"Double-Double" Perovskite $CaMnCrSbO_6$ Structure: ABCD6E_tP40_86_e_c_ab_3g_d-001

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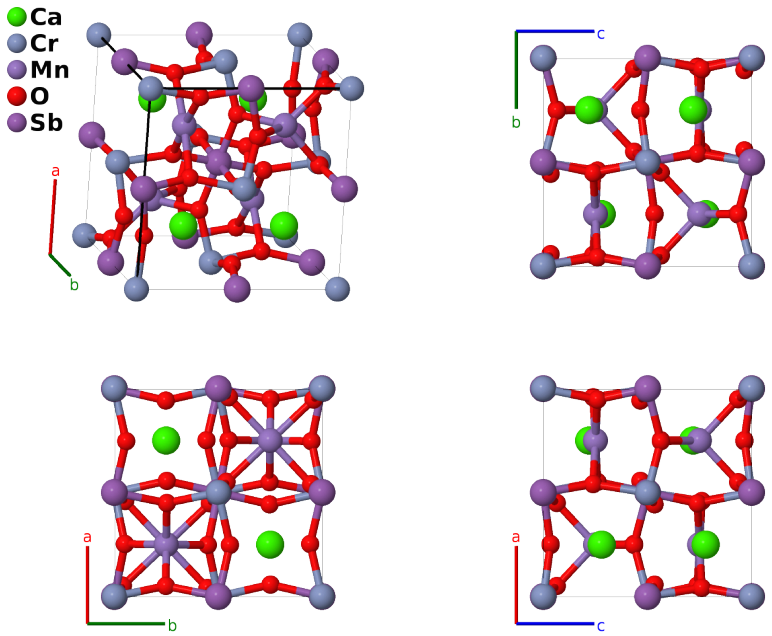
https://aflow.org/p/UT10

https://aflow.org/p/ABCD6E_tP40_86_e_c_ab_3g_d-001



Prototype	$CaCrMnO_6Sb$
AFLOW prototype label	ABCD6E_tP40_86_e_c_ab_3g_d-001
ICSD	none
Pearson symbol	tP40
Space group number	86
Space group symbol	$P4_2/n$
AFLOW prototype command	`aflow --proto=ABCD6E_tP40_86_e_c_ab_3g_d-001 --params=`$a, c/a, z_5, x_6, y_6, z_6, x_7, y_7, z_7, x_8, y_8, z_8$

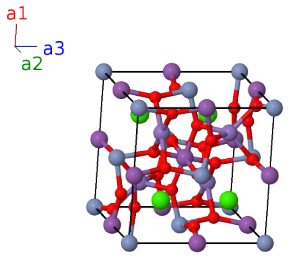
Other compounds with this structure
$CaMnFeSbO_6$

- There is some mixing on the nominal manganese, chromium, and antimony sites (Solana-Madruga, 2021)):
  - Mn-I (2a) is 81% Mn and 19% Cr.
  - Mn-II (2b) is 82% Mn and 18% Cr.
  - Cr (4c) is 95.2% Cr and 4.8% Sb.
  - Sb (4d) is 95.2% Sb and 4.8% Cr.

- This makes actual stoichiometry of this sample $CaMn_{0.815}Cr_{1.37}SbO_6$.

Simple Tetragonal primitive vectors

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



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$\frac{1}{4}\,\mathbf{a}_1+\frac{1}{4}\,\mathbf{a}_2+\frac{1}{4}\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}}+\frac{1}{4}a\,\hat{\mathbf{y}}+\frac{1}{4}c\,\hat{\mathbf{z}}$	(2a)	Mn I
$\mathbf{B_2}$	=	$\frac{3}{4}\,\mathbf{a}_1+\frac{3}{4}\,\mathbf{a}_2+\frac{3}{4}\,\mathbf{a}_3$	=	$\frac{3}{4}a\,\hat{\mathbf{x}}+\frac{3}{4}a\,\hat{\mathbf{y}}+\frac{3}{4}c\,\hat{\mathbf{z}}$	(2a)	Mn I
$\mathbf{B_3}$	=	$\frac{1}{4}\,\mathbf{a}_1+\frac{1}{4}\,\mathbf{a}_2+\frac{3}{4}\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}}+\frac{1}{4}a\,\hat{\mathbf{y}}+\frac{3}{4}c\,\hat{\mathbf{z}}$	(2b)	Mn II
$\mathbf{B_4}$	=	$\frac{3}{4}\,\mathbf{a}_1+\frac{3}{4}\,\mathbf{a}_2+\frac{1}{4}\,\mathbf{a}_3$	=	$\frac{3}{4}a\,\hat{\mathbf{x}}+\frac{3}{4}a\,\hat{\mathbf{y}}+\frac{1}{4}c\,\hat{\mathbf{z}}$	(2b)	Mn II
$\mathbf{B_5}$	=	0	=	0	(4c)	Cr I
$\mathbf{B_6}$	=	$\frac{1}{2}\,\mathbf{a}_1+\frac{1}{2}\,\mathbf{a}_2$	=	$\frac{1}{2}a\,\hat{\mathbf{x}}+\frac{1}{2}a\,\hat{\mathbf{y}}$	(4c)	Cr I
$\mathbf{B_7}$	=	$\frac{1}{2}\,\mathbf{a}_2+\frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{y}}+\frac{1}{2}c\,\hat{\mathbf{z}}$	(4c)	Cr I
$\mathbf{B_8}$	=	$\frac{1}{2}\,\mathbf{a}_1+\frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}}+\frac{1}{2}c\,\hat{\mathbf{z}}$	(4c)	Cr I
$\mathbf{B_9}$	=	$\frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}c\,\hat{\mathbf{z}}$	(4d)	Sb I
$\mathbf{B_{10}}$	=	$\frac{1}{2}\,\mathbf{a}_1+\frac{1}{2}\,\mathbf{a}_2+\frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}}+\frac{1}{2}a\,\hat{\mathbf{y}}+\frac{1}{2}c\,\hat{\mathbf{z}}$	(4d)	Sb I
$\mathbf{B_{11}}$	=	$\frac{1}{2}\,\mathbf{a}_2$	=	$\frac{1}{2}a\,\hat{\mathbf{y}}$	(4d)	Sb I
$\mathbf{B_{12}}$	=	$\frac{1}{2}\,\mathbf{a}_1$	=	$\frac{1}{2}a\,\hat{\mathbf{x}}$	(4d)	Sb I
$\mathbf{B_{13}}$	=	$\frac{3}{4}\,\mathbf{a}_1+\frac{1}{4}\,\mathbf{a}_2+z_5\,\mathbf{a}_3$	=	$\frac{3}{4}a\,\hat{\mathbf{x}}+\frac{1}{4}a\,\hat{\mathbf{y}}+cz_5\,\hat{\mathbf{z}}$	(4e)	Ca I
$\mathbf{B_{14}}$	=	$\frac{3}{4}\,\mathbf{a}_1+\frac{1}{4}\,\mathbf{a}_2+\left(z_5+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{3}{4}a\,\hat{\mathbf{x}}+\frac{1}{4}a\,\hat{\mathbf{y}}+c\left(z_5+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4e)	Ca I
$\mathbf{B_{15}}$	=	$\frac{1}{4}\,\mathbf{a}_1+\frac{3}{4}\,\mathbf{a}_2-z_5\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}}+\frac{3}{4}a\,\hat{\mathbf{y}}-cz_5\,\hat{\mathbf{z}}$	(4e)	Ca I
$\mathbf{B_{16}}$	=	$\frac{1}{4}\,\mathbf{a}_1+\frac{3}{4}\,\mathbf{a}_2-\left(z_5-\frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}}+\frac{3}{4}a\,\hat{\mathbf{y}}-c\left(z_5-\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4e)	Ca I
$\mathbf{B_{17}}$	=	$x_6\,\mathbf{a}_1+y_6\,\mathbf{a}_2+z_6\,\mathbf{a}_3$	=	$ax_6\,\hat{\mathbf{x}}+ay_6\,\hat{\mathbf{y}}+cz_6\,\hat{\mathbf{z}}$	(8g)	O I
$\mathbf{B_{18}}$	=	$-\left(x_6-\frac{1}{2}\right)\,\mathbf{a}_1-\left(y_6-\frac{1}{2}\right)\,\mathbf{a}_2+z_6\,\mathbf{a}_3$	=	$-a\left(x_6-\frac{1}{2}\right)\,\hat{\mathbf{x}}-a\left(y_6-\frac{1}{2}\right)\,\hat{\mathbf{y}}+cz_6\,\hat{\mathbf{z}}$	(8g)	O I
$\mathbf{B_{19}}$	=	$-y_6\,\mathbf{a}_1+\left(x_6+\frac{1}{2}\right)\,\mathbf{a}_2+\left(z_6+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ay_6\,\hat{\mathbf{x}}+a\left(x_6+\frac{1}{2}\right)\,\hat{\mathbf{y}}+c\left(z_6+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8g)	O I
$\mathbf{B_{20}}$	=	$\left(y_6+\frac{1}{2}\right)\,\mathbf{a}_1-x_6\,\mathbf{a}_2+\left(z_6+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$a\left(y_6+\frac{1}{2}\right)\,\hat{\mathbf{x}}-ax_6\,\hat{\mathbf{y}}+c\left(z_6+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8g)	O I
$\mathbf{B_{21}}$	=	$-x_6\,\mathbf{a}_1-y_6\,\mathbf{a}_2-z_6\,\mathbf{a}_3$	=	$-ax_6\,\hat{\mathbf{x}}-ay_6\,\hat{\mathbf{y}}-cz_6\,\hat{\mathbf{z}}$	(8g)	O I
$\mathbf{B_{22}}$	=	$\left(x_6+\frac{1}{2}\right)\,\mathbf{a}_1+\left(y_6+\frac{1}{2}\right)\,\mathbf{a}_2-z_6\,\mathbf{a}_3$	=	$a\left(x_6+\frac{1}{2}\right)\,\hat{\mathbf{x}}+a\left(y_6+\frac{1}{2}\right)\,\hat{\mathbf{y}}-cz_6\,\hat{\mathbf{z}}$	(8g)	O I
$\mathbf{B_{23}}$	=	$y_6\,\mathbf{a}_1-\left(x_6-\frac{1}{2}\right)\,\mathbf{a}_2-\left(z_6-\frac{1}{2}\right)\,\mathbf{a}_3$	=	$ay_6\,\hat{\mathbf{x}}-a\left(x_6-\frac{1}{2}\right)\,\hat{\mathbf{y}}-c\left(z_6-\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8g)	O I
$\mathbf{B_{24}}$	=	$-\left(y_6-\frac{1}{2}\right)\,\mathbf{a}_1+x_6\,\mathbf{a}_2-\left(z_6-\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(y_6-\frac{1}{2}\right)\,\hat{\mathbf{x}}+ax_6\,\hat{\mathbf{y}}-c\left(z_6-\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8g)	O I
$\mathbf{B_{25}}$	=	$x_7\,\mathbf{a}_1+y_7\,\mathbf{a}_2+z_7\,\mathbf{a}_3$	=	$ax_7\,\hat{\mathbf{x}}+ay_7\,\hat{\mathbf{y}}+cz_7\,\hat{\mathbf{z}}$	(8g)	O II

$\mathbf{B_{26}}$	=	$-\left(x_7-\frac{1}{2}\right)\,\mathbf{a}_1-\left(y_7-\frac{1}{2}\right)\,\mathbf{a}_2+z_7\,\mathbf{a}_3$	=	$-a\left(x_7-\frac{1}{2}\right)\,\hat{\mathbf{x}}-a\left(y_7-\frac{1}{2}\right)\,\hat{\mathbf{y}}+cz_7\,\hat{\mathbf{z}}$	(8g)	O II
$\mathbf{B_{27}}$	=	$-y_7\,\mathbf{a}_1+\left(x_7+\frac{1}{2}\right)\,\mathbf{a}_2+\left(z_7+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ay_7\,\hat{\mathbf{x}}+a\left(x_7+\frac{1}{2}\right)\,\hat{\mathbf{y}}+c\left(z_7+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8g)	O II
$\mathbf{B_{28}}$	=	$\left(y_7+\frac{1}{2}\right)\,\mathbf{a}_1-x_7\,\mathbf{a}_2+\left(z_7+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$a\left(y_7+\frac{1}{2}\right)\,\hat{\mathbf{x}}-ax_7\,\hat{\mathbf{y}}+c\left(z_7+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8g)	O II
$\mathbf{B_{29}}$	=	$-x_7\,\mathbf{a}_1-y_7\,\mathbf{a}_2-z_7\,\mathbf{a}_3$	=	$-ax_7\,\hat{\mathbf{x}}-ay_7\,\hat{\mathbf{y}}-cz_7\,\hat{\mathbf{z}}$	(8g)	O II
$\mathbf{B_{30}}$	=	$\left(x_7+\frac{1}{2}\right)\,\mathbf{a}_1+\left(y_7+\frac{1}{2}\right)\,\mathbf{a}_2-z_7\,\mathbf{a}_3$	=	$a\left(x_7+\frac{1}{2}\right)\,\hat{\mathbf{x}}+a\left(y_7+\frac{1}{2}\right)\,\hat{\mathbf{y}}-cz_7\,\hat{\mathbf{z}}$	(8g)	O II
$\mathbf{B_{31}}$	=	$y_7\,\mathbf{a}_1-\left(x_7-\frac{1}{2}\right)\,\mathbf{a}_2-\left(z_7-\frac{1}{2}\right)\,\mathbf{a}_3$	=	$ay_7\,\hat{\mathbf{x}}-a\left(x_7-\frac{1}{2}\right)\,\hat{\mathbf{y}}-c\left(z_7-\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8g)	O II
$\mathbf{B_{32}}$	=	$-\left(y_7-\frac{1}{2}\right)\,\mathbf{a}_1+x_7\,\mathbf{a}_2-\left(z_7-\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(y_7-\frac{1}{2}\right)\,\hat{\mathbf{x}}+ax_7\,\hat{\mathbf{y}}-c\left(z_7-\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8g)	O II
$\mathbf{B_{33}}$	=	$x_8\,\mathbf{a}_1+y_8\,\mathbf{a}_2+z_8\,\mathbf{a}_3$	=	$ax_8\,\hat{\mathbf{x}}+ay_8\,\hat{\mathbf{y}}+cz_8\,\hat{\mathbf{z}}$	(8g)	O III
$\mathbf{B_{34}}$	=	$-\left(x_8-\frac{1}{2}\right)\,\mathbf{a}_1-\left(y_8-\frac{1}{2}\right)\,\mathbf{a}_2+z_8\,\mathbf{a}_3$	=	$-a\left(x_8-\frac{1}{2}\right)\,\hat{\mathbf{x}}-a\left(y_8-\frac{1}{2}\right)\,\hat{\mathbf{y}}+cz_8\,\hat{\mathbf{z}}$	(8g)	O III
$\mathbf{B_{35}}$	=	$-y_8\,\mathbf{a}_1+\left(x_8+\frac{1}{2}\right)\,\mathbf{a}_2+\left(z_8+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ay_8\,\hat{\mathbf{x}}+a\left(x_8+\frac{1}{2}\right)\,\hat{\mathbf{y}}+c\left(z_8+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8g)	O III
$\mathbf{B_{36}}$	=	$\left(y_8+\frac{1}{2}\right)\,\mathbf{a}_1-x_8\,\mathbf{a}_2+\left(z_8+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$a\left(y_8+\frac{1}{2}\right)\,\hat{\mathbf{x}}-ax_8\,\hat{\mathbf{y}}+c\left(z_8+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8g)	O III
$\mathbf{B_{37}}$	=	$-x_8\,\mathbf{a}_1-y_8\,\mathbf{a}_2-z_8\,\mathbf{a}_3$	=	$-ax_8\,\hat{\mathbf{x}}-ay_8\,\hat{\mathbf{y}}-cz_8\,\hat{\mathbf{z}}$	(8g)	O III
$\mathbf{B_{38}}$	=	$\left(x_8+\frac{1}{2}\right)\,\mathbf{a}_1+\left(y_8+\frac{1}{2}\right)\,\mathbf{a}_2-z_8\,\mathbf{a}_3$	=	$a\left(x_8+\frac{1}{2}\right)\,\hat{\mathbf{x}}+a\left(y_8+\frac{1}{2}\right)\,\hat{\mathbf{y}}-cz_8\,\hat{\mathbf{z}}$	(8g)	O III
$\mathbf{B_{39}}$	=	$y_8\,\mathbf{a}_1-\left(x_8-\frac{1}{2}\right)\,\mathbf{a}_2-\left(z_8-\frac{1}{2}\right)\,\mathbf{a}_3$	=	$ay_8\,\hat{\mathbf{x}}-a\left(x_8-\frac{1}{2}\right)\,\hat{\mathbf{y}}-c\left(z_8-\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8g)	O III
$\mathbf{B_{40}}$	=	$-\left(y_8-\frac{1}{2}\right)\,\mathbf{a}_1+x_8\,\mathbf{a}_2-\left(z_8-\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(y_8-\frac{1}{2}\right)\,\hat{\mathbf{x}}+ax_8\,\hat{\mathbf{y}}-c\left(z_8-\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8g)	O III

References

[1] E. Solana-Madruga, P. S. Kearins, K. N. Alharbi, C. T. Lennon, C. Ritter, and J. P. Attfield, *Ferrimagnetism and spin reorientation in the high-pressure double double perovskites $CaMnCrSbO_6$ and $CaMnFeSbO_6$*, Phys. Rev. Materials **5**, 054412 (2021), doi:10.1103/PhysRevMaterials.5.054412.

Found in

[1] R. Dhawan, P. Balasubramanian, and T. Nautiyal, *Origins of multi-sublattice magnetism and superexchange interactions in double-double perovskite $CaMnCrSbO_6$* (2022), doi:10.48550/arXiv.2205.02452. ArXiv:2205.02452 [cond-mat.mtrl-sci].