Ordered $TmBO_3$ Structure: AB3C_hP30_193_g_gk_bd-001

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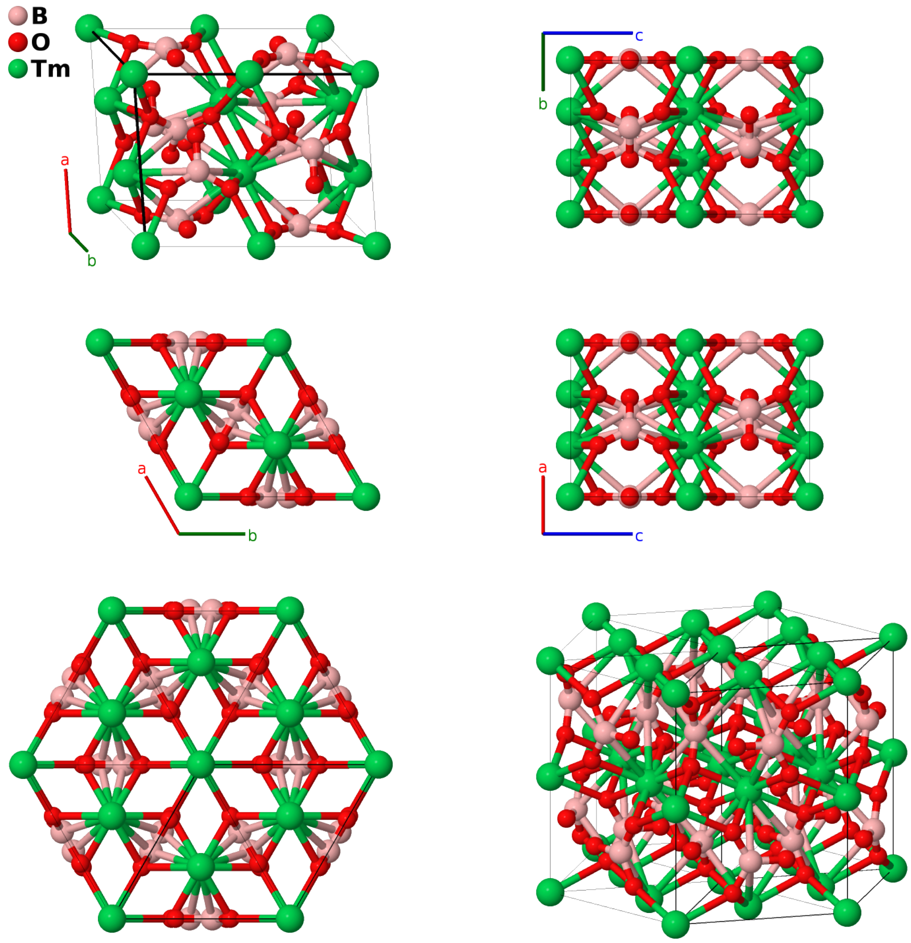
https://aflow.org/p/AE3Q

https://aflow.org/p/AB3C_hP30_193_g_gk_bd-001



Prototype BO_3Tm

AFLOW prototype label AB3C_hP30_193_g_gk_bd-001

ICSD 27942

Pearson symbol hP30

Space group number 193

Space group symbol $P6_3/mcm$

AFLOW prototype command `aflow --proto=AB3C_hP30_193_g_gk_bd-001 --params=`$a, c/a, x_3, x_4, x_5, z_5$

Other compounds with this structure

$DyBO_3$, $ErBO_3$, $EuBO_3$, $GdBO_3$, $HoBO_3$, $LuBO_3$, $SmBO_3$, YBO_3, $YbBO_3$

- (Newnham, 1963) found two possible structures for $TmBO_3$ and YBO_3:
  - A compact hexagonal cell with partially disordered boron and oxygen atoms, and
  - this structure, which has a larger hexagonal cell but completely ordered atoms.
- There are several problems with this structure:
  - The ICSD entry 27942 places this structure in space group $P\bar{6}c2$ #188 even though the positions are such that the structure can be resolved in the higher symmetry $P6_3/mcm$ space group, and
  - the positions of the O I atoms are such that the O-O distance is less than 1Å.
  - The ICSD entry gives what seem to be reasonable O-O distances, so we use those coordinates, using AFLOW to transform the structure into space group $P6_3/mcm$.

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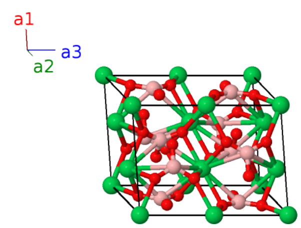
Hexagonal primitive vectors

$$\mathbf{a_1} = \frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a\,\hat{\mathbf{y}}$$
$$\mathbf{a_2} = \frac{1}{2}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a\,\hat{\mathbf{y}}$$
$$\mathbf{a_3} = c\,\hat{\mathbf{z}}$$



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$ =	0	=	0	(2b)	Tm I
$\mathbf{B_2}$ =	$\frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}c\,\hat{\mathbf{z}}$	(2b)	Tm I
$\mathbf{B_3}$ =	$\frac{1}{3}\,\mathbf{a}_1 + \frac{2}{3}\,\mathbf{a}_2$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}}$	(4d)	Tm II
$\mathbf{B_4}$ =	$\frac{2}{3}\,\mathbf{a}_1 + \frac{1}{3}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(4d)	Tm II
$\mathbf{B_5}$ =	$\frac{2}{3}\,\mathbf{a}_1 + \frac{1}{3}\,\mathbf{a}_2$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}}$	(4d)	Tm II
$\mathbf{B_6}$ =	$\frac{1}{3}\,\mathbf{a}_1 + \frac{2}{3}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(4d)	Tm II
$\mathbf{B_7}$ =	$x_3\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_3$	=	$\frac{1}{2}ax_3\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_3\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(6g)	B I
$\mathbf{B_8}$ =	$x_3\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$\frac{1}{2}ax_3\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_3\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(6g)	B I
$\mathbf{B_9}$ =	$-x_3\,\mathbf{a}_1 - x_3\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$-ax_3\,\hat{\mathbf{x}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(6g)	B I
$\mathbf{B_{10}}$ =	$-x_3\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_3$	=	$-\frac{1}{2}ax_3\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_3\,\hat{\mathbf{y}} + \frac{3}{4}c\,\hat{\mathbf{z}}$	(6g)	B I
$\mathbf{B_{11}}$ =	$-x_3\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$-\frac{1}{2}ax_3\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_3\,\hat{\mathbf{y}} + \frac{3}{4}c\,\hat{\mathbf{z}}$	(6g)	B I
$\mathbf{B_{12}}$ =	$x_3\,\mathbf{a}_1 + x_3\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$ax_3\,\hat{\mathbf{x}} + \frac{3}{4}c\,\hat{\mathbf{z}}$	(6g)	B I
$\mathbf{B_{13}}$ =	$x_4\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_3$	=	$\frac{1}{2}ax_4\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_4\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(6g)	O I
$\mathbf{B_{14}}$ =	$x_4\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$\frac{1}{2}ax_4\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_4\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(6g)	O I
$\mathbf{B_{15}}$ =	$-x_4\,\mathbf{a}_1 - x_4\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$-ax_4\,\hat{\mathbf{x}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(6g)	O I
$\mathbf{B_{16}}$ =	$-x_4\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_3$	=	$-\frac{1}{2}ax_4\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_4\,\hat{\mathbf{y}} + \frac{3}{4}c\,\hat{\mathbf{z}}$	(6g)	O I

$\mathbf{B_{17}}$	=	$-x_4\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$-\frac{1}{2}ax_4\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_4\,\hat{\mathbf{y}} + \frac{3}{4}c\,\hat{\mathbf{z}}$	(6g)	O I
$\mathbf{B_{18}}$	=	$x_4\,\mathbf{a}_1 + x_4\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$ax_4\,\hat{\mathbf{x}} + \frac{3}{4}c\,\hat{\mathbf{z}}$	(6g)	O I
$\mathbf{B_{19}}$	=	$x_5\,\mathbf{a}_1 + z_5\,\mathbf{a}_3$	=	$\frac{1}{2}ax_5\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_5\,\hat{\mathbf{y}} + cz_5\,\hat{\mathbf{z}}$	(12k)	O II
$\mathbf{B_{20}}$	=	$x_5\,\mathbf{a}_2 + z_5\,\mathbf{a}_3$	=	$\frac{1}{2}ax_5\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_5\,\hat{\mathbf{y}} + cz_5\,\hat{\mathbf{z}}$	(12k)	O II
$\mathbf{B_{21}}$	=	$-x_5\,\mathbf{a}_1 - x_5\,\mathbf{a}_2 + z_5\,\mathbf{a}_3$	=	$-ax_5\,\hat{\mathbf{x}} + cz_5\,\hat{\mathbf{z}}$	(12k)	O II
$\mathbf{B_{22}}$	=	$-x_5\,\mathbf{a}_1 + \left(z_5 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-\frac{1}{2}ax_5\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_5\,\hat{\mathbf{y}} + c\left(z_5 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(12k)	O II
$\mathbf{B_{23}}$	=	$-x_5\,\mathbf{a}_2 + \left(z_5 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-\frac{1}{2}ax_5\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_5\,\hat{\mathbf{y}} + c\left(z_5 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(12k)	O II
$\mathbf{B_{24}}$	=	$x_5\,\mathbf{a}_1 + x_5\,\mathbf{a}_2 + \left(z_5 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$ax_5\,\hat{\mathbf{x}} + c\left(z_5 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(12k)	O II
$\mathbf{B_{25}}$	=	$x_5\,\mathbf{a}_2 - \left(z_5 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}ax_5\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_5\,\hat{\mathbf{y}} - c\left(z_5 - \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(12k)	O II
$\mathbf{B_{26}}$	=	$x_5\,\mathbf{a}_1 - \left(z_5 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}ax_5\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_5\,\hat{\mathbf{y}} - c\left(z_5 - \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(12k)	O II
$\mathbf{B_{27}}$	=	$-x_5\,\mathbf{a}_1 - x_5\,\mathbf{a}_2 - \left(z_5 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ax_5\,\hat{\mathbf{x}} - c\left(z_5 - \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(12k)	O II
$\mathbf{B_{28}}$	=	$-x_5\,\mathbf{a}_2 - z_5\,\mathbf{a}_3$	=	$-\frac{1}{2}ax_5\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_5\,\hat{\mathbf{y}} - cz_5\,\hat{\mathbf{z}}$	(12k)	O II
$\mathbf{B_{29}}$	=	$-x_5\,\mathbf{a}_1 - z_5\,\mathbf{a}_3$	=	$-\frac{1}{2}ax_5\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_5\,\hat{\mathbf{y}} - cz_5\,\hat{\mathbf{z}}$	(12k)	O II
$\mathbf{B_{30}}$	=	$x_5\,\mathbf{a}_1 + x_5\,\mathbf{a}_2 - z_5\,\mathbf{a}_3$	=	$ax_5\,\hat{\mathbf{x}} - cz_5\,\hat{\mathbf{z}}$	(12k)	O II

References

[1] R. E. Newnham, M. J. Redman, and R. P. Santoro, *Crystal Structure of Yttrium and Other Rare-Earth Borates*, J. Am. Ceram. Soc. **46**, 253–256 (1963), doi:10.1111/j.1151-2916.1963.tb11721.x.