$Nb_2Mn_4O_9$ Structure: A4B2C9_hP30_165_2d_c_fg-001

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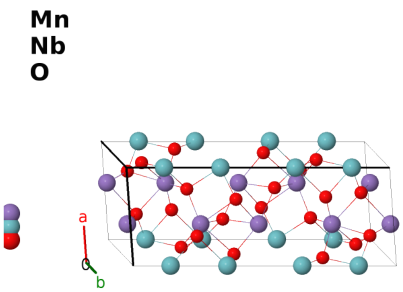
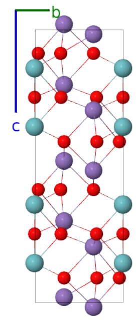
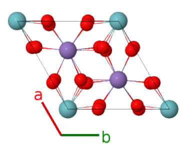
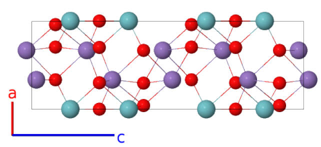
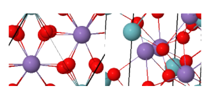
https://aflow.org/prototype-encyclopedia/A4B2C9_hP30_165_2d_c_fg-001











Prototype	$Mn_4Nb_2O_9$
AFLOW prototype label	A4B2C9_hP30_165_2d_c_fg-001
ICSD	29216
CCDC	1604224
Pearson symbol	hP30
Space group number	165
Space group symbol	$P\bar{3}c1$
AFLOW prototype command	`aflow --proto=A4B2C9_hP30_165_2d_c_fg-001 --params=`$a, c/a, z_1, z_2, z_3, x_4, x_5, y_5, z_5$

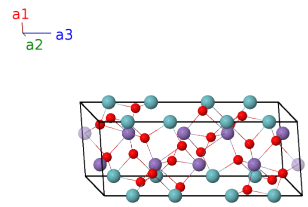
Other compounds with this structure

$Nb_2(Co_xMn_{1-x})O_9$, $Nb_2Co_4O_9$, $Nb_2Fe_4O_9$, $Nb_2Mg_4O_9$, $Nb_2Mn_4O_9$, $Nb_2Zn_4O_9$, $Ta_2(Mg_xMn_{1-x})O_9$, $Ta_2(Mg_xNi_{1-x})O_9$, $Ta_2(Mg_xZn_{1-}$ $Ta_2Co_4O_9$, $Ta_2Mg_4O_9$, $Ta_2Mn_4O_9$, $Ta_2Zn_4O_9$, $W_2(Li_2Mg_2)O_9$, $W_2(Li_2Zn_2)O_9$

- The ICSD uses $Nb_2Co_4O_9$ as the prototype.

Trigonal (Hexagonal) primitive vectors

$$
\begin{aligned}
\mathbf{a_1} &= \tfrac{1}{2}a\,\mathbf{\hat{x}} - \tfrac{\sqrt{3}}{2}a\,\mathbf{\hat{y}} \\
\mathbf{a_2} &= \tfrac{1}{2}a\,\mathbf{\hat{x}} + \tfrac{\sqrt{3}}{2}a\,\mathbf{\hat{y}} \\
\mathbf{a_3} &= c\,\mathbf{\hat{z}}
\end{aligned}
$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$z_1\,\mathbf{a}_3$	=	$cz_1\,\mathbf{\hat{z}}$	(4c)	Nb I
$\mathbf{B_2}$	=	$-\left(z_1-\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-c\left(z_1-\frac{1}{2}\right)\,\mathbf{\hat{z}}$	(4c)	Nb I
$\mathbf{B_3}$	=	$-z_1\,\mathbf{a}_3$	=	$-cz_1\,\mathbf{\hat{z}}$	(4c)	Nb I
$\mathbf{B_4}$	=	$\left(z_1+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$c\left(z_1+\frac{1}{2}\right)\,\mathbf{\hat{z}}$	(4c)	Nb I
$\mathbf{B_5}$	=	$\frac{1}{3}\,\mathbf{a}_1+\frac{2}{3}\,\mathbf{a}_2+z_2\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\mathbf{\hat{x}}+\frac{\sqrt{3}}{6}a\,\mathbf{\hat{y}}+cz_2\,\mathbf{\hat{z}}$	(4d)	Mn I
$\mathbf{B_6}$	=	$\frac{2}{3}\,\mathbf{a}_1+\frac{1}{3}\,\mathbf{a}_2-\left(z_2-\frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\mathbf{\hat{x}}-\frac{\sqrt{3}}{6}a\,\mathbf{\hat{y}}-c\left(z_2-\frac{1}{2}\right)\,\mathbf{\hat{z}}$	(4d)	Mn I
$\mathbf{B_7}$	=	$\frac{2}{3}\,\mathbf{a}_1+\frac{1}{3}\,\mathbf{a}_2-z_2\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\mathbf{\hat{x}}-\frac{\sqrt{3}}{6}a\,\mathbf{\hat{y}}-cz_2\,\mathbf{\hat{z}}$	(4d)	Mn I
$\mathbf{B_8}$	=	$\frac{1}{3}\,\mathbf{a}_1+\frac{2}{3}\,\mathbf{a}_2+\left(z_2+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\mathbf{\hat{x}}+\frac{\sqrt{3}}{6}a\,\mathbf{\hat{y}}+c\left(z_2+\frac{1}{2}\right)\,\mathbf{\hat{z}}$	(4d)	Mn I
$\mathbf{B_9}$	=	$\frac{1}{3}\,\mathbf{a}_1+\frac{2}{3}\,\mathbf{a}_2+z_3\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\mathbf{\hat{x}}+\frac{\sqrt{3}}{6}a\,\mathbf{\hat{y}}+cz_3\,\mathbf{\hat{z}}$	(4d)	Mn II
$\mathbf{B_{10}}$	=	$\frac{2}{3}\,\mathbf{a}_1+\frac{1}{3}\,\mathbf{a}_2-\left(z_3-\frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\mathbf{\hat{x}}-\frac{\sqrt{3}}{6}a\,\mathbf{\hat{y}}-c\left(z_3-\frac{1}{2}\right)\,\mathbf{\hat{z}}$	(4d)	Mn II
$\mathbf{B_{11}}$	=	$\frac{2}{3}\,\mathbf{a}_1+\frac{1}{3}\,\mathbf{a}_2-z_3\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\mathbf{\hat{x}}-\frac{\sqrt{3}}{6}a\,\mathbf{\hat{y}}-cz_3\,\mathbf{\hat{z}}$	(4d)	Mn II
$\mathbf{B_{12}}$	=	$\frac{1}{3}\,\mathbf{a}_1+\frac{2}{3}\,\mathbf{a}_2+\left(z_3+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\mathbf{\hat{x}}+\frac{\sqrt{3}}{6}a\,\mathbf{\hat{y}}+c\left(z_3+\frac{1}{2}\right)\,\mathbf{\hat{z}}$	(4d)	Mn II
$\mathbf{B_{13}}$	=	$x_4\,\mathbf{a}_1+\frac{1}{4}\,\mathbf{a}_3$	=	$\frac{1}{2}ax_4\,\mathbf{\hat{x}}-\frac{\sqrt{3}}{2}ax_4\,\mathbf{\hat{y}}+\frac{1}{4}c\,\mathbf{\hat{z}}$	(6f)	O I
$\mathbf{B_{14}}$	=	$x_4\,\mathbf{a}_2+\frac{1}{4}\,\mathbf{a}_3$	=	$\frac{1}{2}ax_4\,\mathbf{\hat{x}}+\frac{\sqrt{3}}{2}ax_4\,\mathbf{\hat{y}}+\frac{1}{4}c\,\mathbf{\hat{z}}$	(6f)	O I
$\mathbf{B_{15}}$	=	$-x_4\,\mathbf{a}_1-x_4\,\mathbf{a}_2+\frac{1}{4}\,\mathbf{a}_3$	=	$-ax_4\,\mathbf{\hat{x}}+\frac{1}{4}c\,\mathbf{\hat{z}}$	(6f)	O I
$\mathbf{B_{16}}$	=	$-x_4\,\mathbf{a}_1+\frac{3}{4}\,\mathbf{a}_3$	=	$-\frac{1}{2}ax_4\,\mathbf{\hat{x}}+\frac{\sqrt{3}}{2}ax_4\,\mathbf{\hat{y}}+\frac{3}{4}c\,\mathbf{\hat{z}}$	(6f)	O I
$\mathbf{B_{17}}$	=	$-x_4\,\mathbf{a}_2+\frac{3}{4}\,\mathbf{a}_3$	=	$-\frac{1}{2}ax_4\,\mathbf{\hat{x}}-\frac{\sqrt{3}}{2}ax_4\,\mathbf{\hat{y}}+\frac{3}{4}c\,\mathbf{\hat{z}}$	(6f)	O I
$\mathbf{B_{18}}$	=	$x_4\,\mathbf{a}_1+x_4\,\mathbf{a}_2+\frac{3}{4}\,\mathbf{a}_3$	=	$ax_4\,\mathbf{\hat{x}}+\frac{3}{4}c\,\mathbf{\hat{z}}$	(6f)	O I
$\mathbf{B_{19}}$	=	$x_5\,\mathbf{a}_1+y_5\,\mathbf{a}_2+z_5\,\mathbf{a}_3$	=	$\frac{1}{2}a\left(x_5+y_5\right)\,\mathbf{\hat{x}}-\frac{\sqrt{3}}{2}a\left(x_5-y_5\right)\,\mathbf{\hat{y}}+cz_5\,\mathbf{\hat{z}}$	(12g)	O II
$\mathbf{B_{20}}$	=	$-y_5\,\mathbf{a}_1+\left(x_5-y_5\right)\,\mathbf{a}_2+z_5\,\mathbf{a}_3$	=	$\frac{1}{2}a\left(x_5-2y_5\right)\,\mathbf{\hat{x}}+\frac{\sqrt{3}}{2}ax_5\,\mathbf{\hat{y}}+cz_5\,\mathbf{\hat{z}}$	(12g)	O II
$\mathbf{B_{21}}$	=	$-\left(x_5-y_5\right)\,\mathbf{a}_1-x_5\,\mathbf{a}_2+z_5\,\mathbf{a}_3$	=	$-\frac{1}{2}a\left(2x_5-y_5\right)\,\mathbf{\hat{x}}-\frac{\sqrt{3}}{2}ay_5\,\mathbf{\hat{y}}+cz_5\,\mathbf{\hat{z}}$	(12g)	O II
$\mathbf{B_{22}}$	=	$y_5\,\mathbf{a}_1+x_5\,\mathbf{a}_2-\left(z_5-\frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\left(x_5+y_5\right)\,\mathbf{\hat{x}}+\frac{\sqrt{3}}{2}a\left(x_5-y_5\right)\,\mathbf{\hat{y}}-c\left(z_5-\frac{1}{2}\right)\,\mathbf{\hat{z}}$	(12g)	O II

$\mathbf{B_{23}}$	=	$(x_5 - y_5)\,\mathbf{a}_1 - y_5\,\mathbf{a}_2 - \left(z_5 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_5 - 2y_5)\,\mathbf{\hat{x}} - \frac{\sqrt{3}}{2}ax_5\,\mathbf{\hat{y}} - c\left(z_5 - \frac{1}{2}\right)\,\mathbf{\hat{z}}$	(12g)	O II
$\mathbf{B_{24}}$	=	$-x_5\,\mathbf{a}_1 - (x_5 - y_5)\,\mathbf{a}_2 - \left(z_5 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(2x_5 - y_5)\,\mathbf{\hat{x}} + \frac{\sqrt{3}}{2}ay_5\,\mathbf{\hat{y}} - c\left(z_5 - \frac{1}{2}\right)\,\mathbf{\hat{z}}$	(12g)	O II
$\mathbf{B_{25}}$	=	$-x_5\,\mathbf{a}_1 - y_5\,\mathbf{a}_2 - z_5\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(x_5 + y_5)\,\mathbf{\hat{x}} + \frac{\sqrt{3}}{2}a\,(x_5 - y_5)\,\mathbf{\hat{y}} - cz_5\,\mathbf{\hat{z}}$	(12g)	O II
$\mathbf{B_{26}}$	=	$y_5\,\mathbf{a}_1 - (x_5 - y_5)\,\mathbf{a}_2 - z_5\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(-x_5 + 2y_5)\,\mathbf{\hat{x}} - \frac{\sqrt{3}}{2}ax_5\,\mathbf{\hat{y}} - cz_5\,\mathbf{\hat{z}}$	(12g)	O II
$\mathbf{B_{27}}$	=	$(x_5 - y_5)\,\mathbf{a}_1 + x_5\,\mathbf{a}_2 - z_5\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(2x_5 - y_5)\,\mathbf{\hat{x}} + \frac{\sqrt{3}}{2}ay_5\,\mathbf{\hat{y}} - cz_5\,\mathbf{\hat{z}}$	(12g)	O II
$\mathbf{B_{28}}$	=	$-y_5\,\mathbf{a}_1 - x_5\,\mathbf{a}_2 + \left(z_5 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(x_5 + y_5)\,\mathbf{\hat{x}} - \frac{\sqrt{3}}{2}a\,(x_5 - y_5)\,\mathbf{\hat{y}} + c\left(z_5 + \frac{1}{2}\right)\,\mathbf{\hat{z}}$	(12g)	O II
$\mathbf{B_{29}}$	=	$-(x_5 - y_5)\,\mathbf{a}_1 + y_5\,\mathbf{a}_2 + \left(z_5 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(-x_5 + 2y_5)\,\mathbf{\hat{x}} + \frac{\sqrt{3}}{2}ax_5\,\mathbf{\hat{y}} + c\left(z_5 + \frac{1}{2}\right)\,\mathbf{\hat{z}}$	(12g)	O II
$\mathbf{B_{30}}$	=	$x_5\,\mathbf{a}_1 + (x_5 - y_5)\,\mathbf{a}_2 + \left(z_5 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(2x_5 - y_5)\,\mathbf{\hat{x}} - \frac{\sqrt{3}}{2}ay_5\,\mathbf{\hat{y}} + c\left(z_5 + \frac{1}{2}\right)\,\mathbf{\hat{z}}$	(12g)	O II

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[1] E. Fischer, G. Gorodetsky, and R. M. Hornreich, *A new family of magnetoelectric materials: A2M4O9(A = Ta, Nb; M = Mn, Co)*, Solid State Commun. **10**, 1127–1132 (1972), doi:10.1016/0038-1098(72)90927-1.

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