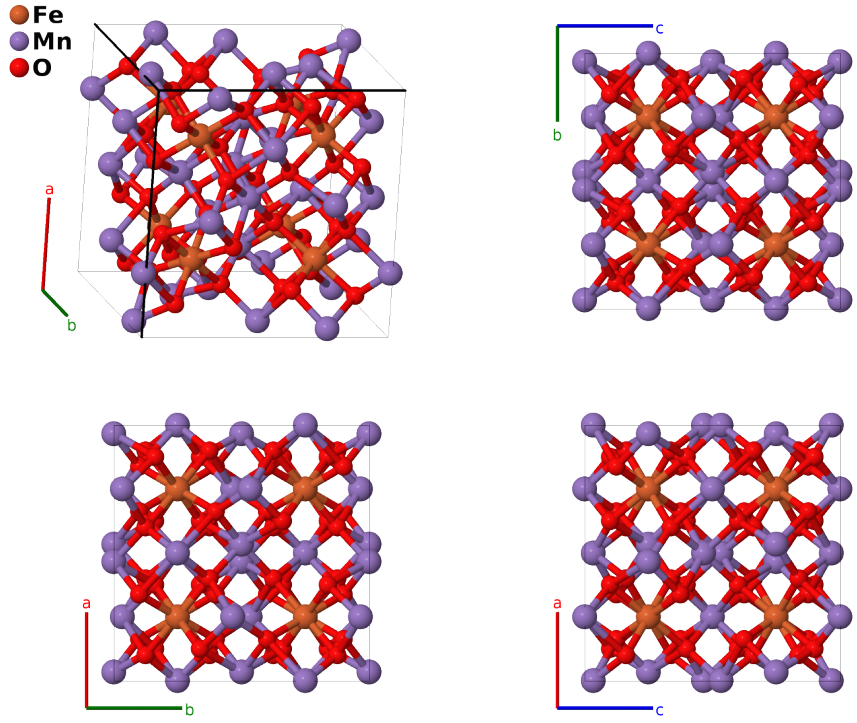
Bixbyite (Mn_2O_3, $D5_3$) Structure: AB3C6_cI80_206_a_d_e-001

This structure originally had the label `AB3C6_cI80_206_b_d_e`. Calls to that address will be redirected here.

Cite this page as: M. J. Mehl, D. Hicks, C. Toher, O. Levy, R. M. Hanson, G. Hart, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 1*, Comput. Mater. Sci. **136**, S1-828 (2017). doi: 10.1016/j.commatsci.2017.01.017

https://aflow.org/p/G3EF

https://aflow.org/p/AB3C6_cI80_206_a_d_e-001



Prototype	Mn_2O_3
AFLOW prototype label	AB3C6_cI80_206_a_d_e-001
***Strukturbericht* designation**	$D5_3$
Mineral name	bixbyite
ICSD	30237
Pearson symbol	cI80
Space group number	206
Space group symbol	$Ia\bar{3}$
AFLOW prototype command	`aflow --proto=AB3C6_cI80_206_a_d_e-001 --params=`a, x_2, x_3, y_3, z_3

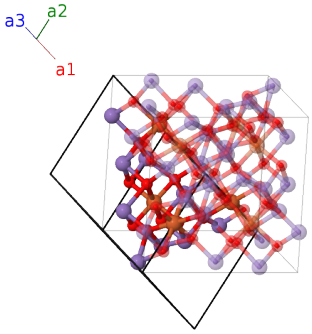
Other compounds with this structure

Am_2O_3, As_2Mg_3, As_2Zn_3, Cd_3P_2, Ce_2O_3, Dy_2O_3, Er_2O_3, Eu_2O_3, Fe_2O_3, Gd_2O_3, Ho_2O_3, In_2O_3, La_2O_3, Lu_2O_3, α-N_2Be_3, N_2Ca_3, N_2Cd_3, N_2Mg_3, N_2Zn_3, P_2Be_3, P_2Mg_3, P_2Zn_3, Pr_2O_3, Pu_2O_3, Sc_2O_3, Sm_2O_3, Tb_2O_3, $TeCu_3O_6$, Tl_2O_3, Tm_2O_3, U_2N_3, Y_2O_3 (yttria), Yb_2O_3

- A search for "bixbyite" on the American Mineralogist Crystal Structure Database (Downs, 2003) shows two structures with the Mn atoms on the (8a) sites and one with Mn on the (8b) site. We use the structure that agrees with the data for pure Mn_2O_3 bixbyite in (Villars, 1991) Vol. IV, 4346-7.
- The referenced data is for $(Mn,Fe)_2O_3$, with Mn and Fe randomly populating the (8b) and (24d) sites.
- The pictures and the CIF file put Fe atoms on the (8b) sites and Mn atoms on the (24d) sites in order to better delineate the difference in the crystallographic behavior of the sites, but both sites are randomly occupied.
- An earlier version of this page (and the article) used the label AB3C6_cI80_206_a_d_e. The label has now been corrected to AB3C6_cI80_206_b_d_e.

Body-centered Cubic primitive vectors

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



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	0	=	0	(8a)	Fe I
$\mathbf{B_2}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{y}}$	(8a)	Fe I
$\mathbf{B_3}$	=	$\frac{1}{2}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}}$	(8a)	Fe I
$\mathbf{B_4}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2$	=	$\frac{1}{2}a\,\hat{\mathbf{z}}$	(8a)	Fe I
$\mathbf{B_5}$	=	$\frac{1}{4}\,\mathbf{a}_1 + \left(x_2 + \frac{1}{4}\right)\,\mathbf{a}_2 + x_2\,\mathbf{a}_3$	=	$ax_2\,\hat{\mathbf{x}} + \frac{1}{4}a\,\hat{\mathbf{z}}$	(24d)	Mn I
$\mathbf{B_6}$	=	$\frac{3}{4}\,\mathbf{a}_1 - \left(x_2 - \frac{1}{4}\right)\,\mathbf{a}_2 - \left(x_2 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ax_2\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{y}} + \frac{1}{4}a\,\hat{\mathbf{z}}$	(24d)	Mn I
$\mathbf{B_7}$	=	$x_2\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 + \left(x_2 + \frac{1}{4}\right)\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + ax_2\,\hat{\mathbf{y}}$	(24d)	Mn I
$\mathbf{B_8}$	=	$-\left(x_2 - \frac{1}{2}\right)\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 - \left(x_2 - \frac{1}{4}\right)\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} - ax_2\,\hat{\mathbf{y}} + \frac{1}{2}a\,\hat{\mathbf{z}}$	(24d)	Mn I
$\mathbf{B_9}$	=	$\left(x_2 + \frac{1}{4}\right)\,\mathbf{a}_1 + x_2\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{y}} + ax_2\,\hat{\mathbf{z}}$	(24d)	Mn I
$\mathbf{B_{10}}$	=	$-\left(x_2 - \frac{1}{4}\right)\,\mathbf{a}_1 - \left(x_2 - \frac{1}{2}\right)\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{4}a\,\hat{\mathbf{y}} - ax_2\,\hat{\mathbf{z}}$	(24d)	Mn I
$\mathbf{B_{11}}$	=	$\frac{3}{4}\,\mathbf{a}_1 - \left(x_2 - \frac{3}{4}\right)\,\mathbf{a}_2 - x_2\,\mathbf{a}_3$	=	$-ax_2\,\hat{\mathbf{x}} + \frac{3}{4}a\,\hat{\mathbf{z}}$	(24d)	Mn I
$\mathbf{B_{12}}$	=	$\frac{1}{4}\,\mathbf{a}_1 + \left(x_2 + \frac{3}{4}\right)\,\mathbf{a}_2 + \left(x_2 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$a\left(x_2 + \frac{1}{2}\right)\,\hat{\mathbf{x}} + \frac{1}{4}a\,\hat{\mathbf{z}}$	(24d)	Mn I
$\mathbf{B_{13}}$	=	$-x_2\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 - \left(x_2 - \frac{3}{4}\right)\,\mathbf{a}_3$	=	$\frac{3}{4}a\,\hat{\mathbf{x}} - ax_2\,\hat{\mathbf{y}}$	(24d)	Mn I
$\mathbf{B_{14}}$	=	$\left(x_2 + \frac{1}{2}\right)\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 + \left(x_2 + \frac{3}{4}\right)\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + a\left(x_2 + \frac{1}{2}\right)\,\hat{\mathbf{y}}$	(24d)	Mn I
$\mathbf{B_{15}}$	=	$-\left(x_2 - \frac{3}{4}\right)\,\mathbf{a}_1 - x_2\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$\frac{3}{4}a\,\hat{\mathbf{y}} - ax_2\,\hat{\mathbf{z}}$	(24d)	Mn I
$\mathbf{B_{16}}$	=	$\left(x_2 + \frac{3}{4}\right)\,\mathbf{a}_1 + \left(x_2 + \frac{1}{2}\right)\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{y}} + a\left(x_2 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(24d)	Mn I
$\mathbf{B_{17}}$	=	$(y_3 + z_3)\,\mathbf{a}_1 + (x_3 + z_3)\,\mathbf{a}_2 + (x_3 + y_3)\,\mathbf{a}_3$	=	$ax_3\,\hat{\mathbf{x}} + ay_3\,\hat{\mathbf{y}} + az_3\,\hat{\mathbf{z}}$	(48e)	O I
$\mathbf{B_{18}}$	=	$\left(-y_3 + z_3 + \frac{1}{2}\right)\,\mathbf{a}_1 - (x_3 - z_3)\,\mathbf{a}_2 - \left(x_3 + y_3 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ax_3\,\hat{\mathbf{x}} - a\left(y_3 - \frac{1}{2}\right)\,\hat{\mathbf{y}} + az_3\,\hat{\mathbf{z}}$	(48e)	O I

$$\mathbf{B_{19}} = (y_3 - z_3)\,\mathbf{a}_1 - \left(x_3 + z_3 - \tfrac{1}{2}\right)\,\mathbf{a}_2 + \left(-x_3 + y_3 + \tfrac{1}{2}\right)\,\mathbf{a}_3 = -a\left(x_3 - \tfrac{1}{2}\right)\,\hat{\mathbf{x}} + a y_3\,\hat{\mathbf{y}} - a z_3\,\hat{\mathbf{z}} \quad (48e) \quad \text{O I}$$

$$\mathbf{B_{20}} = -\left(y_3 + z_3 - \tfrac{1}{2}\right)\,\mathbf{a}_1 + \left(x_3 - z_3 + \tfrac{1}{2}\right)\,\mathbf{a}_2 + (x_3 - y_3)\,\mathbf{a}_3 = a x_3\,\hat{\mathbf{x}} - a y_3\,\hat{\mathbf{y}} - a\left(z_3 - \tfrac{1}{2}\right)\,\hat{\mathbf{z}} \quad (48e) \quad \text{O I}$$

$$\mathbf{B_{21}} = (x_3 + y_3)\,\mathbf{a}_1 + (y_3 + z_3)\,\mathbf{a}_2 + (x_3 + z_3)\,\mathbf{a}_3 = a z_3\,\hat{\mathbf{x}} + a x_3\,\hat{\mathbf{y}} + a y_3\,\hat{\mathbf{z}} \quad (48e) \quad \text{O I}$$

$$\mathbf{B_{22}} = -\left(x_3 + y_3 - \tfrac{1}{2}\right)\,\mathbf{a}_1 + \left(-y_3 + z_3 + \tfrac{1}{2}\right)\,\mathbf{a}_2 - (x_3 - z_3)\,\mathbf{a}_3 = a z_3\,\hat{\mathbf{x}} - a x_3\,\hat{\mathbf{y}} - a\left(y_3 - \tfrac{1}{2}\right)\,\hat{\mathbf{z}} \quad (48e) \quad \text{O I}$$

$$\mathbf{B_{23}} = \left(-x_3 + y_3 + \tfrac{1}{2}\right)\,\mathbf{a}_1 + (y_3 - z_3)\,\mathbf{a}_2 - \left(x_3 + z_3 - \tfrac{1}{2}\right)\,\mathbf{a}_3 = -a z_3\,\hat{\mathbf{x}} - a\left(x_3 - \tfrac{1}{2}\right)\,\hat{\mathbf{y}} + a y_3\,\hat{\mathbf{z}} \quad (48e) \quad \text{O I}$$

$$\mathbf{B_{24}} = (x_3 - y_3)\,\mathbf{a}_1 - \left(y_3 + z_3 - \tfrac{1}{2}\right)\,\mathbf{a}_2 + \left(x_3 - z_3 + \tfrac{1}{2}\right)\,\mathbf{a}_3 = -a\left(z_3 - \tfrac{1}{2}\right)\,\hat{\mathbf{x}} + a x_3\,\hat{\mathbf{y}} - a y_3\,\hat{\mathbf{z}} \quad (48e) \quad \text{O I}$$

$$\mathbf{B_{25}} = (x_3 + z_3)\,\mathbf{a}_1 + (x_3 + y_3)\,\mathbf{a}_2 + (y_3 + z_3)\,\mathbf{a}_3 = a y_3\,\hat{\mathbf{x}} + a z_3\,\hat{\mathbf{y}} + a x_3\,\hat{\mathbf{z}} \quad (48e) \quad \text{O I}$$

$$\mathbf{B_{26}} = -(x_3 - z_3)\,\mathbf{a}_1 - \left(x_3 + y_3 - \tfrac{1}{2}\right)\,\mathbf{a}_2 + \left(-y_3 + z_3 + \tfrac{1}{2}\right)\,\mathbf{a}_3 = -a\left(y_3 - \tfrac{1}{2}\right)\,\hat{\mathbf{x}} + a z_3\,\hat{\mathbf{y}} - a x_3\,\hat{\mathbf{z}} \quad (48e) \quad \text{O I}$$

$$\mathbf{B_{27}} = -\left(x_3 + z_3 - \tfrac{1}{2}\right)\,\mathbf{a}_1 + \left(-x_3 + y_3 + \tfrac{1}{2}\right)\,\mathbf{a}_2 + (y_3 - z_3)\,\mathbf{a}_3 = a y_3\,\hat{\mathbf{x}} - a z_3\,\hat{\mathbf{y}} - a\left(x_3 - \tfrac{1}{2}\right)\,\hat{\mathbf{z}} \quad (48e) \quad \text{O I}$$

$$\mathbf{B_{28}} = \left(x_3 - z_3 + \tfrac{1}{2}\right)\,\mathbf{a}_1 + (x_3 - y_3)\,\mathbf{a}_2 - \left(y_3 + z_3 - \tfrac{1}{2}\right)\,\mathbf{a}_3 = -a y_3\,\hat{\mathbf{x}} - a\left(z_3 - \tfrac{1}{2}\right)\,\hat{\mathbf{y}} + a x_3\,\hat{\mathbf{z}} \quad (48e) \quad \text{O I}$$

$$\mathbf{B_{29}} = -(y_3 + z_3)\,\mathbf{a}_1 - (x_3 + z_3)\,\mathbf{a}_2 - (x_3 + y_3)\,\mathbf{a}_3 = -a x_3\,\hat{\mathbf{x}} - a y_3\,\hat{\mathbf{y}} - a z_3\,\hat{\mathbf{z}} \quad (48e) \quad \text{O I}$$

$$\mathbf{B_{30}} = \left(y_3 - z_3 + \tfrac{1}{2}\right)\,\mathbf{a}_1 + (x_3 - z_3)\,\mathbf{a}_2 + \left(x_3 + y_3 + \tfrac{1}{2}\right)\,\mathbf{a}_3 = a x_3\,\hat{\mathbf{x}} + a\left(y_3 + \tfrac{1}{2}\right)\,\hat{\mathbf{y}} - a z_3\,\hat{\mathbf{z}} \quad (48e) \quad \text{O I}$$

$$\mathbf{B_{31}} = -(y_3 - z_3)\,\mathbf{a}_1 + \left(x_3 + z_3 + \tfrac{1}{2}\right)\,\mathbf{a}_2 + \left(x_3 - y_3 + \tfrac{1}{2}\right)\,\mathbf{a}_3 = a\left(x_3 + \tfrac{1}{2}\right)\,\hat{\mathbf{x}} - a y_3\,\hat{\mathbf{y}} + a z_3\,\hat{\mathbf{z}} \quad (48e) \quad \text{O I}$$

$$\mathbf{B_{32}} = \left(y_3 + z_3 + \tfrac{1}{2}\right)\,\mathbf{a}_1 + \left(-x_3 + z_3 + \tfrac{1}{2}\right)\,\mathbf{a}_2 - (x_3 - y_3)\,\mathbf{a}_3 = -a x_3\,\hat{\mathbf{x}} + a y_3\,\hat{\mathbf{y}} + a\left(z_3 + \tfrac{1}{2}\right)\,\hat{\mathbf{z}} \quad (48e) \quad \text{O I}$$

$$\mathbf{B_{33}} = -(x_3 + y_3)\,\mathbf{a}_1 - (y_3 + z_3)\,\mathbf{a}_2 - (x_3 + z_3)\,\mathbf{a}_3 = -a z_3\,\hat{\mathbf{x}} - a x_3\,\hat{\mathbf{y}} - a y_3\,\hat{\mathbf{z}} \quad (48e) \quad \text{O I}$$

$$\mathbf{B_{34}} = \left(x_3 + y_3 + \tfrac{1}{2}\right)\,\mathbf{a}_1 + \left(y_3 - z_3 + \tfrac{1}{2}\right)\,\mathbf{a}_2 + (x_3 - z_3)\,\mathbf{a}_3 = -a z_3\,\hat{\mathbf{x}} + a x_3\,\hat{\mathbf{y}} + a\left(y_3 + \tfrac{1}{2}\right)\,\hat{\mathbf{z}} \quad (48e) \quad \text{O I}$$

$$\mathbf{B_{35}} = \left(x_3 - y_3 + \tfrac{1}{2}\right)\,\mathbf{a}_1 - (y_3 - z_3)\,\mathbf{a}_2 + \left(x_3 + z_3 + \tfrac{1}{2}\right)\,\mathbf{a}_3 = a z_3\,\hat{\mathbf{x}} + a\left(x_3 + \tfrac{1}{2}\right)\,\hat{\mathbf{y}} - a y_3\,\hat{\mathbf{z}} \quad (48e) \quad \text{O I}$$

$$\mathbf{B_{36}} = -(x_3 - y_3)\,\mathbf{a}_1 + \left(y_3 + z_3 + \tfrac{1}{2}\right)\,\mathbf{a}_2 + \left(-x_3 + z_3 + \tfrac{1}{2}\right)\,\mathbf{a}_3 = a\left(z_3 + \tfrac{1}{2}\right)\,\hat{\mathbf{x}} - a x_3\,\hat{\mathbf{y}} + a y_3\,\hat{\mathbf{z}} \quad (48e) \quad \text{O I}$$

$$\mathbf{B_{37}} = -(x_3 + z_3)\,\mathbf{a}_1 - (x_3 + y_3)\,\mathbf{a}_2 - (y_3 + z_3)\,\mathbf{a}_3 = -a y_3\,\hat{\mathbf{x}} - a z_3\,\hat{\mathbf{y}} - a x_3\,\hat{\mathbf{z}} \quad (48e) \quad \text{O I}$$

$$\mathbf{B_{38}} = (x_3 - z_3)\,\mathbf{a}_1 + \left(x_3 + y_3 + \tfrac{1}{2}\right)\,\mathbf{a}_2 + \left(y_3 - z_3 + \tfrac{1}{2}\right)\,\mathbf{a}_3 = a\left(y_3 + \tfrac{1}{2}\right)\,\hat{\mathbf{x}} - a z_3\,\hat{\mathbf{y}} + a x_3\,\hat{\mathbf{z}} \quad (48e) \quad \text{O I}$$

$$\mathbf{B_{39}} = \left(x_3 + z_3 + \tfrac{1}{2}\right)\,\mathbf{a}_1 + \left(x_3 - y_3 + \tfrac{1}{2}\right)\,\mathbf{a}_2 - (y_3 - z_3)\,\mathbf{a}_3 = -a y_3\,\hat{\mathbf{x}} + a z_3\,\hat{\mathbf{y}} + a\left(x_3 + \tfrac{1}{2}\right)\,\hat{\mathbf{z}} \quad (48e) \quad \text{O I}$$

$$\mathbf{B_{40}} = \left(-x_3 + z_3 + \tfrac{1}{2}\right)\,\mathbf{a}_1 - (x_3 - y_3)\,\mathbf{a}_2 + \left(y_3 + z_3 + \tfrac{1}{2}\right)\,\mathbf{a}_3 = a y_3\,\hat{\mathbf{x}} + a\left(z_3 + \tfrac{1}{2}\right)\,\hat{\mathbf{y}} - a x_3\,\hat{\mathbf{z}} \quad (48e) \quad \text{O I}$$

References

[1] H. Dachs, *Die Kristallstruktur des Bixbyits (Fe,Mn)$_2O_3$*, Z. Krystallogr. **107**, S, 370–395 (1956), doi:10.1524/zkri.1956.107.5-6.370.

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

Found in

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