathbf{x}} + cz_9\sin\beta\,\hat{\mathbf{z}}$	(4i)	Pr IV
$\mathbf{B_{18}}$	=	$-x_9\,\mathbf{a_1} - x_9\,\mathbf{a_2} - z_9\,\mathbf{a_3}$	=	$-(ax_9 + cz_9\cos\beta)\,\hat{\mathbf{x}} - cz_9\sin\beta\,\hat{\mathbf{z}}$	(4i)	Pr IV
$\mathbf{B_{19}}$	=	$x_{10}\,\mathbf{a_1} + x_{10}\,\mathbf{a_2} + z_{10}\,\mathbf{a_3}$	=	$(ax_{10} + cz_{10}\cos\beta)\,\hat{\mathbf{x}} + cz_{10}\sin\beta\,\hat{\mathbf{z}}$	(4i)	Pr V
$\mathbf{B_{20}}$	=	$-x_{10}\,\mathbf{a_1} - x_{10}\,\mathbf{a_2} - z_{10}\,\mathbf{a_3}$	=	$-(ax_{10} + cz_{10}\cos\beta)\,\hat{\mathbf{x}} - cz_{10}\sin\beta\,\hat{\mathbf{z}}$	(4i)	Pr V

References

[1] Q. Lin, K. Aguirre, S. M. Saunders, T. A. Hackett, Y. Liu, V. Taufour, D. Paudyal, S. Budko, P. C. Canfield, and G. J. Miller, *Polar Intermetallics $Pr_5Co_2Ge_3$ and $Pr_7Co_2Ge_4$ with Planar Hydrocarbon-Like Metal Clusters*, Chem. Europ. J. **23**, 10516–10521 (2017), doi:10.1002/chem.201702798.

Found in

[1] L. Xiang, E. Gati, S. L. Bud'ko, S. M. Saunders, and P. C. Canfield, *Avoided ferromagnetic quantum critical point in pressurized $La_5Co_2Ge_3$*, Phys. Rev. B **103**, 054419 (2021), doi:10.1103/PhysRevB.103.054419.