$Co_8Zn_9Mn_3$ Structure: A2B3_cP20_213_c_d-001

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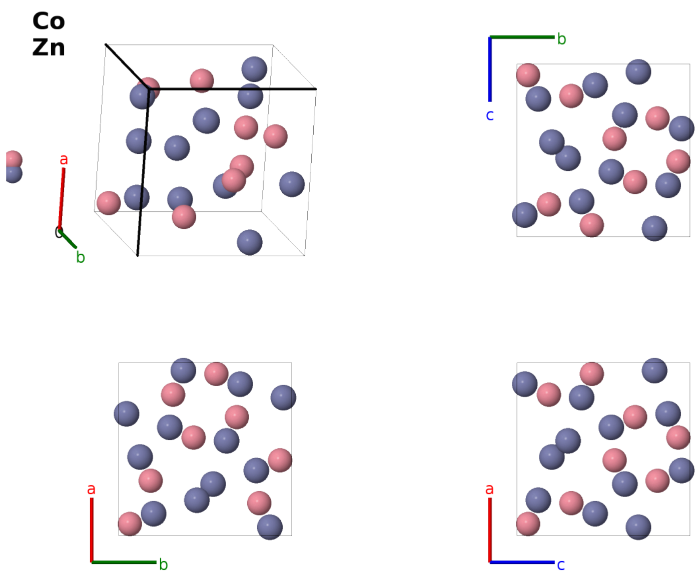
https://aflow.org/prototype-encyclopedia/KXT1

https://aflow.org/prototype-encyclopedia/A2B3_cP20_213_c_d-001

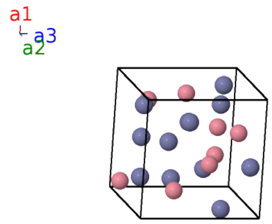


Prototype	$Co_8Mn_3Zn_9$
AFLOW prototype label	A2B3_cP20_213_c_d-001
ICSD	19272
CCDC	2185005
Pearson symbol	cP20
Space group number	213
Space group symbol	$P4_132$
AFLOW prototype command	`aflow --proto=A2B3_cP20_213_c_d-001 --params=`a, x_1, y_2

- The composition of the site we label "Co (8c)" is actually $Co_{7.616}Mn_{0.834}$, and the site labeled "Zn (12d)" is $Zn_{8.7756}Co_{0.684}Mn_{2.448}$. (Bocarsly, 2019)
- Many other compositions are observed.
- We use the synchrotron data taken by (Bocarsly, 2019) at 100K.
- This structure can also be found in the enantiomorphic space group $P4_332$ #212.

Simple Cubic primitive vectors

$$
\begin{aligned}
\mathbf{a_1} &= a\,\mathbf{\hat{x}} \\
\mathbf{a_2} &= a\,\mathbf{\hat{y}} \\
\mathbf{a_3} &= a\,\mathbf{\hat{z}}
\end{aligned}
$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$x_1\,\mathbf{a}_1 + x_1\,\mathbf{a}_2 + x_1\,\mathbf{a}_3$	=	$ax_1\,\mathbf{\hat{x}} + ax_1\,\mathbf{\hat{y}} + ax_1\,\mathbf{\hat{z}}$	(8c)	Co I
$\mathbf{B_2}$	=	$-\left(x_1 - \frac{1}{2}\right)\,\mathbf{a}_1 - x_1\,\mathbf{a}_2 + \left(x_1 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(x_1 - \frac{1}{2}\right)\,\mathbf{\hat{x}} - ax_1\,\mathbf{\hat{y}} + a\left(x_1 + \frac{1}{2}\right)\,\mathbf{\hat{z}}$	(8c)	Co I
$\mathbf{B_3}$	=	$-x_1\,\mathbf{a}_1 + \left(x_1 + \frac{1}{2}\right)\,\mathbf{a}_2 - \left(x_1 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ax_1\,\mathbf{\hat{x}} + a\left(x_1 + \frac{1}{2}\right)\,\mathbf{\hat{y}} - a\left(x_1 - \frac{1}{2}\right)\,\mathbf{\hat{z}}$	(8c)	Co I
$\mathbf{B_4}$	=	$\left(x_1 + \frac{1}{2}\right)\,\mathbf{a}_1 - \left(x_1 - \frac{1}{2}\right)\,\mathbf{a}_2 - x_1\,\mathbf{a}_3$	=	$a\left(x_1 + \frac{1}{2}\right)\,\mathbf{\hat{x}} - a\left(x_1 - \frac{1}{2}\right)\,\mathbf{\hat{y}} - ax_1\,\mathbf{\hat{z}}$	(8c)	Co I
$\mathbf{B_5}$	=	$\left(x_1 + \frac{3}{4}\right)\,\mathbf{a}_1 + \left(x_1 + \frac{1}{4}\right)\,\mathbf{a}_2 - \left(x_1 - \frac{1}{4}\right)\,\mathbf{a}_3$	=	$a\left(x_1 + \frac{3}{4}\right)\,\mathbf{\hat{x}} + a\left(x_1 + \frac{1}{4}\right)\,\mathbf{\hat{y}} - a\left(x_1 - \frac{1}{4}\right)\,\mathbf{\hat{z}}$	(8c)	Co I
$\mathbf{B_6}$	=	$-\left(x_1 - \frac{3}{4}\right)\,\mathbf{a}_1 - \left(x_1 - \frac{3}{4}\right)\,\mathbf{a}_2 - \left(x_1 - \frac{3}{4}\right)\,\mathbf{a}_3$	=	$-a\left(x_1 - \frac{3}{4}\right)\,\mathbf{\hat{x}} - a\left(x_1 - \frac{3}{4}\right)\,\mathbf{\hat{y}} - a\left(x_1 - \frac{3}{4}\right)\,\mathbf{\hat{z}}$	(8c)	Co I
$\mathbf{B_7}$	=	$\left(x_1 + \frac{1}{4}\right)\,\mathbf{a}_1 - \left(x_1 - \frac{1}{4}\right)\,\mathbf{a}_2 + \left(x_1 + \frac{3}{4}\right)\,\mathbf{a}_3$	=	$a\left(x_1 + \frac{1}{4}\right)\,\mathbf{\hat{x}} - a\left(x_1 - \frac{1}{4}\right)\,\mathbf{\hat{y}} + a\left(x_1 + \frac{3}{4}\right)\,\mathbf{\hat{z}}$	(8c)	Co I
$\mathbf{B_8}$	=	$-\left(x_1 - \frac{1}{4}\right)\,\mathbf{a}_1 + \left(x_1 + \frac{3}{4}\right)\,\mathbf{a}_2 + \left(x_1 + \frac{1}{4}\right)\,\mathbf{a}_3$	=	$-a\left(x_1 - \frac{1}{4}\right)\,\mathbf{\hat{x}} + a\left(x_1 + \frac{3}{4}\right)\,\mathbf{\hat{y}} + a\left(x_1 + \frac{1}{4}\right)\,\mathbf{\hat{z}}$	(8c)	Co I
$\mathbf{B_9}$	=	$\frac{1}{8}\,\mathbf{a}_1 + y_2\,\mathbf{a}_2 + \left(y_2 + \frac{1}{4}\right)\,\mathbf{a}_3$	=	$\frac{1}{8}a\,\mathbf{\hat{x}} + ay_2\,\mathbf{\hat{y}} + a\left(y_2 + \frac{1}{4}\right)\,\mathbf{\hat{z}}$	(12d)	Zn I
$\mathbf{B_{10}}$	=	$\frac{3}{8}\,\mathbf{a}_1 - y_2\,\mathbf{a}_2 + \left(y_2 + \frac{3}{4}\right)\,\mathbf{a}_3$	=	$\frac{3}{8}a\,\mathbf{\hat{x}} - ay_2\,\mathbf{\hat{y}} + a\left(y_2 + \frac{3}{4}\right)\,\mathbf{\hat{z}}$	(12d)	Zn I
$\mathbf{B_{11}}$	=	$\frac{7}{8}\,\mathbf{a}_1 + \left(y_2 + \frac{1}{2}\right)\,\mathbf{a}_2 - \left(y_2 - \frac{1}{4}\right)\,\mathbf{a}_3$	=	$\frac{7}{8}a\,\mathbf{\hat{x}} + a\left(y_2 + \frac{1}{2}\right)\,\mathbf{\hat{y}} - a\left(y_2 - \frac{1}{4}\right)\,\mathbf{\hat{z}}$	(12d)	Zn I
$\mathbf{B_{12}}$	=	$\frac{5}{8}\,\mathbf{a}_1 - \left(y_2 - \frac{1}{2}\right)\,\mathbf{a}_2 - \left(y_2 - \frac{3}{4}\right)\,\mathbf{a}_3$	=	$\frac{5}{8}a\,\mathbf{\hat{x}} - a\left(y_2 - \frac{1}{2}\right)\,\mathbf{\hat{y}} - a\left(y_2 - \frac{3}{4}\right)\,\mathbf{\hat{z}}$	(12d)	Zn I
$\mathbf{B_{13}}$	=	$\left(y_2 + \frac{1}{4}\right)\,\mathbf{a}_1 + \frac{1}{8}\,\mathbf{a}_2 + y_2\,\mathbf{a}_3$	=	$a\left(y_2 + \frac{1}{4}\right)\,\mathbf{\hat{x}} + \frac{1}{8}a\,\mathbf{\hat{y}} + ay_2\,\mathbf{\hat{z}}$	(12d)	Zn I
$\mathbf{B_{14}}$	=	$\left(y_2 + \frac{3}{4}\right)\,\mathbf{a}_1 + \frac{3}{8}\,\mathbf{a}_2 - y_2\,\mathbf{a}_3$	=	$a\left(y_2 + \frac{3}{4}\right)\,\mathbf{\hat{x}} + \frac{3}{8}a\,\mathbf{\hat{y}} - ay_2\,\mathbf{\hat{z}}$	(12d)	Zn I
$\mathbf{B_{15}}$	=	$-\left(y_2 - \frac{1}{4}\right)\,\mathbf{a}_1 + \frac{7}{8}\,\mathbf{a}_2 + \left(y_2 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(y_2 - \frac{1}{4}\right)\,\mathbf{\hat{x}} + \frac{7}{8}a\,\mathbf{\hat{y}} + a\left(y_2 + \frac{1}{2}\right)\,\mathbf{\hat{z}}$	(12d)	Zn I
$\mathbf{B_{16}}$	=	$-\left(y_2 - \frac{3}{4}\right)\,\mathbf{a}_1 + \frac{5}{8}\,\mathbf{a}_2 - \left(y_2 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(y_2 - \frac{3}{4}\right)\,\mathbf{\hat{x}} + \frac{5}{8}a\,\mathbf{\hat{y}} - a\left(y_2 - \frac{1}{2}\right)\,\mathbf{\hat{z}}$	(12d)	Zn I
$\mathbf{B_{17}}$	=	$y_2\,\mathbf{a}_1 + \left(y_2 + \frac{1}{4}\right)\,\mathbf{a}_2 + \frac{1}{8}\,\mathbf{a}_3$	=	$ay_2\,\mathbf{\hat{x}} + a\left(y_2 + \frac{1}{4}\right)\,\mathbf{\hat{y}} + \frac{1}{8}a\,\mathbf{\hat{z}}$	(12d)	Zn I
$\mathbf{B_{18}}$	=	$-y_2\,\mathbf{a}_1 + \left(y_2 + \frac{3}{4}\right)\,\mathbf{a}_2 + \frac{3}{8}\,\mathbf{a}_3$	=	$-ay_2\,\mathbf{\hat{x}} + a\left(y_2 + \frac{3}{4}\right)\,\mathbf{\hat{y}} + \frac{3}{8}a\,\mathbf{\hat{z}}$	(12d)	Zn I
$\mathbf{B_{19}}$	=	$\left(y_2 + \frac{1}{2}\right)\,\mathbf{a}_1 - \left(y_2 - \frac{1}{4}\right)\,\mathbf{a}_2 + \frac{7}{8}\,\mathbf{a}_3$	=	$a\left(y_2 + \frac{1}{2}\right)\,\mathbf{\hat{x}} - a\left(y_2 - \frac{1}{4}\right)\,\mathbf{\hat{y}} + \frac{7}{8}a\,\mathbf{\hat{z}}$	(12d)	Zn I
$\mathbf{B_{20}}$	=	$-\left(y_2 - \frac{1}{2}\right)\,\mathbf{a}_1 - \left(y_2 - \frac{3}{4}\right)\,\mathbf{a}_2 + \frac{5}{8}\,\mathbf{a}_3$	=	$-a\left(y_2 - \frac{1}{2}\right)\,\mathbf{\hat{x}} - a\left(y_2 - \frac{3}{4}\right)\,\mathbf{\hat{y}} + \frac{5}{8}a\,\mathbf{\hat{z}}$	(12d)	Zn I

References

[1] J. D. Bocarsly, C. Heikes, C. M. Brown, S. D. Wilson, and R. Seshadri, *Deciphering structural and magnetic disorder in the chiral skyrmion host materials* $Co_xZn_yMn_z$ $(x + y + z = 20)$, Phys. Rev. Materials **3**, 014402 (2019), doi:10.1103/PhysRevMaterials.3.014402.

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