Mn_2Co_2C Structure: AB2C2_tP5_123_b_e_ac-001

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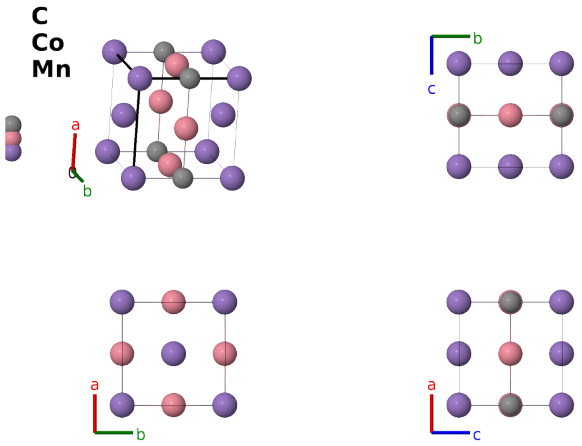
https://aflow.org/prototype-encyclopedia/8ZWP

https://aflow.org/prototype-encyclopedia/AB2C2_tP5_123_b_e_ac-001

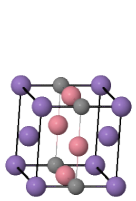


Prototype	CCo_2Mn_2
AFLOW prototype label	AB2C2_tP5_123_b_e_ac-001
ICSD	44353
CCDC	1613756
Pearson symbol	tP5
Space group number	123
Space group symbol	$P4/mmm$
AFLOW prototype command	`aflow --proto=AB2C2_tP5_123_b_e_ac-001 --params=`$a, c/a$

- We have inferred the value of a and the positions of the atoms from Figure 2(a) of (Holtzman, 1959) and Figure 3 of (Murthy, 1969), shifting the origin to be on the Mn_{II} atom. The value of c was inferred from the C-Mn_{II} distance given in the paper. This is a pseudo-cubic lattice, with $c/a \approx 1$.

Simple Tetragonal primitive vectors

$$\mathbf{a_1} = a\,\hat{\mathbf{x}}$$
$$\mathbf{a_2} = a\,\hat{\mathbf{y}}$$
$$\mathbf{a_3} = c\,\hat{\mathbf{z}}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	0	=	0	(1a)	Mn I
$\mathbf{B_2}$	=	$\frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}c\,\hat{\mathbf{z}}$	(1b)	C I
$\mathbf{B_3}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{y}}$	(1c)	Mn II
$\mathbf{B_4}$	=	$\frac{1}{2}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(2e)	Co I
$\mathbf{B_5}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(2e)	Co I

References

[1] A. H. Holtzman and I. G. P. Conrad, *Structural and Magnetic Properties of Mn-Co-C Alloys*, J. Appl. Phys. **30**, 103S–104S (1959), doi:10.1063/1.2185842.

[2] N. S. S. Murthy, R. J. Begum, C. S. Somanathan, B. S. Srinivasan, and M. R. L. N. Murthy, *Ferrimagnetic structure of Mn_2Co_2C*, J. Phys.: Conf. Ser. **30**, 939–945 (1969), doi:10.1016/0022-3697(69)90291-1.

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