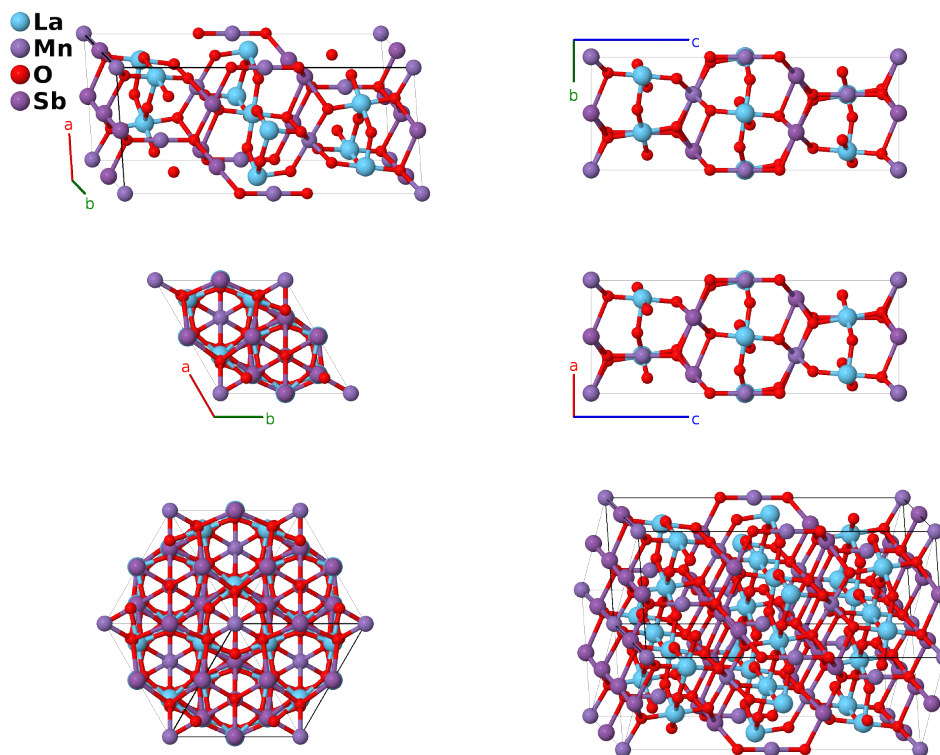


# Mn<sub>2</sub>La<sub>3</sub>Sb<sub>3</sub>O<sub>14</sub> Structure: A3B2C14D3\_hR22\_166\_d\_ab\_c2h\_e-001

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<https://aflow.org/p/6NJM>

[https://aflow.org/p/A3B2C14D3\\_hR22\\_166\\_d\\_ab\\_c2h\\_e-001](https://aflow.org/p/A3B2C14D3_hR22_166_d_ab_c2h_e-001)



<b>Prototype</b>	La <sub>3</sub> Mn <sub>2</sub> O <sub>14</sub> Sb <sub>3</sub>
<b>AFLOW prototype label</b>	A3B2C14D3_hR22_166_d_ab_c2h_e-001
<b>ICSD</b>	191137
<b>Pearson symbol</b>	hR22
<b>Space group number</b>	166
<b>Space group symbol</b>	$R\bar{3}m$
<b>AFLOW prototype command</b>	aflow --proto=A3B2C14D3_hR22_166_d_ab_c2h_e-001 --params=a, c/a, x <sub>3</sub> , x <sub>6</sub> , z <sub>6</sub> , x <sub>7</sub> , z <sub>7</sub>

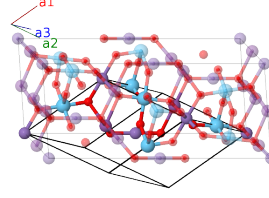
## Other compounds with this structure

Mg<sub>2</sub>Dy<sub>3</sub>Sb<sub>3</sub>O<sub>14</sub>, Mg<sub>2</sub>Er<sub>3</sub>Sb<sub>3</sub>O<sub>14</sub>, Mg<sub>2</sub>Gd<sub>3</sub>Sb<sub>3</sub>O<sub>14</sub>, Mg<sub>2</sub>Ho<sub>3</sub>Sb<sub>3</sub>O<sub>14</sub>, Mg<sub>2</sub>Nd<sub>3</sub>Sb<sub>3</sub>O<sub>14</sub>, Mg<sub>2</sub>Pr<sub>3</sub>Sb<sub>3</sub>O<sub>14</sub>, Mg<sub>2</sub>Tb<sub>3</sub>Sb<sub>3</sub>O<sub>14</sub>, Mg<sub>2</sub>Tm<sub>3</sub>Sb<sub>3</sub>O<sub>14</sub>, Mg<sub>2</sub>Yb<sub>3</sub>Sb<sub>3</sub>O<sub>14</sub>, Mn<sub>2</sub>Pr<sub>3</sub>Sb<sub>3</sub>O<sub>14</sub>, Mn<sub>2</sub>Nd<sub>3</sub>Sb<sub>3</sub>O<sub>14</sub>, Zn<sub>2</sub>Dy<sub>3</sub>Sb<sub>3</sub>O<sub>14</sub>, Zn<sub>2</sub>Er<sub>3</sub>Sb<sub>3</sub>O<sub>14</sub>, Zn<sub>2</sub>Gd<sub>3</sub>Sb<sub>3</sub>O<sub>14</sub>, Zn<sub>2</sub>Ho<sub>3</sub>Sb<sub>3</sub>O<sub>14</sub>, Zn<sub>2</sub>Nd<sub>3</sub>Sb<sub>3</sub>O<sub>14</sub>, Zn<sub>2</sub>Pr<sub>3</sub>Sb<sub>3</sub>O<sub>14</sub>, Zn<sub>2</sub>Tb<sub>3</sub>Sb<sub>3</sub>O<sub>14</sub>, Zn<sub>2</sub>Tm<sub>3</sub>Sb<sub>3</sub>O<sub>14</sub>, Zn<sub>2</sub>Yb<sub>3</sub>Sb<sub>3</sub>O<sub>14</sub>

- Hexagonal settings of this structure can be obtained with the option `--hex`.

## Rhombohedral primitive vectors

$$\begin{aligned}\mathbf{a}_1 &= \frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + \frac{1}{3}c \hat{\mathbf{z}} \\ \mathbf{a}_2 &= \frac{1}{\sqrt{3}}a \hat{\mathbf{y}} + \frac{1}{3}c \hat{\mathbf{z}} \\ \mathbf{a}_3 &= -\frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + \frac{1}{3}c \hat{\mathbf{z}}\end{aligned}$$



## Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$0$	$=$	$0$	(1a)	Mn I
$\mathbf{B}_2$	$\frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2}c \hat{\mathbf{z}}$	(1b)	Mn II
$\mathbf{B}_3$	$x_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 + x_3 \mathbf{a}_3$	$=$	$cx_3 \hat{\mathbf{z}}$	(2c)	O I
$\mathbf{B}_4$	$-x_3 \mathbf{a}_1 - x_3 \mathbf{a}_2 - x_3 \mathbf{a}_3$	$=$	$-cx_3 \hat{\mathbf{z}}$	(2c)	O I
$\mathbf{B}_5$	$\frac{1}{2} \mathbf{a}_1$	$=$	$\frac{1}{4}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{12}a \hat{\mathbf{y}} + \frac{1}{6}c \hat{\mathbf{z}}$	(3d)	La I
$\mathbf{B}_6$	$\frac{1}{2} \mathbf{a}_2$	$=$	$\frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + \frac{1}{6}c \hat{\mathbf{z}}$	(3d)	La I
$\mathbf{B}_7$	$\frac{1}{2} \mathbf{a}_3$	$=$	$-\frac{1}{4}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{12}a \hat{\mathbf{y}} + \frac{1}{6}c \hat{\mathbf{z}}$	(3d)	La I
$\mathbf{B}_8$	$\frac{1}{2} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$-\frac{1}{4}a \hat{\mathbf{x}} + \frac{\sqrt{3}}{12}a \hat{\mathbf{y}} + \frac{1}{3}c \hat{\mathbf{z}}$	(3e)	Sb I
$\mathbf{B}_9$	$\frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_3$	$=$	$-\frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + \frac{1}{3}c \hat{\mathbf{z}}$	(3e)	Sb I
$\mathbf{B}_{10}$	$\frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2$	$=$	$\frac{1}{4}a \hat{\mathbf{x}} + \frac{\sqrt{3}}{12}a \hat{\mathbf{y}} + \frac{1}{3}c \hat{\mathbf{z}}$	(3e)	Sb I
$\mathbf{B}_{11}$	$x_6 \mathbf{a}_1 + x_6 \mathbf{a}_2 + z_6 \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_6 - z_6) \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a(x_6 - z_6) \hat{\mathbf{y}} + \frac{1}{3}c(2x_6 + z_6) \hat{\mathbf{z}}$	(6h)	O II
$\mathbf{B}_{12}$	$z_6 \mathbf{a}_1 + x_6 \mathbf{a}_2 + x_6 \mathbf{a}_3$	$=$	$-\frac{1}{2}a(x_6 - z_6) \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a(x_6 - z_6) \hat{\mathbf{y}} + \frac{1}{3}c(2x_6 + z_6) \hat{\mathbf{z}}$	(6h)	O II
$\mathbf{B}_{13}$	$x_6 \mathbf{a}_1 + z_6 \mathbf{a}_2 + x_6 \mathbf{a}_3$	$=$	$-\frac{1}{\sqrt{3}}a(x_6 - z_6) \hat{\mathbf{y}} + \frac{1}{3}c(2x_6 + z_6) \hat{\mathbf{z}}$	(6h)	O II
$\mathbf{B}_{14}$	$-z_6 \mathbf{a}_1 - x_6 \mathbf{a}_2 - x_6 \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_6 - z_6) \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a(x_6 - z_6) \hat{\mathbf{y}} - \frac{1}{3}c(2x_6 + z_6) \hat{\mathbf{z}}$	(6h)	O II
$\mathbf{B}_{15}$	$-x_6 \mathbf{a}_1 - x_6 \mathbf{a}_2 - z_6 \mathbf{a}_3$	$=$	$-\frac{1}{2}a(x_6 - z_6) \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a(x_6 - z_6) \hat{\mathbf{y}} - \frac{1}{3}c(2x_6 + z_6) \hat{\mathbf{z}}$	(6h)	O II
$\mathbf{B}_{16}$	$-x_6 \mathbf{a}_1 - z_6 \mathbf{a}_2 - x_6 \mathbf{a}_3$	$=$	$\frac{1}{\sqrt{3}}a(x_6 - z_6) \hat{\mathbf{y}} - \frac{1}{3}c(2x_6 + z_6) \hat{\mathbf{z}}$	(6h)	O II
$\mathbf{B}_{17}$	$x_7 \mathbf{a}_1 + x_7 \mathbf{a}_2 + z_7 \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_7 - z_7) \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a(x_7 - z_7) \hat{\mathbf{y}} + \frac{1}{3}c(2x_7 + z_7) \hat{\mathbf{z}}$	(6h)	O III
$\mathbf{B}_{18}$	$z_7 \mathbf{a}_1 + x_7 \mathbf{a}_2 + x_7 \mathbf{a}_3$	$=$	$-\frac{1}{2}a(x_7 - z_7) \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a(x_7 - z_7) \hat{\mathbf{y}} + \frac{1}{3}c(2x_7 + z_7) \hat{\mathbf{z}}$	(6h)	O III
$\mathbf{B}_{19}$	$x_7 \mathbf{a}_1 + z_7 \mathbf{a}_2 + x_7 \mathbf{a}_3$	$=$	$-\frac{1}{\sqrt{3}}a(x_7 - z_7) \hat{\mathbf{y}} + \frac{1}{3}c(2x_7 + z_7) \hat{\mathbf{z}}$	(6h)	O III
$\mathbf{B}_{20}$	$-z_7 \mathbf{a}_1 - x_7 \mathbf{a}_2 - x_7 \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_7 - z_7) \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a(x_7 - z_7) \hat{\mathbf{y}} - \frac{1}{3}c(2x_7 + z_7) \hat{\mathbf{z}}$	(6h)	O III
$\mathbf{B}_{21}$	$-x_7 \mathbf{a}_1 - x_7 \mathbf{a}_2 - z_7 \mathbf{a}_3$	$=$	$-\frac{1}{2}a(x_7 - z_7) \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a(x_7 - z_7) \hat{\mathbf{y}} - \frac{1}{3}c(2x_7 + z_7) \hat{\mathbf{z}}$	(6h)	O III
$\mathbf{B}_{22}$	$-x_7 \mathbf{a}_1 - z_7 \mathbf{a}_2 - x_7 \mathbf{a}_3$	$=$	$\frac{1}{\sqrt{3}}a(x_7 - z_7) \hat{\mathbf{y}} - \frac{1}{3}c(2x_7 + z_7) \hat{\mathbf{z}}$	(6h)	O III

## References

- [1] W. T. Fu and D. J. W. Ijdo, *Crystal structure of  $Mn_2Ln_3Sb_3O_{14}$  ( $Ln=La, Pr$  and  $Nd$ ): A new ordered rhombohedral pyrochlore*, J. Solid State Chem. **213**, 165–168 (2014), doi:10.1016/j.jssc.2014.02.025.

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- [1] *Inorganic Crystal Structure Database*. Entry 191137 (La3Mn2Sb3O14).