Sc_3CoC_4 Structure: A4BC3_oI16_71_m_a_bf-001

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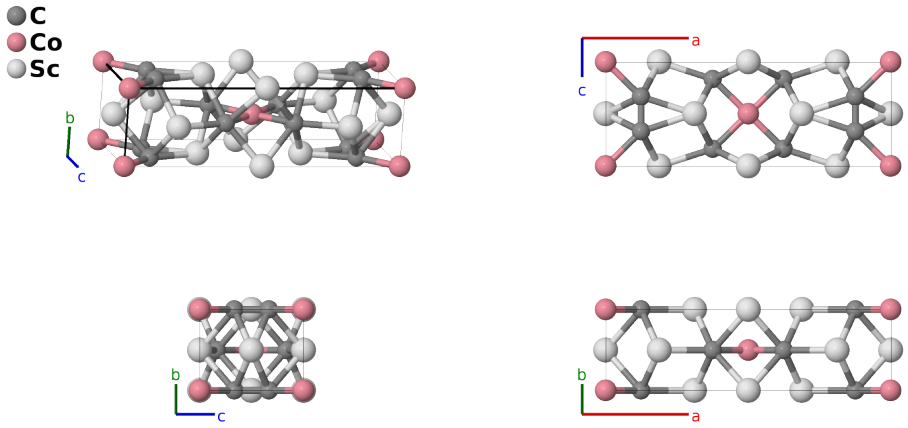
https://aflow.org/p/A4BC3_oI16_71_m_a_bf-001



Prototype	C_4CoSc_3
AFLOW prototype label	A4BC3_oI16_71_m_a_bf-001
ICSD	236393
Pearson symbol	oI16
Space group number	71
Space group symbol	$Immm$
AFLOW prototype command	`aflow --proto=A4BC3_oI16_71_m_a_bf-001 --params=`$a, b/a, c/a, x_3, x_4, z_4$

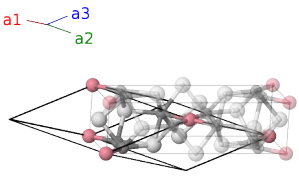
Other compounds with this structure

Sc_3FeC_4, Sc_3IrC_4, Sc_3NiC_4, Sc_3OsC_4, Sc_3RhC_4, Sc_3RuC_4

- This is the high temperature structure of Sc_3CoC_4. Below 72K it transforms into the monoclinic Sc_3RhC_4 structure. Data for the current structure was taken at 293K.
- (Vogt, 2005) found that in Sc_3IrC_4 and Sc_3RhC_4 the transition metal atom is not exactly on the (2a) site, but instead is on the (4i) Wyckoff position (0,0,±0.04), with each site 50% occupied.

Body-centered Orthorhombic primitive vectors

$$\mathbf{a_1} = -\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}b\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$$
$$\mathbf{a_2} = \frac{1}{2}a\,\hat{\mathbf{x}} - \frac{1}{2}b\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$$
$$\mathbf{a_3} = \frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}b\,\hat{\mathbf{y}} - \frac{1}{2}c\,\hat{\mathbf{z}}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	0	=	0	(2a)	Co I
$\mathbf{B_2}$	=	$\frac{1}{2}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}}$	(2b)	Sc I
$\mathbf{B_3}$	=	$\frac{1}{2}\,\mathbf{a}_1 + x_3\,\mathbf{a}_2 + \left(x_3 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$ax_3\,\hat{\mathbf{x}} + \frac{1}{2}b\,\hat{\mathbf{y}}$	(4f)	Sc II
$\mathbf{B_4}$	=	$\frac{1}{2}\,\mathbf{a}_1 - x_3\,\mathbf{a}_2 - \left(x_3 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ax_3\,\hat{\mathbf{x}} + \frac{1}{2}b\,\hat{\mathbf{y}}$	(4f)	Sc II
$\mathbf{B_5}$	=	$z_4\,\mathbf{a}_1 + (x_4 + z_4)\,\mathbf{a}_2 + x_4\,\mathbf{a}_3$	=	$ax_4\,\hat{\mathbf{x}} + cz_4\,\hat{\mathbf{z}}$	(8m)	C I
$\mathbf{B_6}$	=	$z_4\,\mathbf{a}_1 - (x_4 - z_4)\,\mathbf{a}_2 - x_4\,\mathbf{a}_3$	=	$-ax_4\,\hat{\mathbf{x}} + cz_4\,\hat{\mathbf{z}}$	(8m)	C I
$\mathbf{B_7}$	=	$-z_4\,\mathbf{a}_1 - (x_4 + z_4)\,\mathbf{a}_2 - x_4\,\mathbf{a}_3$	=	$-ax_4\,\hat{\mathbf{x}} - cz_4\,\hat{\mathbf{z}}$	(8m)	C I
$\mathbf{B_8}$	=	$-z_4\,\mathbf{a}_1 + (x_4 - z_4)\,\mathbf{a}_2 + x_4\,\mathbf{a}_3$	=	$ax_4\,\hat{\mathbf{x}} - cz_4\,\hat{\mathbf{z}}$	(8m)	C I

References

[1] G. Eickerling, C. Hauf, E. Scheidt, L. Reichardt, C. Schneider, A. M. noz, S. Lopez-Moreno, A. H. Romero, F. Porcher, G. André, R. Pöttgen, and W. Scherer, *On the Control Parameters of the Quasi-One Dimensional Superconductivity in Sc_3CoC_4*, Z. Anorganische und Allgemeine Chemie **639**, 1985–1995 (2013), doi:10.1002/zaac.201200517.

[2] C. Vogt, R.-D. Hoffmann, and R. Pöttgen, *The superstructure of Sc_3RhC_4 and Sc_3IrC_4*, Solid State Sci. **7**, 1003–1009 (2005), doi:10.1016/j.solidstatesciences.2005.04.004.

Found in

[1] *Sc_3CoC_4 (T = 223.7 K) Crystal Structure: Datasheet from "PAULING FILE Multinaries Edition – 2012" in SpringerMaterials.* Copyright 2016 Springer-Verlag Berlin Heidelberg & Material Phases Data System (MPDS), Switzerland & National Institute for Materials Science (NIMS), Japan.