Haussmannite (Mn_3O_4) Structure: A3B4_tI28_141_ad_h-001

This structure originally had the label `A3B4_tI28_141_ad_h`. Calls to that address will be redirected here.

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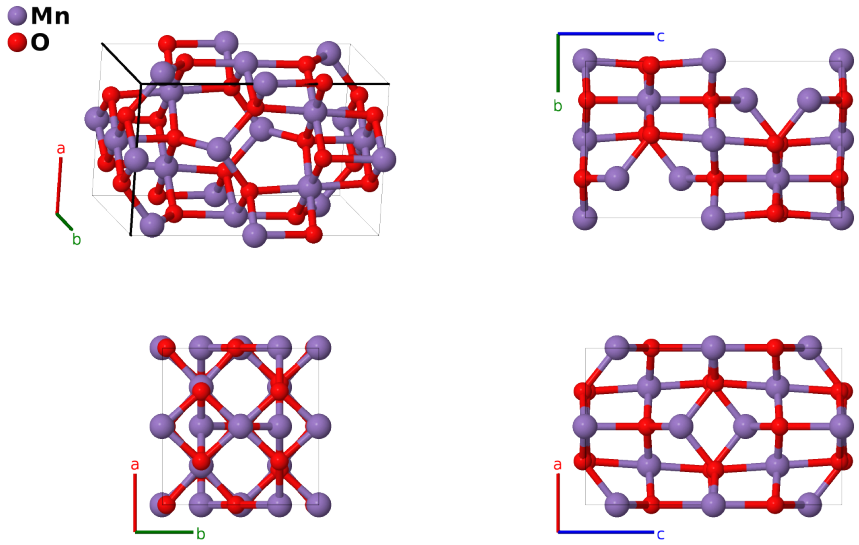
https://aflow.org/p/KP7A

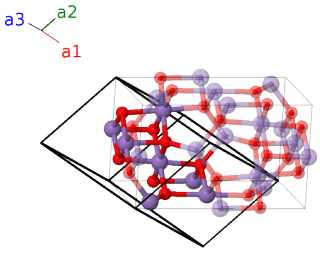
https://aflow.org/p/A3B4_tI28_141_ad_h-001



Prototype	Mn_3O_4
AFLOW prototype label	A3B4_tI28_141_ad_h-001
Mineral name	haussmannite
ICSD	68174
Pearson symbol	tI28
Space group number	141
Space group symbol	$I4_1/amd$
AFLOW prototype command	`aflow --proto=A3B4_tI28_141_ad_h-001 --params=`$a, c/a, y_3, z_3$

Body-centered Tetragonal primitive vectors

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



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$\frac{7}{8}\,\mathbf{a}_1 + \frac{1}{8}\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$\frac{3}{4}a\,\hat{\mathbf{y}} + \frac{1}{8}c\,\hat{\mathbf{z}}$	(4a)	Mn I
$\mathbf{B_2}$	=	$\frac{1}{8}\,\mathbf{a}_1 + \frac{7}{8}\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - \frac{1}{4}a\,\hat{\mathbf{y}} + \frac{3}{8}c\,\hat{\mathbf{z}}$	(4a)	Mn I
$\mathbf{B_3}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2$	=	$\frac{1}{2}c\,\hat{\mathbf{z}}$	(8d)	Mn II
$\mathbf{B_4}$	=	$\frac{1}{2}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}}$	(8d)	Mn II
$\mathbf{B_5}$	=	$\frac{1}{2}\,\mathbf{a}_1$	=	$-\frac{1}{4}a\,\hat{\mathbf{x}} + \frac{1}{4}a\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(8d)	Mn II
$\mathbf{B_6}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + \frac{1}{4}a\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(8d)	Mn II
$\mathbf{B_7}$	=	$(y_3 + z_3)\,\mathbf{a}_1 + z_3\,\mathbf{a}_2 + y_3\,\mathbf{a}_3$	=	$ay_3\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$	(16h)	O I
$\mathbf{B_8}$	=	$\left(-y_3 + z_3 + \frac{1}{2}\right)\,\mathbf{a}_1 + z_3\,\mathbf{a}_2 - \left(y_3 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(y_3 - \frac{1}{2}\right)\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$	(16h)	O I
$\mathbf{B_9}$	=	$z_3\,\mathbf{a}_1 + \left(-y_3 + z_3 + \frac{1}{2}\right)\,\mathbf{a}_2 - y_3\,\mathbf{a}_3$	=	$-a\left(y_3 - \frac{1}{4}\right)\,\hat{\mathbf{x}} - \frac{1}{4}a\,\hat{\mathbf{y}} + c\left(z_3 + \frac{1}{4}\right)\,\hat{\mathbf{z}}$	(16h)	O I
$\mathbf{B_{10}}$	=	$z_3\,\mathbf{a}_1 + (y_3 + z_3)\,\mathbf{a}_2 + \left(y_3 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$a\left(y_3 + \frac{1}{4}\right)\,\hat{\mathbf{x}} + \frac{1}{4}a\,\hat{\mathbf{y}} + c\left(z_3 - \frac{1}{4}\right)\,\hat{\mathbf{z}}$	(16h)	O I
$\mathbf{B_{11}}$	=	$\left(y_3 - z_3 + \frac{1}{2}\right)\,\mathbf{a}_1 - z_3\,\mathbf{a}_2 + \left(y_3 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$a\left(y_3 + \frac{1}{2}\right)\,\hat{\mathbf{y}} - cz_3\,\hat{\mathbf{z}}$	(16h)	O I
$\mathbf{B_{12}}$	=	$-(y_3 + z_3)\,\mathbf{a}_1 - z_3\,\mathbf{a}_2 - y_3\,\mathbf{a}_3$	=	$-ay_3\,\hat{\mathbf{y}} - cz_3\,\hat{\mathbf{z}}$	(16h)	O I
$\mathbf{B_{13}}$	=	$-z_3\,\mathbf{a}_1 + \left(y_3 - z_3 + \frac{1}{2}\right)\,\mathbf{a}_2 + y_3\,\mathbf{a}_3$	=	$a\left(y_3 + \frac{1}{4}\right)\,\hat{\mathbf{x}} - \frac{1}{4}a\,\hat{\mathbf{y}} - c\left(z_3 - \frac{1}{4}\right)\,\hat{\mathbf{z}}$	(16h)	O I
$\mathbf{B_{14}}$	=	$-z_3\,\mathbf{a}_1 - (y_3 + z_3)\,\mathbf{a}_2 - \left(y_3 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(y_3 - \frac{1}{4}\right)\,\hat{\mathbf{x}} + \frac{1}{4}a\,\hat{\mathbf{y}} - c\left(z_3 + \frac{1}{4}\right)\,\hat{\mathbf{z}}$	(16h)	O I

References

[1] D. Jarosch, *Crystal structure refinement and reflectance measurements of hausmannite, Mn_3O_4*, Mineralogy and Petrology **37**, 15–23 (1987), doi:10.1007/BF01163155.

Found in

[1] P. Villars and L. Calvert, *Pearson's Handbook of Crystallographic Data for Intermetallic Phases* (ASM International, Materials Park, OH, 1991), 2nd edn.