$HoMn_2O_5$ Structure: AB2C5_oP32_55_g_eh_fghi-001

This structure originally had the label `AB2C5_oP32_55_g_fh_eghi`. Calls to that address will be redirected here.

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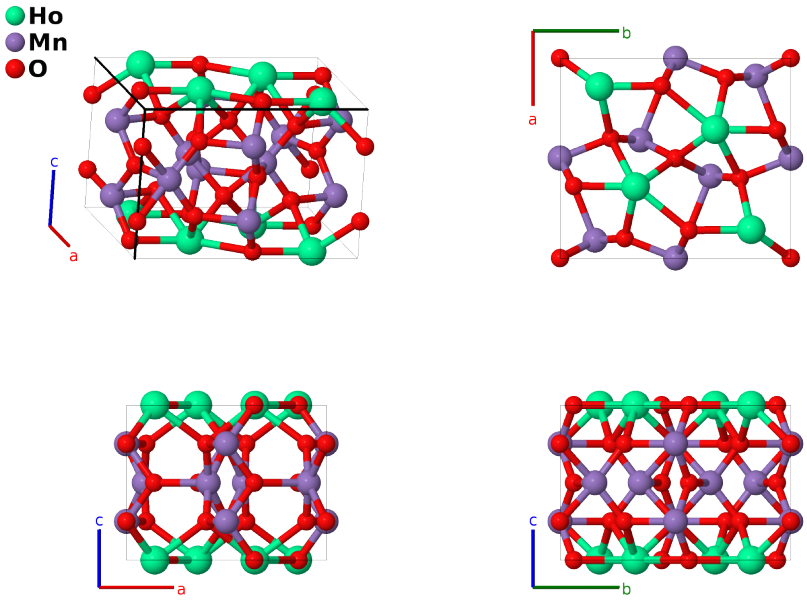
https://aflow.org/p/KF2N

https://aflow.org/p/AB2C5_oP32_55_g_eh_fghi-001



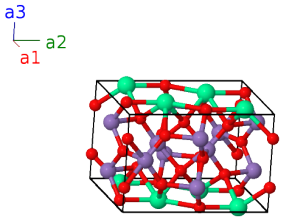
Prototype	$HoMn_2O_5$
AFLOW prototype label	AB2C5_oP32_55_g_eh_fghi-001
ICSD	none
Pearson symbol	oP32
Space group number	55
Space group symbol	*Pbam*
AFLOW prototype command	`aflow --proto=AB2C5_oP32_55_g_eh_fghi-001 --params=`$a, b/a, c/a, z_1, z_2, x_3, y_3, x_4, y_4, x_5, y_5, x_6, y_6, x_7, y_7, z_7$

Other compounds with this structure
$DyMn_2O_5$, $ErMn_2O_5$, $EuMn_2O_5$, $LaMn_2O_5$, $NdMn_2O_5$, $PrMn_2O_5$, $SmMn_2O_5$, $TbMn_2O_5$

- We found no definitive definition for the prototype of the structure XMn_2O_5, where X is a rare earth. (Quezel-Ambrunaz, 1964) has the earliest description of the structure we could find, so we use $HoMn_2O_5$ as the prototype.

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
$\mathbf{B_1}$	=	$z_1\,\mathbf{a}_3$	=	$cz_1\,\hat{\mathbf{z}}$	(4e)	Mn I
$\mathbf{B_2}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 - z_1\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}b\,\hat{\mathbf{y}} - cz_1\,\hat{\mathbf{z}}$	(4e)	Mn I
$\mathbf{B_3}$	=	$-z_1\,\mathbf{a}_3$	=	$-cz_1\,\hat{\mathbf{z}}$	(4e)	Mn I
$\mathbf{B_4}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 + z_1\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}b\,\hat{\mathbf{y}} + cz_1\,\hat{\mathbf{z}}$	(4e)	Mn I
$\mathbf{B_5}$	=	$\frac{1}{2}\,\mathbf{a}_2 + z_2\,\mathbf{a}_3$	=	$\frac{1}{2}b\,\hat{\mathbf{y}} + cz_2\,\hat{\mathbf{z}}$	(4f)	O I
$\mathbf{B_6}$	=	$\frac{1}{2}\,\mathbf{a}_1 - z_2\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - cz_2\,\hat{\mathbf{z}}$	(4f)	O I
$\mathbf{B_7}$	=	$\frac{1}{2}\,\mathbf{a}_2 - z_2\,\mathbf{a}_3$	=	$\frac{1}{2}b\,\hat{\mathbf{y}} - cz_2\,\hat{\mathbf{z}}$	(4f)	O I
$\mathbf{B_8}$	=	$\frac{1}{2}\,\mathbf{a}_1 + z_2\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + cz_2\,\hat{\mathbf{z}}$	(4f)	O I
$\mathbf{B_9}$	=	$x_3\,\mathbf{a}_1 + y_3\,\mathbf{a}_2$	=	$ax_3\,\hat{\mathbf{x}} + by_3\,\hat{\mathbf{y}}$	(4g)	Ho I
$\mathbf{B_{10}}$	=	$-x_3\,\mathbf{a}_1 - y_3\,\mathbf{a}_2$	=	$-ax_3\,\hat{\mathbf{x}} - by_3\,\hat{\mathbf{y}}$	(4g)	Ho I
$\mathbf{B_{11}}$	=	$-\left(x_3 - \frac{1}{2}\right)\,\mathbf{a}_1 + \left(y_3 + \frac{1}{2}\right)\,\mathbf{a}_2$	=	$-a\left(x_3 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + b\left(y_3 + \frac{1}{2}\right)\,\hat{\mathbf{y}}$	(4g)	Ho I
$\mathbf{B_{12}}$	=	$\left(x_3 + \frac{1}{2}\right)\,\mathbf{a}_1 - \left(y_3 - \frac{1}{2}\right)\,\mathbf{a}_2$	=	$a\left(x_3 + \frac{1}{2}\right)\,\hat{\mathbf{x}} - b\left(y_3 - \frac{1}{2}\right)\,\hat{\mathbf{y}}$	(4g)	Ho I
$\mathbf{B_{13}}$	=	$x_4\,\mathbf{a}_1 + y_4\,\mathbf{a}_2$	=	$ax_4\,\hat{\mathbf{x}} + by_4\,\hat{\mathbf{y}}$	(4g)	O II
$\mathbf{B_{14}}$	=	$-x_4\,\mathbf{a}_1 - y_4\,\mathbf{a}_2$	=	$-ax_4\,\hat{\mathbf{x}} - by_4\,\hat{\mathbf{y}}$	(4g)	O II
$\mathbf{B_{15}}$	=	$-\left(x_4 - \frac{1}{2}\right)\,\mathbf{a}_1 + \left(y_4 + \frac{1}{2}\right)\,\mathbf{a}_2$	=	$-a\left(x_4 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + b\left(y_4 + \frac{1}{2}\right)\,\hat{\mathbf{y}}$	(4g)	O II
$\mathbf{B_{16}}$	=	$\left(x_4 + \frac{1}{2}\right)\,\mathbf{a}_1 - \left(y_4 - \frac{1}{2}\right)\,\mathbf{a}_2$	=	$a\left(x_4 + \frac{1}{2}\right)\,\hat{\mathbf{x}} - b\left(y_4 - \frac{1}{2}\right)\,\hat{\mathbf{y}}$	(4g)	O II
$\mathbf{B_{17}}$	=	$x_5\,\mathbf{a}_1 + y_5\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$ax_5\,\hat{\mathbf{x}} + by_5\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(4h)	Mn II
$\mathbf{B_{18}}$	=	$-x_5\,\mathbf{a}_1 - y_5\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$-ax_5\,\hat{\mathbf{x}} - by_5\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(4h)	Mn II
$\mathbf{B_{19}}$	=	$-\left(x_5 - \frac{1}{2}\right)\,\mathbf{a}_1 + \left(y_5 + \frac{1}{2}\right)\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$-a\left(x_5 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + b\left(y_5 + \frac{1}{2}\right)\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(4h)	Mn II
$\mathbf{B_{20}}$	=	$\left(x_5 + \frac{1}{2}\right)\,\mathbf{a}_1 - \left(y_5 - \frac{1}{2}\right)\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$a\left(x_5 + \frac{1}{2}\right)\,\hat{\mathbf{x}} - b\left(y_5 - \frac{1}{2}\right)\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(4h)	Mn II
$\mathbf{B_{21}}$	=	$x_6\,\mathbf{a}_1 + y_6\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$ax_6\,\hat{\mathbf{x}} + by_6\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(4h)	O III
$\mathbf{B_{22}}$	=	$-x_6\,\mathbf{a}_1 - y_6\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$-ax_6\,\hat{\mathbf{x}} - by_6\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(4h)	O III
$\mathbf{B_{23}}$	=	$-\left(x_6 - \frac{1}{2}\right)\,\mathbf{a}_1 + \left(y_6 + \frac{1}{2}\right)\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$-a\left(x_6 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + b\left(y_6 + \frac{1}{2}\right)\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(4h)	O III
$\mathbf{B_{24}}$	=	$\left(x_6 + \frac{1}{2}\right)\,\mathbf{a}_1 - \left(y_6 - \frac{1}{2}\right)\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$a\left(x_6 + \frac{1}{2}\right)\,\hat{\mathbf{x}} - b\left(y_6 - \frac{1}{2}\right)\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(4h)	O III
$\mathbf{B_{25}}$	=	$x_7\,\mathbf{a}_1 + y_7\,\mathbf{a}_2 + z_7\,\mathbf{a}_3$	=	$ax_7\,\hat{\mathbf{x}} + by_7\,\hat{\mathbf{y}} + cz_7\,\hat{\mathbf{z}}$	(8i)	O IV
$\mathbf{B_{26}}$	=	$-x_7\,\mathbf{a}_1 - y_7\,\mathbf{a}_2 + z_7\,\mathbf{a}_3$	=	$-ax_7\,\hat{\mathbf{x}} - by_7\,\hat{\mathbf{y}} + cz_7\,\hat{\mathbf{z}}$	(8i)	O IV
$\mathbf{B_{27}}$	=	$-\left(x_7 - \frac{1}{2}\right)\,\mathbf{a}_1 + \left(y_7 + \frac{1}{2}\right)\,\mathbf{a}_2 - z_7\,\mathbf{a}_3$	=	$-a\left(x_7 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + b\left(y_7 + \frac{1}{2}\right)\,\hat{\mathbf{y}} - cz_7\,\hat{\mathbf{z}}$	(8i)	O IV

$\mathbf{B_{28}}$	=	$\left(x_7+\frac{1}{2}\right)\,\mathbf{a}_1-\left(y_7-\frac{1}{2}\right)\,\mathbf{a}_2-z_7\,\mathbf{a}_3$	=	$a\left(x_7+\frac{1}{2}\right)\,\hat{\mathbf{x}}-b\left(y_7-\frac{1}{2}\right)\,\hat{\mathbf{y}}-cz_7\,\hat{\mathbf{z}}$	(8i)	O IV
$\mathbf{B_{29}}$	=	$-x_7\,\mathbf{a}_1-y_7\,\mathbf{a}_2-z_7\,\mathbf{a}_3$	=	$-ax_7\,\hat{\mathbf{x}}-by_7\,\hat{\mathbf{y}}-cz_7\,\hat{\mathbf{z}}$	(8i)	O IV
$\mathbf{B_{30}}$	=	$x_7\,\mathbf{a}_1+y_7\,\mathbf{a}_2-z_7\,\mathbf{a}_3$	=	$ax_7\,\hat{\mathbf{x}}+by_7\,\hat{\mathbf{y}}-cz_7\,\hat{\mathbf{z}}$	(8i)	O IV
$\mathbf{B_{31}}$	=	$\left(x_7+\frac{1}{2}\right)\,\mathbf{a}_1-\left(y_7-\frac{1}{2}\right)\,\mathbf{a}_2+z_7\,\mathbf{a}_3$	=	$a\left(x_7+\frac{1}{2}\right)\,\hat{\mathbf{x}}-b\left(y_7-\frac{1}{2}\right)\,\hat{\mathbf{y}}+cz_7\,\hat{\mathbf{z}}$	(8i)	O IV
$\mathbf{B_{32}}$	=	$-\left(x_7-\frac{1}{2}\right)\,\mathbf{a}_1+\left(y_7+\frac{1}{2}\right)\,\mathbf{a}_2+z_7\,\mathbf{a}_3$	=	$-a\left(x_7-\frac{1}{2}\right)\,\hat{\mathbf{x}}+b\left(y_7+\frac{1}{2}\right)\,\hat{\mathbf{y}}+cz_7\,\hat{\mathbf{z}}$	(8i)	O IV

References

[1] S. Quezel-Ambrunaz, F. Bertaut, and G. Buisson, *Structure des composés d'oxydes de terres rares et de manganése de formule TMn_2O_5*, C. R. Acd. Sc. Paris **258**, 3025–3027 (1964).

Found in

[1] P. Euzen, P. Leone, C. Gueho, and P. Palvadeu, *Structure of $NdMn_2O_5$* **49**, 1875–1877 (1993).