α-HBO$_2$ (orthorhombic) Structure: ABC2_oP48_62_3c_3c_6c-001

https://aflow.org/p/XYXT

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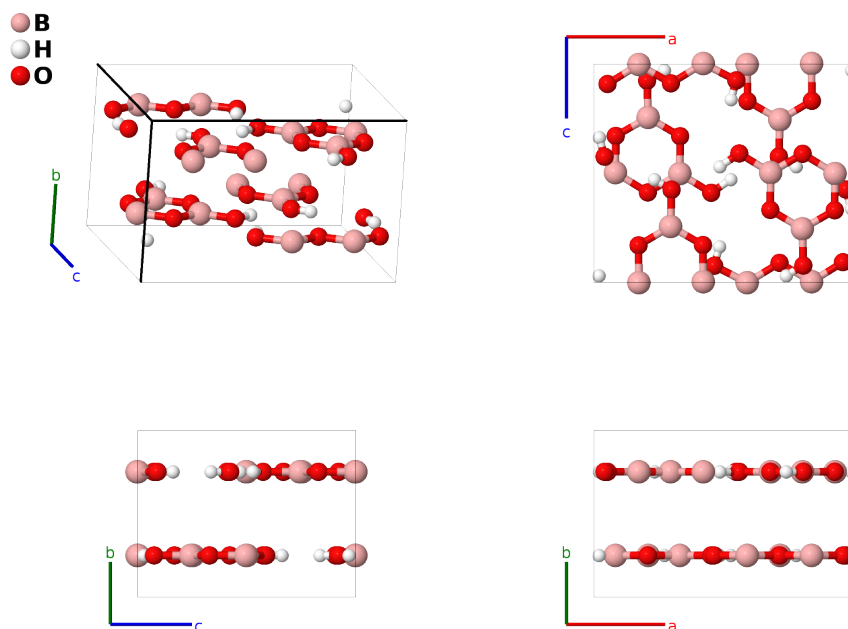
Prototype	BHO$_2$
AFLOW prototype label	ABC2_oP48_62_3c_3c_6c-001
ICSD	16545
Pearson symbol	oP48
Space group number	62
Space group symbol	$Pnma$
AFLOW prototype command	aflow --proto=ABC2_oP48_62_3c_3c_6c-001

$\qquad$ --params=$a, b/a, c/a, x_1, z_1, x_2, z_2, x_3, z_3, x_4, z_4, x_5, z_5, x_6, z_6, x_7, z_7, x_8, z_8, x_9, z_9, x_{10},$
$z_{10}, x_{11}, z_{11}, x_{12}, z_{12}$

- Metaboric acid, HBO$_2$, is found in three forms (Kracke, 1938):

    - orthorhombic α-HBO$_2$, also known as HBO$_2$ I (this structure),
    - monoclinic β-HBO$_2$, also known as HBO$_2$ II, and
    - cubic γ-HBO$_2$, also known as HBO$_2$ III.

- The structures are named in order of stability, although all can exist at room temperature.

- (Peters, 1980) give the structure of α-HBO$_2$ in the *Pbnm* setting of space group #62. We used FINDSYM to transform this to the standard *Pnma* setting.

Simple Orthorhombic primitive vectors

$$\mathbf{a_1} = a\,\hat{\mathbf{x}}$$
$$\mathbf{a_2} = b\,\hat{\mathbf{y}}$$
$$\mathbf{a_3} = c\,\hat{\mathbf{z}}$$
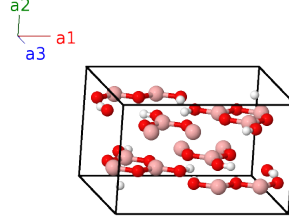
Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	$=$	$x_1\,\mathbf{a_1} + \frac{1}{4}\,\mathbf{a_2} + z_1\,\mathbf{a_3}$	$=$	$ax_1\,\hat{\mathbf{x}} + \frac{1}{4}b\,\hat{\mathbf{y}} + cz_1\,\hat{\mathbf{z}}$	(4c)	B I
$\mathbf{B_2}$	$=$	$-\left(x_1 - \frac{1}{2}\right)\mathbf{a_1} + \frac{3}{4}\,\mathbf{a_2} + \left(z_1 + \frac{1}{2}\right)\mathbf{a_3}$	$=$	$-a\left(x_1 - \frac{1}{2}\right)\hat{\mathbf{x}} + \frac{3}{4}b\,\hat{\mathbf{y}} + c\left(z_1 + \frac{1}{2}\right)\hat{\mathbf{z}}$	(4c)	B I
$\mathbf{B_3}$	$=$	$-x_1\,\mathbf{a_1} + \frac{3}{4}\,\mathbf{a_2} - z_1\,\mathbf{a_3}$	$=$	$-ax_1\,\hat{\mathbf{x}} + \frac{3}{4}b\,\hat{\mathbf{y}} - cz_1\,\hat{\mathbf{z}}$	(4c)	B I
$\mathbf{B_4}$	$=$	$\left(x_1 + \frac{1}{2}\right)\mathbf{a_1} + \frac{1}{4}\,\mathbf{a_2} - \left(z_1 - \frac{1}{2}\right)\mathbf{a_3}$	$=$	$a\left(x_1 + \frac{1}{2}\right)\hat{\mathbf{x}} + \frac{1}{4}b\,\hat{\mathbf{y}} - c\left(z_1 - \frac{1}{2}\right)\hat{\mathbf{z}}$	(4c)	B I
$\mathbf{B_5}$	$=$	$x_2\,\mathbf{a_1} + \frac{1}{4}\,\mathbf{a_2} + z_2\,\mathbf{a_3}$	$=$	$ax_2\,\hat{\mathbf{x}} + \frac{1}{4}b\,\hat{\mathbf{y}} + cz_2\,\hat{\mathbf{z}}$	(4c)	B II
$\mathbf{B_6}$	$=$	$-\left(x_2 - \frac{1}{2}\right)\mathbf{a_1} + \frac{3}{4}\,\mathbf{a_2} + \left(z_2 + \frac{1}{2}\right)\mathbf{a_3}$	$=$	$-a\left(x_2 - \frac{1}{2}\right)\hat{\mathbf{x}} + \frac{3}{4}b\,\hat{\mathbf{y}} + c\left(z_2 + \frac{1}{2}\right)\hat{\mathbf{z}}$	(4c)	B II
$\mathbf{B_7}$	$=$	$-x_2\,\mathbf{a_1} + \frac{3}{4}\,\mathbf{a_2} - z_2\,\mathbf{a_3}$	$=$	$-ax_2\,\hat{\mathbf{x}} + \frac{3}{4}b\,\hat{\mathbf{y}} - cz_2\,\hat{\mathbf{z}}$	(4c)	B II
$\mathbf{B_8}$	$=$	$\left(x_2 + \frac{1}{2}\right)\mathbf{a_1} + \frac{1}{4}\,\mathbf{a_2} - \left(z_2 - \frac{1}{2}\right)\mathbf{a_3}$	$=$	$a\left(x_2 + \frac{1}{2}\right)\hat{\mathbf{x}} + \frac{1}{4}b\,\hat{\mathbf{y}} - c\left(z_2 - \frac{1}{2}\right)\hat{\mathbf{z}}$	(4c)	B II
$\mathbf{B_9}$	$=$	$x_3\,\mathbf{a_1} + \frac{1}{4}\,\mathbf{a_2} + z_3\,\mathbf{a_3}$	$=$	$ax_3\,\hat{\mathbf{x}} + \frac{1}{4}b\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$	(4c)	B III
$\mathbf{B_{10}}$	$=$	$-\left(x_3 - \frac{1}{2}\right)\mathbf{a_1} + \frac{3}{4}\,\mathbf{a_2} + \left(z_3 + \frac{1}{2}\right)\mathbf{a_3}$	$=$	$-a\left(x_3 - \frac{1}{2}\right)\hat{\mathbf{x}} + \frac{3}{4}b\,\hat{\mathbf{y}} + c\left(z_3 + \frac{1}{2}\right)\hat{\mathbf{z}}$	(4c)	B III
$\mathbf{B_{11}}$	$=$	$-x_3\,\mathbf{a_1} + \frac{3}{4}\,\mathbf{a_2} - z_3\,\mathbf{a_3}$	$=$	$-ax_3\,\hat{\mathbf{x}} + \frac{3}{4}b\,\hat{\mathbf{y}} - cz_3\,\hat{\mathbf{z}}$	(4c)	B III
$\mathbf{B_{12}}$	$=$	$\left(x_3 + \frac{1}{2}\right)\mathbf{a_1} + \frac{1}{4}\,\mathbf{a_2} - \left(z_3 - \frac{1}{2}\right)\mathbf{a_3}$	$=$	$a\left(x_3 + \frac{1}{2}\right)\hat{\mathbf{x}} + \frac{1}{4}b\,\hat{\mathbf{y}} - c\left(z_3 - \frac{1}{2}\right)\hat{\mathbf{z}}$	(4c)	B III
$\mathbf{B_{13}}$	$=$	$x_4\,\mathbf{a_1} + \frac{1}{4}\,\mathbf{a_2} + z_4\,\mathbf{a_3}$	$=$	$ax_4\,\hat{\mathbf{x}} + \frac{1}{4}b\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$	(4c)	H I
$\mathbf{B_{14}}$	$=$	$-\left(x_4 - \frac{1}{2}\right)\mathbf{a_1} + \frac{3}{4}\,\mathbf{a_2} + \left(z_4 + \frac{1}{2}\right)\mathbf{a_3}$	$=$	$-a\left(x_4 - \frac{1}{2}\right)\hat{\mathbf{x}} + \frac{3}{4}b\,\hat{\mathbf{y}} + c\left(z_4 + \frac{1}{2}\right)\hat{\mathbf{z}}$	(4c)	H I
$\mathbf{B_{15}}$	$=$	$-x_4\,\mathbf{a_1} + \frac{3}{4}\,\mathbf{a_2} - z_4\,\mathbf{a_3}$	$=$	$-ax_4\,\hat{\mathbf{x}} + \frac{3}{4}b\,\hat{\mathbf{y}} - cz_4\,\hat{\mathbf{z}}$	(4c)	H I
$\mathbf{B_{16}}$	$=$	$\left(x_4 + \frac{1}{2}\right)\mathbf{a_1} + \frac{1}{4}\,\mathbf{a_2} - \left(z_4 - \frac{1}{2}\right)\mathbf{a_3}$	$=$	$a\left(x_4 + \frac{1}{2}\right)\hat{\mathbf{x}} + \frac{1}{4}b\,\hat{\mathbf{y}} - c\left(z_4 - \frac{1}{2}\right)\hat{\mathbf{z}}$	(4c)	H I
$\mathbf{B_{17}}$	$=$	$x_5\,\mathbf{a_1} + \frac{1}{4}\,\mathbf{a_2} + z_5\,\mathbf{a_3}$	$=$	$ax_5\,\hat{\mathbf{x}} + \frac{1}{4}b\,\hat{\mathbf{y}} + cz_5\,\hat{\mathbf{z}}$	(4c)	H II
$\mathbf{B_{18}}$	$=$	$-\left(x_5 - \frac{1}{2}\right)\mathbf{a_1} + \frac{3}{4}\,\mathbf{a_2} + \left(z_5 + \frac{1}{2}\right)\mathbf{a_3}$	$=$	$-a\left(x_5 - \frac{1}{2}\right)\hat{\mathbf{x}} + \frac{3}{4}b\,\hat{\mathbf{y}} + c\left(z_5 + \frac{1}{2}\right)\hat{\mathbf{z}}$	(4c)	H II
$\mathbf{B_{19}}$	$=$	$-x_5\,\mathbf{a_1} + \frac{3}{4}\,\mathbf{a_2} - z_5\,\mathbf{a_3}$	$=$	$-ax_5\,\hat{\mathbf{x}} + \frac{3}{4}b\,\hat{\mathbf{y}} - cz_5\,\hat{\mathbf{z}}$	(4c)	H II
$\mathbf{B_{20}}$	$=$	$\left(x_5 + \frac{1}{2}\right)\mathbf{a_1} + \frac{1}{4}\,\mathbf{a_2} - \left(z_5 - \frac{1}{2}\right)\mathbf{a_3}$	$=$	$a\left(x_5 + \frac{1}{2}\right)\hat{\mathbf{x}} + \frac{1}{4}b\,\hat{\mathbf{y}} - c\left(z_5 - \frac{1}{2}\right)\hat{\mathbf{z}}$	(4c)	H II
$\mathbf{B_{21}}$	$=$	$x_6\,\mathbf{a_1} + \frac{1}{4}\,\mathbf{a_2} + z_6\,\mathbf{a_3}$	$=$	$ax_6\,\hat{\mathbf{x}} + \frac{1}{4}b\,\hat{\mathbf{y}} + cz_6\,\hat{\mathbf{z}}$	(4c)	H III
$\mathbf{B_{22}}$	$=$	$-\left(x_6 - \frac{1}{2}\right)\mathbf{a_1} + \frac{3}{4}\,\mathbf{a_2} + \left(z_6 + \frac{1}{2}\right)\mathbf{a_3}$	$=$	$-a\left(x_6 - \frac{1}{2}\right)\hat{\mathbf{x}} + \frac{3}{4}b\,\hat{\mathbf{y}} + c\left(z_6 + \frac{1}{2}\right)\hat{\mathbf{z}}$	(4c)	H III
$\mathbf{B_{23}}$	$=$	$-x_6\,\mathbf{a_1} + \frac{3}{4}\,\mathbf{a_2} - z_6\,\mathbf{a_3}$	$=$	$-ax_6\,\hat{\mathbf{x}} + \frac{3}{4}b\,\hat{\mathbf{y}} - cz_6\,\hat{\mathbf{z}}$	(4c)	H III

$$\mathbf{B_{24}} = \left(x_6 + \tfrac{1}{2}\right)\mathbf{a}_1 + \tfrac{1}{4}\mathbf{a}_2 - \left(z_6 - \tfrac{1}{2}\right)\mathbf{a}_3 = a\left(x_6 + \tfrac{1}{2}\right)\hat{\mathbf{x}} + \tfrac{1}{4}b\hat{\mathbf{y}} - c\left(z_6 - \tfrac{1}{2}\right)\hat{\mathbf{z}} \quad (4c) \quad \text{H III}$$

$$\mathbf{B_{25}} = x_7\mathbf{a}_1 + \tfrac{1}{4}\mathbf{a}_2 + z_7\mathbf{a}_3 = ax_7\hat{\mathbf{x}} + \tfrac{1}{4}b\hat{\mathbf{y}} + cz_7\hat{\mathbf{z}} \quad (4c) \quad \text{O I}$$

$$\mathbf{B_{26}} = -\left(x_7 - \tfrac{1}{2}\right)\mathbf{a}_1 + \tfrac{3}{4}\mathbf{a}_2 + \left(z_7 + \tfrac{1}{2}\right)\mathbf{a}_3 = -a\left(x_7 - \tfrac{1}{2}\right)\hat{\mathbf{x}} + \tfrac{3}{4}b\hat{\mathbf{y}} + c\left(z_7 + \tfrac{1}{2}\right)\hat{\mathbf{z}} \quad (4c) \quad \text{O I}$$

$$\mathbf{B_{27}} = -x_7\mathbf{a}_1 + \tfrac{3}{4}\mathbf{a}_2 - z_7\mathbf{a}_3 = -ax_7\hat{\mathbf{x}} + \tfrac{3}{4}b\hat{\mathbf{y}} - cz_7\hat{\mathbf{z}} \quad (4c) \quad \text{O I}$$

$$\mathbf{B_{28}} = \left(x_7 + \tfrac{1}{2}\right)\mathbf{a}_1 + \tfrac{1}{4}\mathbf{a}_2 - \left(z_7 - \tfrac{1}{2}\right)\mathbf{a}_3 = a\left(x_7 + \tfrac{1}{2}\right)\hat{\mathbf{x}} + \tfrac{1}{4}b\hat{\mathbf{y}} - c\left(z_7 - \tfrac{1}{2}\right)\hat{\mathbf{z}} \quad (4c) \quad \text{O I}$$

$$\mathbf{B_{29}} = x_8\mathbf{a}_1 + \tfrac{1}{4}\mathbf{a}_2 + z_8\mathbf{a}_3 = ax_8\hat{\mathbf{x}} + \tfrac{1}{4}b\hat{\mathbf{y}} + cz_8\hat{\mathbf{z}} \quad (4c) \quad \text{O II}$$

$$\mathbf{B_{30}} = -\left(x_8 - \tfrac{1}{2}\right)\mathbf{a}_1 + \tfrac{3}{4}\mathbf{a}_2 + \left(z_8 + \tfrac{1}{2}\right)\mathbf{a}_3 = -a\left(x_8 - \tfrac{1}{2}\right)\hat{\mathbf{x}} + \tfrac{3}{4}b\hat{\mathbf{y}} + c\left(z_8 + \tfrac{1}{2}\right)\hat{\mathbf{z}} \quad (4c) \quad \text{O II}$$

$$\mathbf{B_{31}} = -x_8\mathbf{a}_1 + \tfrac{3}{4}\mathbf{a}_2 - z_8\mathbf{a}_3 = -ax_8\hat{\mathbf{x}} + \tfrac{3}{4}b\hat{\mathbf{y}} - cz_8\hat{\mathbf{z}} \quad (4c) \quad \text{O II}$$

$$\mathbf{B_{32}} = \left(x_8 + \tfrac{1}{2}\right)\mathbf{a}_1 + \tfrac{1}{4}\mathbf{a}_2 - \left(z_8 - \tfrac{1}{2}\right)\mathbf{a}_3 = a\left(x_8 + \tfrac{1}{2}\right)\hat{\mathbf{x}} + \tfrac{1}{4}b\hat{\mathbf{y}} - c\left(z_8 - \tfrac{1}{2}\right)\hat{\mathbf{z}} \quad (4c) \quad \text{O II}$$

$$\mathbf{B_{33}} = x_9\mathbf{a}_1 + \tfrac{1}{4}\mathbf{a}_2 + z_9\mathbf{a}_3 = ax_9\hat{\mathbf{x}} + \tfrac{1}{4}b\hat{\mathbf{y}} + cz_9\hat{\mathbf{z}} \quad (4c) \quad \text{O III}$$

$$\mathbf{B_{34}} = -\left(x_9 - \tfrac{1}{2}\right)\mathbf{a}_1 + \tfrac{3}{4}\mathbf{a}_2 + \left(z_9 + \tfrac{1}{2}\right)\mathbf{a}_3 = -a\left(x_9 - \tfrac{1}{2}\right)\hat{\mathbf{x}} + \tfrac{3}{4}b\hat{\mathbf{y}} + c\left(z_9 + \tfrac{1}{2}\right)\hat{\mathbf{z}} \quad (4c) \quad \text{O III}$$

$$\mathbf{B_{35}} = -x_9\mathbf{a}_1 + \tfrac{3}{4}\mathbf{a}_2 - z_9\mathbf{a}_3 = -ax_9\hat{\mathbf{x}} + \tfrac{3}{4}b\hat{\mathbf{y}} - cz_9\hat{\mathbf{z}} \quad (4c) \quad \text{O III}$$

$$\mathbf{B_{36}} = \left(x_9 + \tfrac{1}{2}\right)\mathbf{a}_1 + \tfrac{1}{4}\mathbf{a}_2 - \left(z_9 - \tfrac{1}{2}\right)\mathbf{a}_3 = a\left(x_9 + \tfrac{1}{2}\right)\hat{\mathbf{x}} + \tfrac{1}{4}b\hat{\mathbf{y}} - c\left(z_9 - \tfrac{1}{2}\right)\hat{\mathbf{z}} \quad (4c) \quad \text{O III}$$

$$\mathbf{B_{37}} = x_{10}\mathbf{a}_1 + \tfrac{1}{4}\mathbf{a}_2 + z_{10}\mathbf{a}_3 = ax_{10}\hat{\mathbf{x}} + \tfrac{1}{4}b\hat{\mathbf{y}} + cz_{10}\hat{\mathbf{z}} \quad (4c) \quad \text{O IV}$$

$$\mathbf{B_{38}} = -\left(x_{10} - \tfrac{1}{2}\right)\mathbf{a}_1 + \tfrac{3}{4}\mathbf{a}_2 + \left(z_{10} + \tfrac{1}{2}\right)\mathbf{a}_3 = -a\left(x_{10} - \tfrac{1}{2}\right)\hat{\mathbf{x}} + \tfrac{3}{4}b\hat{\mathbf{y}} + c\left(z_{10} + \tfrac{1}{2}\right)\hat{\mathbf{z}} \quad (4c) \quad \text{O IV}$$

$$\mathbf{B_{39}} = -x_{10}\mathbf{a}_1 + \tfrac{3}{4}\mathbf{a}_2 - z_{10}\mathbf{a}_3 = -ax_{10}\hat{\mathbf{x}} + \tfrac{3}{4}b\hat{\mathbf{y}} - cz_{10}\hat{\mathbf{z}} \quad (4c) \quad \text{O IV}$$

$$\mathbf{B_{40}} = \left(x_{10} + \tfrac{1}{2}\right)\mathbf{a}_1 + \tfrac{1}{4}\mathbf{a}_2 - \left(z_{10} - \tfrac{1}{2}\right)\mathbf{a}_3 = a\left(x_{10} + \tfrac{1}{2}\right)\hat{\mathbf{x}} + \tfrac{1}{4}b\hat{\mathbf{y}} - c\left(z_{10} - \tfrac{1}{2}\right)\hat{\mathbf{z}} \quad (4c) \quad \text{O IV}$$

$$\mathbf{B_{41}} = x_{11}\mathbf{a}_1 + \tfrac{1}{4}\mathbf{a}_2 + z_{11}\mathbf{a}_3 = ax_{11}\hat{\mathbf{x}} + \tfrac{1}{4}b\hat{\mathbf{y}} + cz_{11}\hat{\mathbf{z}} \quad (4c) \quad \text{O V}$$

$$\mathbf{B_{42}} = -\left(x_{11} - \tfrac{1}{2}\right)\mathbf{a}_1 + \tfrac{3}{4}\mathbf{a}_2 + \left(z_{11} + \tfrac{1}{2}\right)\mathbf{a}_3 = -a\left(x_{11} - \tfrac{1}{2}\right)\hat{\mathbf{x}} + \tfrac{3}{4}b\hat{\mathbf{y}} + c\left(z_{11} + \tfrac{1}{2}\right)\hat{\mathbf{z}} \quad (4c) \quad \text{O V}$$

$$\mathbf{B_{43}} = -x_{11}\mathbf{a}_1 + \tfrac{3}{4}\mathbf{a}_2 - z_{11}\mathbf{a}_3 = -ax_{11}\hat{\mathbf{x}} + \tfrac{3}{4}b\hat{\mathbf{y}} - cz_{11}\hat{\mathbf{z}} \quad (4c) \quad \text{O V}$$

$$\mathbf{B_{44}} = \left(x_{11} + \tfrac{1}{2}\right)\mathbf{a}_1 + \tfrac{1}{4}\mathbf{a}_2 - \left(z_{11} - \tfrac{1}{2}\right)\mathbf{a}_3 = a\left(x_{11} + \tfrac{1}{2}\right)\hat{\mathbf{x}} + \tfrac{1}{4}b\hat{\mathbf{y}} - c\left(z_{11} - \tfrac{1}{2}\right)\hat{\mathbf{z}} \quad (4c) \quad \text{O V}$$

$$\mathbf{B_{45}} = x_{12}\mathbf{a}_1 + \tfrac{1}{4}\mathbf{a}_2 + z_{12}\mathbf{a}_3 = ax_{12}\hat{\mathbf{x}} + \tfrac{1}{4}b\hat{\mathbf{y}} + cz_{12}\hat{\mathbf{z}} \quad (4c) \quad \text{O VI}$$

$$\mathbf{B_{46}} = -\left(x_{12} - \tfrac{1}{2}\right)\mathbf{a}_1 + \tfrac{3}{4}\mathbf{a}_2 + \left(z_{12} + \tfrac{1}{2}\right)\mathbf{a}_3 = -a\left(x_{12} - \tfrac{1}{2}\right)\hat{\mathbf{x}} + \tfrac{3}{4}b\hat{\mathbf{y}} + c\left(z_{12} + \tfrac{1}{2}\right)\hat{\mathbf{z}} \quad (4c) \quad \text{O VI}$$

$$\mathbf{B_{47}} = -x_{12}\mathbf{a}_1 + \tfrac{3}{4}\mathbf{a}_2 - z_{12}\mathbf{a}_3 = -ax_{12}\hat{\mathbf{x}} + \tfrac{3}{4}b\hat{\mathbf{y}} - cz_{12}\hat{\mathbf{z}} \quad (4c) \quad \text{O VI}$$

$$\mathbf{B_{48}} = \left(x_{12} + \tfrac{1}{2}\right)\mathbf{a}_1 + \tfrac{1}{4}\mathbf{a}_2 - \left(z_{12} - \tfrac{1}{2}\right)\mathbf{a}_3 = a\left(x_{12} + \tfrac{1}{2}\right)\hat{\mathbf{x}} + \tfrac{1}{4}b\hat{\mathbf{y}} - c\left(z_{12} - \tfrac{1}{2}\right)\hat{\mathbf{z}} \quad (4c) \quad \text{O VI}$$

References

[1] C. R. Peters and M. E. Milberg, *The refined structure of orthorhombic metaboric acid*, Acta Cryst. **17**, 229–234 (1964), doi:10.1107/S0365110X64000597.

[2] F. C. Kracek, G. W. Morey, and H. E. Merwin, *The system. Water-boron oxide*, Amer. J. Sci. **A35**, 143–171 (1938).

Found in

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