Mn_3As ($D0_d$) Structure: AB3_oC16_63_c_3c-001

This structure previously used the label(s) `AB3_oC16_63_c_3c`. Calls to these addresses will be redirected here.

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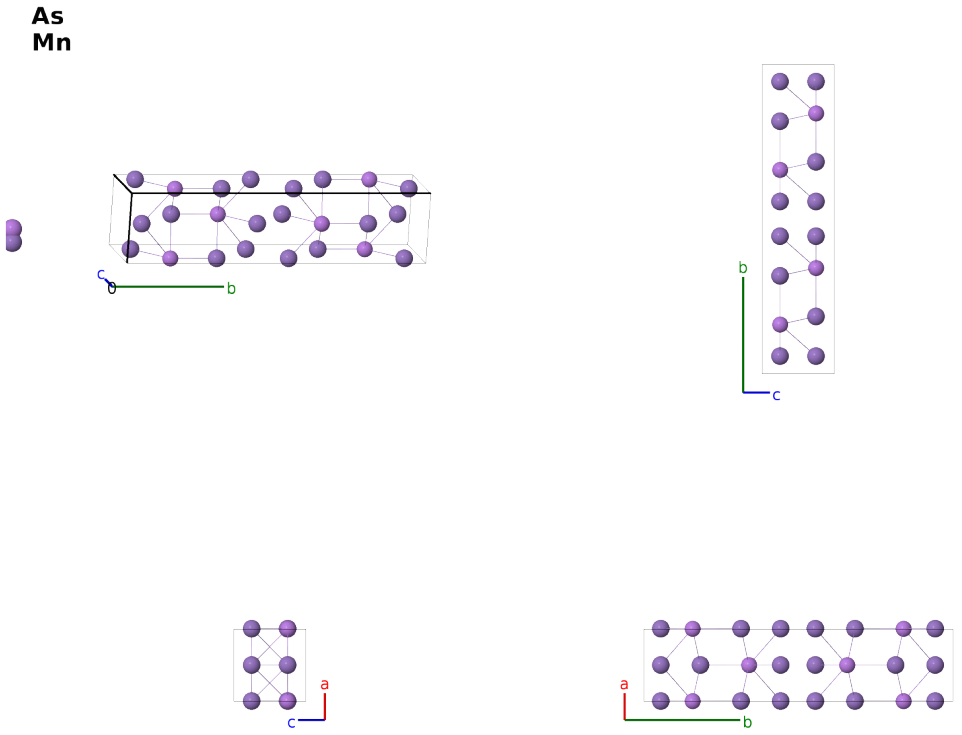
https://aflow.org/prototype-encyclopedia/DPFG

https://aflow.org/prototype-encyclopedia/AB3_oC16_63_c_3c-001



Prototype	$AsMn_3$
AFLOW prototype label	AB3_oC16_63_c_3c-001
ICSD	40437
CCDC	1610291
Pearson symbol	oC16
Space group number	63
Space group symbol	*Cmcm*

AFLOW prototype command `aflow --proto=AB3_oC16_63_c_3c-001 --params=`$a, b/a, c/a, y_1, y_2, y_3, y_4$

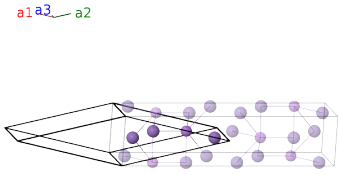
Other compounds with this structure

Te_3Nd, $DyGe_3$

- (Nowotny, 1951) set the structure of Mn_3As in space group $Pmmn$ #59. This was repeated by (Villars, 1991) and (Brandes, 1992). However, (Carrillo-Cabrera, 1983) showed that the structure actually reduces to space group $Cmcm$ #63, and this was recognized by (Parthé, 1993). We follow that latter two works and assign the $D0_e$ structure to space group $Cmcm$.
- (Carrillo-Cabrera, 1983) placed the structure in setting $Bmmb$ of space group #63, but we have shifted it to the standard $Cmcm$ setting.
- Mn_3As ($D0_d$) and $NdTe_3$ have the same AFLOW prototype label, AB3_oC16_63_c_3c. They are generated by the same symmetry operations with different sets of parameters (`--params`) specified in their corresponding CIF files.

Base-centered Orthorhombic primitive vectors

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



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$-y_1\,\mathbf{a}_1 + y_1\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$by_1\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(4c)	As I
$\mathbf{B_2}$	=	$y_1\,\mathbf{a}_1 - y_1\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$-by_1\,\hat{\mathbf{y}} + \frac{3}{4}c\,\hat{\mathbf{z}}$	(4c)	As I
$\mathbf{B_3}$	=	$-y_2\,\mathbf{a}_1 + y_2\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$by_2\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(4c)	Mn I
$\mathbf{B_4}$	=	$y_2\,\mathbf{a}_1 - y_2\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$-by_2\,\hat{\mathbf{y}} + \frac{3}{4}c\,\hat{\mathbf{z}}$	(4c)	Mn I
$\mathbf{B_5}$	=	$-y_3\,\mathbf{a}_1 + y_3\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$by_3\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(4c)	Mn II
$\mathbf{B_6}$	=	$y_3\,\mathbf{a}_1 - y_3\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$-by_3\,\hat{\mathbf{y}} + \frac{3}{4}c\,\hat{\mathbf{z}}$	(4c)	Mn II
$\mathbf{B_7}$	=	$-y_4\,\mathbf{a}_1 + y_4\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$by_4\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(4c)	Mn III
$\mathbf{B_8}$	=	$y_4\,\mathbf{a}_1 - y_4\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$-by_4\,\hat{\mathbf{y}} + \frac{3}{4}c\,\hat{\mathbf{z}}$	(4c)	Mn III

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