$CaMnSb_2$ Structure: ABC2_oP16_62_c_c_2c-003

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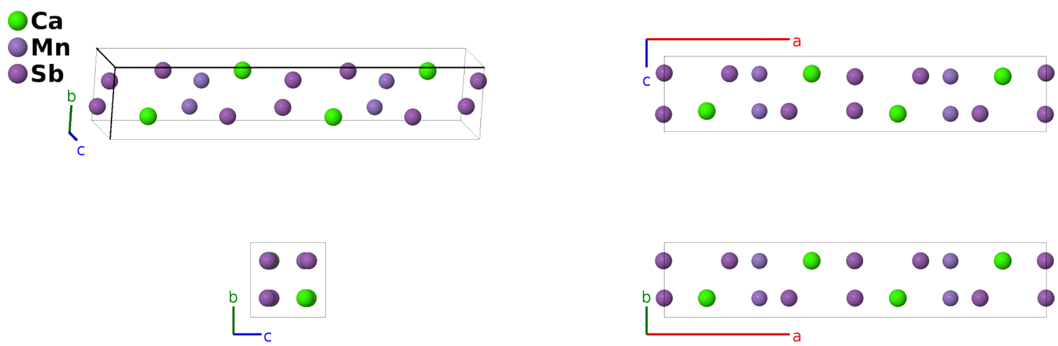
https://aflow.org/p/JHY5

https://aflow.org/p/ABC2_oP16_62_c_c_2c-003



Prototype	$CaMnSb_2$
AFLOW prototype label	ABC2_oP16_62_c_c_2c-003
ICSD	52705
Pearson symbol	oP16
Space group number	62
Space group symbol	*Pnma*
AFLOW prototype command	`aflow --proto=ABC2_oP16_62_c_c_2c-003` `--params=`$a, b/a, c/a, x_1, z_1, x_2, z_2, x_3, z_3, x_4, z_4$

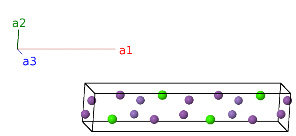
Other compounds with this structure

$EuMnSb_2$, $SrMnSb_2$, $ZrMnSb_2$

- This structure has the same AFLOW label as diaspore, AlOOH ($E0_2$), ABC2_oP16_62_c_c_2c. The structures are generated by the same symmetry operations with different sets of parameters (`--params`) specified in their corresponding CIF files.

Simple Orthorhombic primitive vectors

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



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$x_1\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 + z_1\,\mathbf{a}_3$	=	$ax_1\,\mathbf{\hat{x}} + \frac{1}{4}b\,\mathbf{\hat{y}} + cz_1\,\mathbf{\hat{z}}$	(4c)	Ca I
$\mathbf{B_2}$	=	$-\left(x_1 - \frac{1}{2}\right)\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 + \left(z_1 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(x_1 - \frac{1}{2}\right)\,\mathbf{\hat{x}} + \frac{3}{4}b\,\mathbf{\hat{y}} + c\left(z_1 + \frac{1}{2}\right)\,\mathbf{\hat{z}}$	(4c)	Ca I
$\mathbf{B_3}$	=	$-x_1\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 - z_1\,\mathbf{a}_3$	=	$-ax_1\,\mathbf{\hat{x}} + \frac{3}{4}b\,\mathbf{\hat{y}} - cz_1\,\mathbf{\hat{z}}$	(4c)	Ca I
$\mathbf{B_4}$	=	$\left(x_1 + \frac{1}{2}\right)\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 - \left(z_1 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$a\left(x_1 + \frac{1}{2}\right)\,\mathbf{\hat{x}} + \frac{1}{4}b\,\mathbf{\hat{y}} - c\left(z_1 - \frac{1}{2}\right)\,\mathbf{\hat{z}}$	(4c)	Ca I
$\mathbf{B_5}$	=	$x_2\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 + z_2\,\mathbf{a}_3$	=	$ax_2\,\mathbf{\hat{x}} + \frac{1}{4}b\,\mathbf{\hat{y}} + cz_2\,\mathbf{\hat{z}}$	(4c)	Mn I
$\mathbf{B_6}$	=	$-\left(x_2 - \frac{1}{2}\right)\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 + \left(z_2 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(x_2 - \frac{1}{2}\right)\,\mathbf{\hat{x}} + \frac{3}{4}b\,\mathbf{\hat{y}} + c\left(z_2 + \frac{1}{2}\right)\,\mathbf{\hat{z}}$	(4c)	Mn I
$\mathbf{B_7}$	=	$-x_2\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 - z_2\,\mathbf{a}_3$	=	$-ax_2\,\mathbf{\hat{x}} + \frac{3}{4}b\,\mathbf{\hat{y}} - cz_2\,\mathbf{\hat{z}}$	(4c)	Mn I
$\mathbf{B_8}$	=	$\left(x_2 + \frac{1}{2}\right)\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 - \left(z_2 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$a\left(x_2 + \frac{1}{2}\right)\,\mathbf{\hat{x}} + \frac{1}{4}b\,\mathbf{\hat{y}} - c\left(z_2 - \frac{1}{2}\right)\,\mathbf{\hat{z}}$	(4c)	Mn I
$\mathbf{B_9}$	=	$x_3\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 + z_3\,\mathbf{a}_3$	=	$ax_3\,\mathbf{\hat{x}} + \frac{1}{4}b\,\mathbf{\hat{y}} + cz_3\,\mathbf{\hat{z}}$	(4c)	Sb I
$\mathbf{B_{10}}$	=	$-\left(x_3 - \frac{1}{2}\right)\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 + \left(z_3 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(x_3 - \frac{1}{2}\right)\,\mathbf{\hat{x}} + \frac{3}{4}b\,\mathbf{\hat{y}} + c\left(z_3 + \frac{1}{2}\right)\,\mathbf{\hat{z}}$	(4c)	Sb I
$\mathbf{B_{11}}$	=	$-x_3\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 - z_3\,\mathbf{a}_3$	=	$-ax_3\,\mathbf{\hat{x}} + \frac{3}{4}b\,\mathbf{\hat{y}} - cz_3\,\mathbf{\hat{z}}$	(4c)	Sb I
$\mathbf{B_{12}}$	=	$\left(x_3 + \frac{1}{2}\right)\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 - \left(z_3 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$a\left(x_3 + \frac{1}{2}\right)\,\mathbf{\hat{x}} + \frac{1}{4}b\,\mathbf{\hat{y}} - c\left(z_3 - \frac{1}{2}\right)\,\mathbf{\hat{z}}$	(4c)	Sb I
$\mathbf{B_{13}}$	=	$x_4\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 + z_4\,\mathbf{a}_3$	=	$ax_4\,\mathbf{\hat{x}} + \frac{1}{4}b\,\mathbf{\hat{y}} + cz_4\,\mathbf{\hat{z}}$	(4c)	Sb II
$\mathbf{B_{14}}$	=	$-\left(x_4 - \frac{1}{2}\right)\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 + \left(z_4 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(x_4 - \frac{1}{2}\right)\,\mathbf{\hat{x}} + \frac{3}{4}b\,\mathbf{\hat{y}} + c\left(z_4 + \frac{1}{2}\right)\,\mathbf{\hat{z}}$	(4c)	Sb II
$\mathbf{B_{15}}$	=	$-x_4\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 - z_4\,\mathbf{a}_3$	=	$-ax_4\,\mathbf{\hat{x}} + \frac{3}{4}b\,\mathbf{\hat{y}} - cz_4\,\mathbf{\hat{z}}$	(4c)	Sb II
$\mathbf{B_{16}}$	=	$\left(x_4 + \frac{1}{2}\right)\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 - \left(z_4 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$a\left(x_4 + \frac{1}{2}\right)\,\mathbf{\hat{x}} + \frac{1}{4}b\,\mathbf{\hat{y}} - c\left(z_4 - \frac{1}{2}\right)\,\mathbf{\hat{z}}$	(4c)	Sb II

References

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