Double Perovskite (Ba_2MnWO_6) Structure: A2BC6D_cF40_225_c_a_e_b-001

This structure originally had the label `A2BC6D_cF40_225_c_a_e_b`. Calls to that address will be redirected here.

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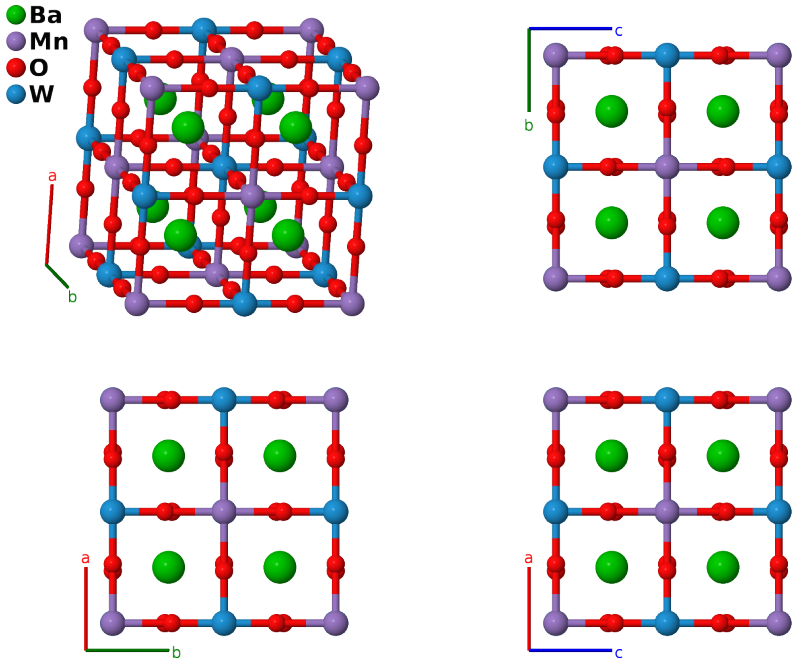
https://aflow.org/p/83J5

https://aflow.org/p/A2BC6D_cF40_225_c_a_e_b-001



Prototype	Ba_2MnO_6W
AFLOW prototype label	A2BC6D_cF40_225_c_a_e_b-001
Mineral name	double perovskite
ICSD	51613
Pearson symbol	cF40
Space group number	225
Space group symbol	$Fm\bar{3}m$
AFLOW prototype command	`aflow --proto=A2BC6D_cF40_225_c_a_e_b-001 --params=`a, x_4

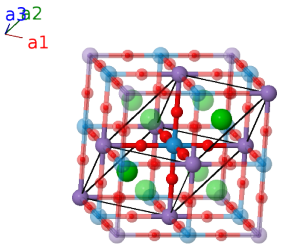
Other compounds with this structure

Ba_2CaReO_6, Ba_2CaWO_6, Ba_2CdReO_6, Ba_2DyIrO_6, Ba_2IrNiO_6, Ba_2LiOsO_6, Ba_2MgReO_6, Ba_2NaOsO_6, Ba_2NdIrO_6, Ba_2SmIrO_6, Ba_2ZnReO_6, Bi_2FeCrO_6, Ca_2MnReO_6, Cs_2AgBBr_6, Cs_2AgBCl_6, $Cs_2AgBiBr_6$, $Cs_2AgInBr_6$, $Cs_2AgInCl_6$, Cs_2LiTlF_6, Cs_2NaBBr_6, Cs_2NaBCl_6, $Cs_2NaBiCl_6$, $Cs_2NaInBr_6$, $Cs_2NaInCl_6$, $Cs_2NaLaCl_6$, Cu_2TiSiO_6, K_2NaAlF_6 (elpasolite), $K_2NaBiCl_6$, La_2TcNiO_6, Mn_2FeSbO_6, $Rb_2NaBiCl_6$, Sr_2CrReO_6, Sr_2FeMoO_6, Sr_2ReMoO_6, Sr_2TiFeO_6, Sr_2YIrO_6, $(La_{0.5}Sc_{0.5})_2MnCoO_6$

- We use the data taken at room temperature.

Face-centered Cubic primitive vectors

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



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	0	=	0	(4a)	Mn I
$\mathbf{B_2}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{y}} + \frac{1}{2}a\,\hat{\mathbf{z}}$	(4b)	W I
$\mathbf{B_3}$	=	$\frac{1}{4}\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + \frac{1}{4}a\,\hat{\mathbf{y}} + \frac{1}{4}a\,\hat{\mathbf{z}}$	(8c)	Ba I
$\mathbf{B_4}$	=	$\frac{3}{4}\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$\frac{3}{4}a\,\hat{\mathbf{x}} + \frac{3}{4}a\,\hat{\mathbf{y}} + \frac{3}{4}a\,\hat{\mathbf{z}}$	(8c)	Ba I
$\mathbf{B_5}$	=	$-x_4\,\mathbf{a}_1 + x_4\,\mathbf{a}_2 + x_4\,\mathbf{a}_3$	=	$ax_4\,\hat{\mathbf{x}}$	(24e)	O I
$\mathbf{B_6}$	=	$x_4\,\mathbf{a}_1 - x_4\,\mathbf{a}_2 - x_4\,\mathbf{a}_3$	=	$-ax_4\,\hat{\mathbf{x}}$	(24e)	O I
$\mathbf{B_7}$	=	$x_4\,\mathbf{a}_1 - x_4\,\mathbf{a}_2 + x_4\,\mathbf{a}_3$	=	$ax_4\,\hat{\mathbf{y}}$	(24e)	O I
$\mathbf{B_8}$	=	$-x_4\,\mathbf{a}_1 + x_4\,\mathbf{a}_2 - x_4\,\mathbf{a}_3$	=	$-ax_4\,\hat{\mathbf{y}}$	(24e)	O I
$\mathbf{B_9}$	=	$x_4\,\mathbf{a}_1 + x_4\,\mathbf{a}_2 - x_4\,\mathbf{a}_3$	=	$ax_4\,\hat{\mathbf{z}}$	(24e)	O I
$\mathbf{B_{10}}$	=	$-x_4\,\mathbf{a}_1 - x_4\,\mathbf{a}_2 + x_4\,\mathbf{a}_3$	=	$-ax_4\,\hat{\mathbf{z}}$	(24e)	O I

References

[1] A. K. Azad, S. A. Ivanov, S.-G. Eriksson, J. Eriksen, H. Rundlöf, R. Mathieu, and P. Svedlindh, *Synthesis, crystal structure, and magnetic characterization of the double perovskite Ba_2MnWO_6*, Mater. Res. Bull. **36**, 2215–2228 (2001), doi:10.1016/S0025-5408(01)00707-3.