Mn_3As ($D0_d$) Structure: AB3_oC16_63_c_3c-001

This structure originally had the label `AB3_oC16_63_c_3c`. Calls to that address will be redirected here.

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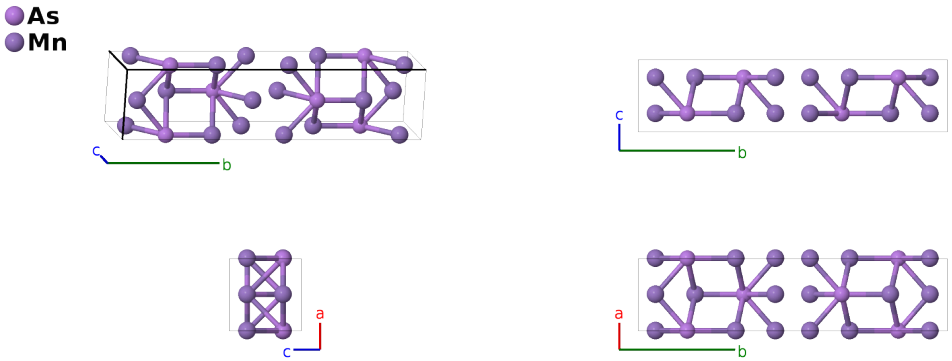
https://aflow.org/p/DPFG

https://aflow.org/p/AB3_oC16_63_c_3c-001



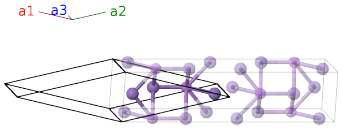
Prototype	$AsMn_3$
AFLOW prototype label	AB3_oC16_63_c_3c-001
ICSD	40437
Pearson symbol	oC16
Space group number	63
Space group symbol	*Cmcm*
AFLOW prototype command	`aflow --proto=AB3_oC16_63_c_3c-001 --params=`$a, b/a, c/a, y_1, y_2, y_3, y_4$

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.

Base-centered Orthorhombic primitive vectors

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



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

References

[1] W. Carrillo-Cabrera, *The Crystal Structure of $TiCu_2P$ and Its Relationship to the Structure of Mn_3As*, Acta Chem. Scand. **37A**, 93–98 (1983), doi:10.3891/acta.chem.scand.37a-0093.

[2] H. Nowotny, R. Funk, and J. Pesi, *Kristallchemische Untersuchungen in den Systemen Mn-As, V-Sb, Ti-Sb*, Monat. Chem. **82**, 513–525 (1951), doi:10.1007/BF00900849.

[3] E. Parthé, L. Gelato, B. Chabot, M. Penso, K. Cenzula, and R. Gladyshevskii, *Standardized Data and Crystal Chemical Characterization of Inorganic Structure Types*, *Gmelin Handbook of Inorganic and Organometallic Chemistry*, vol. 2 (Springer-Verlag, Berlin, Heidelberg, 1993), 8 edn., doi:10.1007/978-3-662-02909-1_3.

[4] E. A. Brandes and G. B. Brook, eds., *Smithells Metals Reference Book* (Butterworth Heinemann, Oxford, Auckland, Boston, Johannesburg, Melbourne, New Delhi, 1992), seventh edn.

[5] P. Villars and L. D. Calvert, eds., *Pearson's Handbook of Crystallographic Data for Intermetallic Phases* (ASM International, Materials Park, Ohio, 1991), 2^{nd} edn.