Alluaudite [$NaMnFe_2(PO_4)_3$] Structure: A2BCD12E3_mC76_15_f_e_a_6f_ef-001

This structure originally had the label `A2BCD12E3_mC76_15_f_e_b_6f_ef`. Calls to that address will be redirected here.

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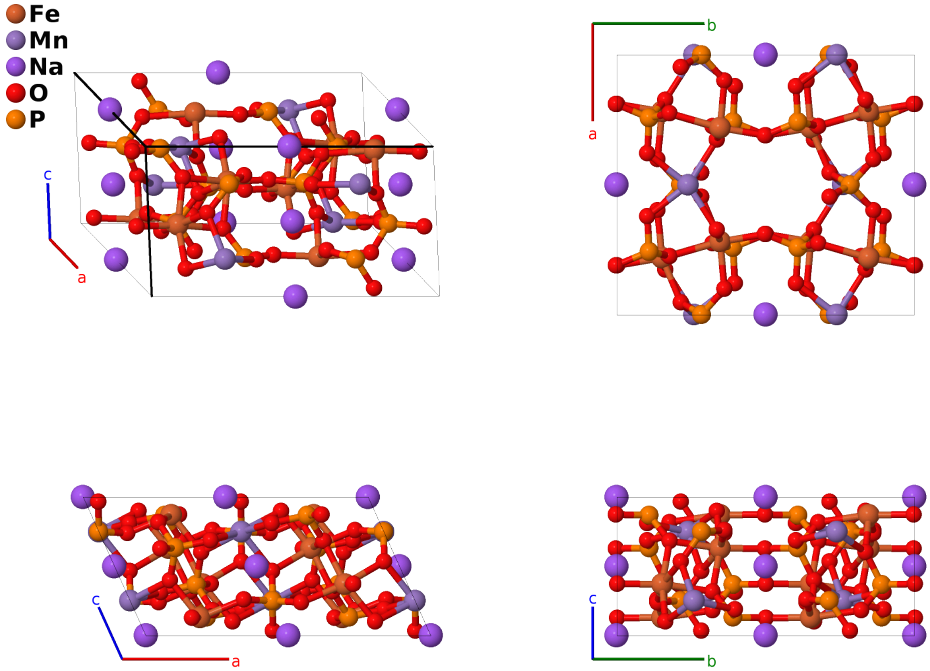
https://aflow.org/p/8ZWK

https://aflow.org/p/A2BCD12E3_mC76_15_f_e_a_6f_ef-001



Prototype	$Fe_2MnNaO_{12}P_3$
AFLOW prototype label	A2BCD12E3_mC76_15_f_e_a_6f_ef-001
Mineral name	alluaudite
ICSD	15241
Pearson symbol	mC76
Space group number	15
Space group symbol	$C2/c$
AFLOW prototype command	`aflow --proto=A2BCD12E3_mC76_15_f_e_a_6f_ef-001 --params=`$a, b/a, c/a, \beta, y_2, y_3, x_4, y_4, z_4, x_5, y_5, z_5, x_6, y_6, z_6, x_7, y_7, z_7, x_8, y_8, z_8, x_9, y_9, z_9, x_{10}, y_{10}, z_{10}, x_{11}, y_{11}, z_{11}$

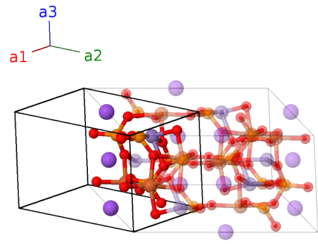
Other compounds with this structure

$Ag_xNa_{1-x}Mn_3(PO_4)_3$, $Li_xNa_{1-x}CdIn_2(PO_4)_3$, $Li_xNa_{1-x}MnFe_2(PO_4)_3$, $Na_2(Fe, Co)Fe(VO_4)_3$, $Na_2Co_2Cr(PO_4)_3$, $Na_2Fe_2V(PO_4)_3$, $Na_2Zn_2Fe(VO_4)_3$, $Na_3Bi_2(AsO_4)_3$, $Na_4Co(MnO_4)_3$, $Na_xMn_yAl_{5-x-y}(PO_4)_3$

- This is a rather idealized version of alluaudite. (Moore, 1971) gives the composition of the sodium site (Na) as $Na_{0.625}Mn_{0.175}Ca_{0.125}$, with vacancies on the remaining sites; the manganese (Mn) site is $Mn_{0.950}Mg_{0.025}Li_{0.025}$; and the iron (Fe) site as $Fe_{0.988}Mg_{0.012}$. (Hatert, 2005) puts some sodium atoms on another (4e) site, with $y \approx 0$; the exact placement and concentration depends upon the manganese content. We may expect similar variations in other compounds having this structure.

Base-centered Monoclinic primitive vectors

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



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	0	=	0	(4a)	Na I
$\mathbf{B_2}$	=	$\frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}c\cos\beta\,\hat{\mathbf{x}} + \frac{1}{2}c\sin\beta\,\hat{\mathbf{z}}$	(4a)	Na I
$\mathbf{B_3}$	=	$-y_2\,\mathbf{a}_1 + y_2\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$\frac{1}{4}c\cos\beta\,\hat{\mathbf{x}} + by_2\,\hat{\mathbf{y}} + \frac{1}{4}c\sin\beta\,\hat{\mathbf{z}}$	(4e)	Mn I
$\mathbf{B_4}$	=	$y_2\,\mathbf{a}_1 - y_2\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$\frac{3}{4}c\cos\beta\,\hat{\mathbf{x}} - by_2\,\hat{\mathbf{y}} + \frac{3}{4}c\sin\beta\,\hat{\mathbf{z}}$	(4e)	Mn I
$\mathbf{B_5}$	=	$-y_3\,\mathbf{a}_1 + y_3\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$\frac{1}{4}c\cos\beta\,\hat{\mathbf{x}} + by_3\,\hat{\mathbf{y}} + \frac{1}{4}c\sin\beta\,\hat{\mathbf{z}}$	(4e)	P I
$\mathbf{B_6}$	=	$y_3\,\mathbf{a}_1 - y_3\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$\frac{3}{4}c\cos\beta\,\hat{\mathbf{x}} - by_3\,\hat{\mathbf{y}} + \frac{3}{4}c\sin\beta\,\hat{\mathbf{z}}$	(4e)	P I
$\mathbf{B_7}$	=	$(x_4 - y_4)\,\mathbf{a}_1 + (x_4 + y_4)\,\mathbf{a}_2 + z_4\,\mathbf{a}_3$	=	$(ax_4 + cz_4\cos\beta)\,\hat{\mathbf{x}} + by_4\,\hat{\mathbf{y}} + cz_4\sin\beta\,\hat{\mathbf{z}}$	(8f)	Fe I
$\mathbf{B_8}$	=	$-(x_4 + y_4)\,\mathbf{a}_1 - (x_4 - y_4)\,\mathbf{a}_2 - \left(z_4 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-\left(ax_4 + c\left(z_4 - \frac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}} + by_4\,\hat{\mathbf{y}} - c\left(z_4 - \frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(8f)	Fe I
$\mathbf{B_9}$	=	$-(x_4 - y_4)\,\mathbf{a}_1 - (x_4 + y_4)\,\mathbf{a}_2 - z_4\,\mathbf{a}_3$	=	$-(ax_4 + cz_4\cos\beta)\,\hat{\mathbf{x}} - by_4\,\hat{\mathbf{y}} - cz_4\sin\beta\,\hat{\mathbf{z}}$	(8f)	Fe I
$\mathbf{B_{10}}$	=	$(x_4 + y_4)\,\mathbf{a}_1 + (x_4 - y_4)\,\mathbf{a}_2 + \left(z_4 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\left(ax_4 + c\left(z_4 + \frac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}} - by_4\,\hat{\mathbf{y}} + c\left(z_4 + \frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(8f)	Fe I
$\mathbf{B_{11}}$	=	$(x_5 - y_5)\,\mathbf{a}_1 + (x_5 + y_5)\,\mathbf{a}_2 + z_5\,\mathbf{a}_3$	=	$(ax_5 + cz_5\cos\beta)\,\hat{\mathbf{x}} + by_5\,\hat{\mathbf{y}} + cz_5\sin\beta\,\hat{\mathbf{z}}$	(8f)	O I
$\mathbf{B_{12}}$	=	$-(x_5 + y_5)\,\mathbf{a}_1 - (x_5 - y_5)\,\mathbf{a}_2 - \left(z_5 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-\left(ax_5 + c\left(z_5 - \frac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}} + by_5\,\hat{\mathbf{y}} - c\left(z_5 - \frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(8f)	O I
$\mathbf{B_{13}}$	=	$-(x_5 - y_5)\,\mathbf{a}_1 - (x_5 + y_5)\,\mathbf{a}_2 - z_5\,\mathbf{a}_3$	=	$-(ax_5 + cz_5\cos\beta)\,\hat{\mathbf{x}} - by_5\,\hat{\mathbf{y}} - cz_5\sin\beta\,\hat{\mathbf{z}}$	(8f)	O I
$\mathbf{B_{14}}$	=	$(x_5 + y_5)\,\mathbf{a}_1 + (x_5 - y_5)\,\mathbf{a}_2 + \left(z_5 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\left(ax_5 + c\left(z_5 + \frac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}} - by_5\,\hat{\mathbf{y}} + c\left(z_5 + \frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(8f)	O I
$\mathbf{B_{15}}$	=	$(x_6 - y_6)\,\mathbf{a}_1 + (x_6 + y_6)\,\mathbf{a}_2 + z_6\,\mathbf{a}_3$	=	$(ax_6 + cz_6\cos\beta)\,\hat{\mathbf{x}} + by_6\,\hat{\mathbf{y}} + cz_6\sin\beta\,\hat{\mathbf{z}}$	(8f)	O II
$\mathbf{B_{16}}$	=	$-(x_6 + y_6)\,\mathbf{a}_1 - (x_6 - y_6)\,\mathbf{a}_2 - \left(z_6 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-\left(ax_6 + c\left(z_6 - \frac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}} + by_6\,\hat{\mathbf{y}} - c\left(z_6 - \frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(8f)	O II
$\mathbf{B_{17}}$	=	$-(x_6 - y_6)\,\mathbf{a}_1 - (x_6 + y_6)\,\mathbf{a}_2 - z_6\,\mathbf{a}_3$	=	$-(ax_6 + cz_6\cos\beta)\,\hat{\mathbf{x}} - by_6\,\hat{\mathbf{y}} - cz_6\sin\beta\,\hat{\mathbf{z}}$	(8f)	O II

$\mathbf{B_{18}}$	=	$(x_6+y_6)\,\mathbf{a}_1+(x_6-y_6)\,\mathbf{a}_2+\left(z_6+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$\left(ax_6+c\left(z_6+\frac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}}-by_6\,\hat{\mathbf{y}}+c\left(z_6+\frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(8f)	O II
$\mathbf{B_{19}}$	=	$(x_7-y_7)\,\mathbf{a}_1+(x_7+y_7)\,\mathbf{a}_2+z_7\,\mathbf{a}_3$	=	$(ax_7+cz_7\cos\beta)\,\hat{\mathbf{x}}+by_7\,\hat{\mathbf{y}}+cz_7\sin\beta\,\hat{\mathbf{z}}$	(8f)	O III
$\mathbf{B_{20}}$	=	$-(x_7+y_7)\,\mathbf{a}_1-(x_7-y_7)\,\mathbf{a}_2-\left(z_7-\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-\left(ax_7+c\left(z_7-\frac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}}+by_7\,\hat{\mathbf{y}}-c\left(z_7-\frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(8f)	O III
$\mathbf{B_{21}}$	=	$-(x_7-y_7)\,\mathbf{a}_1-(x_7+y_7)\,\mathbf{a}_2-z_7\,\mathbf{a}_3$	=	$-(ax_7+cz_7\cos\beta)\,\hat{\mathbf{x}}-by_7\,\hat{\mathbf{y}}-cz_7\sin\beta\,\hat{\mathbf{z}}$	(8f)	O III
$\mathbf{B_{22}}$	=	$(x_7+y_7)\,\mathbf{a}_1+(x_7-y_7)\,\mathbf{a}_2+\left(z_7+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$\left(ax_7+c\left(z_7+\frac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}}-by_7\,\hat{\mathbf{y}}+c\left(z_7+\frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(8f)	O III
$\mathbf{B_{23}}$	=	$(x_8-y_8)\,\mathbf{a}_1+(x_8+y_8)\,\mathbf{a}_2+z_8\,\mathbf{a}_3$	=	$(ax_8+cz_8\cos\beta)\,\hat{\mathbf{x}}+by_8\,\hat{\mathbf{y}}+cz_8\sin\beta\,\hat{\mathbf{z}}$	(8f)	O IV
$\mathbf{B_{24}}$	=	$-(x_8+y_8)\,\mathbf{a}_1-(x_8-y_8)\,\mathbf{a}_2-\left(z_8-\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-\left(ax_8+c\left(z_8-\frac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}}+by_8\,\hat{\mathbf{y}}-c\left(z_8-\frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(8f)	O IV
$\mathbf{B_{25}}$	=	$-(x_8-y_8)\,\mathbf{a}_1-(x_8+y_8)\,\mathbf{a}_2-z_8\,\mathbf{a}_3$	=	$-(ax_8+cz_8\cos\beta)\,\hat{\mathbf{x}}-by_8\,\hat{\mathbf{y}}-cz_8\sin\beta\,\hat{\mathbf{z}}$	(8f)	O IV
$\mathbf{B_{26}}$	=	$(x_8+y_8)\,\mathbf{a}_1+(x_8-y_8)\,\mathbf{a}_2+\left(z_8+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$\left(ax_8+c\left(z_8+\frac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}}-by_8\,\hat{\mathbf{y}}+c\left(z_8+\frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(8f)	O IV
$\mathbf{B_{27}}$	=	$(x_9-y_9)\,\mathbf{a}_1+(x_9+y_9)\,\mathbf{a}_2+z_9\,\mathbf{a}_3$	=	$(ax_9+cz_9\cos\beta)\,\hat{\mathbf{x}}+by_9\,\hat{\mathbf{y}}+cz_9\sin\beta\,\hat{\mathbf{z}}$	(8f)	O V
$\mathbf{B_{28}}$	=	$-(x_9+y_9)\,\mathbf{a}_1-(x_9-y_9)\,\mathbf{a}_2-\left(z_9-\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-\left(ax_9+c\left(z_9-\frac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}}+by_9\,\hat{\mathbf{y}}-c\left(z_9-\frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(8f)	O V
$\mathbf{B_{29}}$	=	$-(x_9-y_9)\,\mathbf{a}_1-(x_9+y_9)\,\mathbf{a}_2-z_9\,\mathbf{a}_3$	=	$-(ax_9+cz_9\cos\beta)\,\hat{\mathbf{x}}-by_9\,\hat{\mathbf{y}}-cz_9\sin\beta\,\hat{\mathbf{z}}$	(8f)	O V
$\mathbf{B_{30}}$	=	$(x_9+y_9)\,\mathbf{a}_1+(x_9-y_9)\,\mathbf{a}_2+\left(z_9+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$\left(ax_9+c\left(z_9+\frac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}}-by_9\,\hat{\mathbf{y}}+c\left(z_9+\frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(8f)	O V
$\mathbf{B_{31}}$	=	$(x_{10}-y_{10})\,\mathbf{a}_1+(x_{10}+y_{10})\,\mathbf{a}_2+z_{10}\,\mathbf{a}_3$	=	$(ax_{10}+cz_{10}\cos\beta)\,\hat{\mathbf{x}}+by_{10}\,\hat{\mathbf{y}}+cz_{10}\sin\beta\,\hat{\mathbf{z}}$	(8f)	O VI
$\mathbf{B_{32}}$	=	$-(x_{10}+y_{10})\,\mathbf{a}_1-(x_{10}-y_{10})\,\mathbf{a}_2-\left(z_{10}-\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-\left(ax_{10}+c\left(z_{10}-\frac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}}+by_{10}\,\hat{\mathbf{y}}-c\left(z_{10}-\frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(8f)	O VI
$\mathbf{B_{33}}$	=	$-(x_{10}-y_{10})\,\mathbf{a}_1-(x_{10}+y_{10})\,\mathbf{a}_2-z_{10}\,\mathbf{a}_3$	=	$-(ax_{10}+cz_{10}\cos\beta)\,\hat{\mathbf{x}}-by_{10}\,\hat{\mathbf{y}}-cz_{10}\sin\beta\,\hat{\mathbf{z}}$	(8f)	O VI
$\mathbf{B_{34}}$	=	$(x_{10}+y_{10})\,\mathbf{a}_1+(x_{10}-y_{10})\,\mathbf{a}_2+\left(z_{10}+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$\left(ax_{10}+c\left(z_{10}+\frac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}}-by_{10}\,\hat{\mathbf{y}}+c\left(z_{10}+\frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(8f)	O VI
$\mathbf{B_{35}}$	=	$(x_{11}-y_{11})\,\mathbf{a}_1+(x_{11}+y_{11})\,\mathbf{a}_2+z_{11}\,\mathbf{a}_3$	=	$(ax_{11}+cz_{11}\cos\beta)\,\hat{\mathbf{x}}+by_{11}\,\hat{\mathbf{y}}+cz_{11}\sin\beta\,\hat{\mathbf{z}}$	(8f)	P II
$\mathbf{B_{36}}$	=	$-(x_{11}+y_{11})\,\mathbf{a}_1-(x_{11}-y_{11})\,\mathbf{a}_2-\left(z_{11}-\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-\left(ax_{11}+c\left(z_{11}-\frac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}}+by_{11}\,\hat{\mathbf{y}}-c\left(z_{11}-\frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(8f)	P II
$\mathbf{B_{37}}$	=	$-(x_{11}-y_{11})\,\mathbf{a}_1-(x_{11}+y_{11})\,\mathbf{a}_2-z_{11}\,\mathbf{a}_3$	=	$-(ax_{11}+cz_{11}\cos\beta)\,\hat{\mathbf{x}}-by_{11}\,\hat{\mathbf{y}}-cz_{11}\sin\beta\,\hat{\mathbf{z}}$	(8f)	P II
$\mathbf{B_{38}}$	=	$(x_{11}+y_{11})\,\mathbf{a}_1+(x_{11}-y_{11})\,\mathbf{a}_2+\left(z_{11}+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$\left(ax_{11}+c\left(z_{11}+\frac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}}-by_{11}\,\hat{\mathbf{y}}+c\left(z_{11}+\frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(8f)	P II

References

[1] P. B. Moore, *Crystal Chemistry of the Alluaudite Structure Type: Contribution to the Paragenesis of Pegmatite Phosphate Giant Crystals*, Am. Mineral. **56**, 1955–1975 (1971).

Found in

[1] R. T. Downs and M. Hall-Wallace, *The American Mineralogist Crystal Structure Database*, Am. Mineral. **88**, 247–250 (2003).