

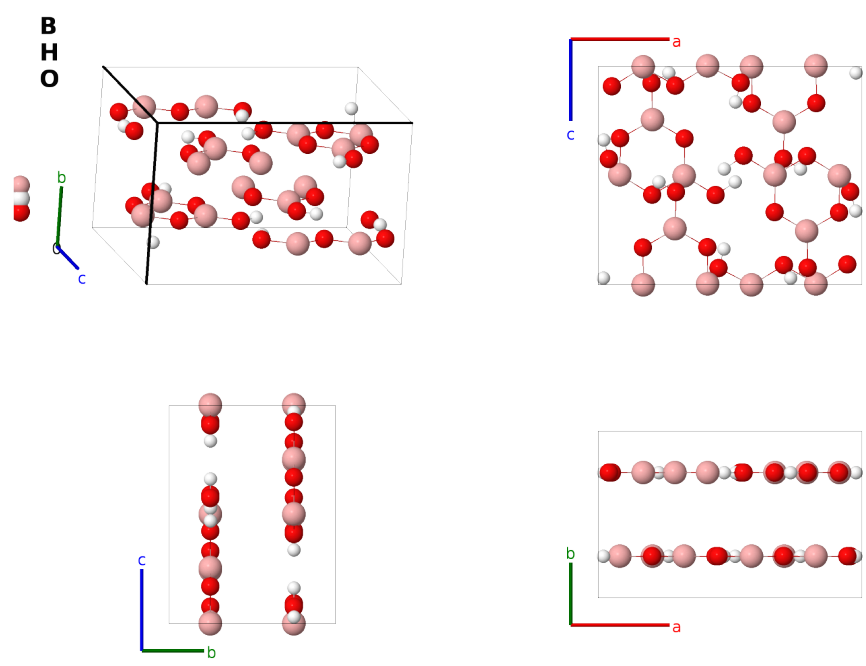
α -HBO₂ (orthorhombic) Structure: ABC2_oP48_62_3c_3c_6c-001

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- D. Hicks, M. J. Mehl, M. Esters, C. Oses, O. Levy, G. L. W. Hart, C. Toher, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 3*, Comput. Mater. Sci. **199**, 110450 (2021), doi: 10.1016/j.commatsci.2021.110450.

<https://aflow.org/prototype-encyclopedia/XYXT>

https://aflow.org/prototype-encyclopedia/ABC2_oP48_62_3c_3c_6c-001



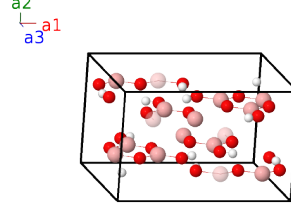
Prototype	BHO ₂
AFLOW prototype label	ABC2_oP48_62_3c_3c_6c-001
ICSD	16545
CCDC	1597109
Pearson symbol	oP48
Space group number	62
Space group symbol	<i>Pnma</i>
AFLOW prototype command	<code>aflow --proto=ABC2_oP48_62_3c_3c_6c-001</code> <code>--params=a,b/a,c/a,x₁,z₁,x₂,z₂,x₃,z₃,x₄,z₄,x₅,z₅,x₆,z₆,x₇,z₇,x₈,z₈,x₉,z₉,x₁₀,z₁₀,x₁₁,z₁₁,x₁₂,z₁₂</code>

- Metaboric acid, HBO₂, is found in three forms (Kracke, 1938):
 - orthorhombic α -HBO₂, also known as HBO₂ I (this structure),

- monoclinic β -HBO₂, also known as HBO₂ II, and
- cubic γ -HBO₂, also known as HBO₂ III.
- The structures are named in order of stability, although all can exist at room temperature.
- (Peters, 1980) give the structure of α -HBO₂ in the $Pbnm$ setting of space group #62. We used FINDSYM to transform this to the standard $Pnma$ setting.

Simple Orthorhombic primitive vectors

$$\begin{aligned} \mathbf{a}_1 &= a \hat{\mathbf{x}} \\ \mathbf{a}_2 &= b \hat{\mathbf{y}} \\ \mathbf{a}_3 &= c \hat{\mathbf{z}} \end{aligned}$$



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
$\mathbf{B}_2$	$= -(x_1 - \frac{1}{2}) \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + (z_1 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-a(x_1 - \frac{1}{2}) \hat{\mathbf{x}} + \frac{3}{4}b \hat{\mathbf{y}} + c(z_1 + \frac{1}{2}) \hat{\mathbf{z}}$	(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
$\mathbf{B}_4$	$= (x_1 + \frac{1}{2}) \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 - (z_1 - \frac{1}{2}) \mathbf{a}_3$	$=$	$a(x_1 + \frac{1}{2}) \hat{\mathbf{x}} + \frac{1}{4}b \hat{\mathbf{y}} - c(z_1 - \frac{1}{2}) \hat{\mathbf{z}}$	(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
$\mathbf{B}_6$	$= -(x_2 - \frac{1}{2}) \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + (z_2 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-a(x_2 - \frac{1}{2}) \hat{\mathbf{x}} + \frac{3}{4}b \hat{\mathbf{y}} + c(z_2 + \frac{1}{2}) \hat{\mathbf{z}}$	(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
$\mathbf{B}_8$	$= (x_2 + \frac{1}{2}) \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 - (z_2 - \frac{1}{2}) \mathbf{a}_3$	$=$	$a(x_2 + \frac{1}{2}) \hat{\mathbf{x}} + \frac{1}{4}b \hat{\mathbf{y}} - c(z_2 - \frac{1}{2}) \hat{\mathbf{z}}$	(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
$\mathbf{B}_{10}$	$= -(x_3 - \frac{1}{2}) \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + (z_3 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-a(x_3 - \frac{1}{2}) \hat{\mathbf{x}} + \frac{3}{4}b \hat{\mathbf{y}} + c(z_3 + \frac{1}{2}) \hat{\mathbf{z}}$	(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
$\mathbf{B}_{12}$	$= (x_3 + \frac{1}{2}) \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 - (z_3 - \frac{1}{2}) \mathbf{a}_3$	$=$	$a(x_3 + \frac{1}{2}) \hat{\mathbf{x}} + \frac{1}{4}b \hat{\mathbf{y}} - c(z_3 - \frac{1}{2}) \hat{\mathbf{z}}$	(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
$\mathbf{B}_{14}$	$= -(x_4 - \frac{1}{2}) \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + (z_4 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-a(x_4 - \frac{1}{2}) \hat{\mathbf{x}} + \frac{3}{4}b \hat{\mathbf{y}} + c(z_4 + \frac{1}{2}) \hat{\mathbf{z}}$	(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
$\mathbf{B}_{16}$	$= (x_4 + \frac{1}{2}) \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 - (z_4 - \frac{1}{2}) \mathbf{a}_3$	$=$	$a(x_4 + \frac{1}{2}) \hat{\mathbf{x}} + \frac{1}{4}b \hat{\mathbf{y}} - c(z_4 - \frac{1}{2}) \hat{\mathbf{z}}$	(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
$\mathbf{B}_{18}$	$= -(x_5 - \frac{1}{2}) \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + (z_5 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-a(x_5 - \frac{1}{2}) \hat{\mathbf{x}} + \frac{3}{4}b \hat{\mathbf{y}} + c(z_5 + \frac{1}{2}) \hat{\mathbf{z}}$	(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
$\mathbf{B}_{20}$	$= (x_5 + \frac{1}{2}) \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 - (z_5 - \frac{1}{2}) \mathbf{a}_3$	$=$	$a(x_5 + \frac{1}{2}) \hat{\mathbf{x}} + \frac{1}{4}b \hat{\mathbf{y}} - c(z_5 - \frac{1}{2}) \hat{\mathbf{z}}$	(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
$\mathbf{B}_{22} =$	$-(x_6 - \frac{1}{2}) \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + (z_6 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-a(x_6 - \frac{1}{2}) \hat{\mathbf{x}} + \frac{3}{4} b \hat{\mathbf{y}} + c(z_6 + \frac{1}{2}) \hat{\mathbf{z}}$	(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
$\mathbf{B}_{24} =$	$(x_6 + \frac{1}{2}) \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 - (z_6 - \frac{1}{2}) \mathbf{a}_3$	$=$	$a(x_6 + \frac{1}{2}) \hat{\mathbf{x}} + \frac{1}{4} b \hat{\mathbf{y}} - c(z_6 - \frac{1}{2}) \hat{\mathbf{z}}$	(4c)	H III
$\mathbf{B}_{25} =$	$x_7 \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_7 \mathbf{a}_3$	$=$	$ax_7 \hat{\mathbf{x}} + \frac{1}{4} b \hat{\mathbf{y}} + cz_7 \hat{\mathbf{z}}$	(4c)	O I
$\mathbf{B}_{26} =$	$-(x_7 - \frac{1}{2}) \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + (z_7 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-a(x_7 - \frac{1}{2}) \hat{\mathbf{x}} + \frac{3}{4} b \hat{\mathbf{y}} + c(z_7 + \frac{1}{2}) \hat{\mathbf{z}}$	(4c)	O I
$\mathbf{B}_{27} =$	$-x_7 \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_7 \mathbf{a}_3$	$=$	$-ax_7 \hat{\mathbf{x}} + \frac{3}{4} b \hat{\mathbf{y}} - cz_7 \hat{\mathbf{z}}$	(4c)	O I
$\mathbf{B}_{28} =$	$(x_7 + \frac{1}{2}) \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 - (z_7 - \frac{1}{2}) \mathbf{a}_3$	$=$	$a(x_7 + \frac{1}{2}) \hat{\mathbf{x}} + \frac{1}{4} b \hat{\mathbf{y}} - c(z_7 - \frac{1}{2}) \hat{\mathbf{z}}$	(4c)	O I
$\mathbf{B}_{29} =$	$x_8 \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_8 \mathbf{a}_3$	$=$	$ax_8 \hat{\mathbf{x}} + \frac{1}{4} b \hat{\mathbf{y}} + cz_8 \hat{\mathbf{z}}$	(4c)	O II
$\mathbf{B}_{30} =$	$-(x_8 - \frac{1}{2}) \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + (z_8 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-a(x_8 - \frac{1}{2}) \hat{\mathbf{x}} + \frac{3}{4} b \hat{\mathbf{y}} + c(z_8 + \frac{1}{2}) \hat{\mathbf{z}}$	(4c)	O II
$\mathbf{B}_{31} =$	$-x_8 \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_8 \mathbf{a}_3$	$=$	$-ax_8 \hat{\mathbf{x}} + \frac{3}{4} b \hat{\mathbf{y}} - cz_8 \hat{\mathbf{z}}$	(4c)	O II
$\mathbf{B}_{32} =$	$(x_8 + \frac{1}{2}) \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 - (z_8 - \frac{1}{2}) \mathbf{a}_3$	$=$	$a(x_8 + \frac{1}{2}) \hat{\mathbf{x}} + \frac{1}{4} b \hat{\mathbf{y}} - c(z_8 - \frac{1}{2}) \hat{\mathbf{z}}$	(4c)	O II
$\mathbf{B}_{33} =$	$x_9 \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_9 \mathbf{a}_3$	$=$	$ax_9 \hat{\mathbf{x}} + \frac{1}{4} b \hat{\mathbf{y}} + cz_9 \hat{\mathbf{z}}$	(4c)	O III
$\mathbf{B}_{34} =$	$-(x_9 - \frac{1}{2}) \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + (z_9 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-a(x_9 - \frac{1}{2}) \hat{\mathbf{x}} + \frac{3}{4} b \hat{\mathbf{y}} + c(z_9 + \frac{1}{2}) \hat{\mathbf{z}}$	(4c)	O III
$\mathbf{B}_{35} =$	$-x_9 \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_9 \mathbf{a}_3$	$=$	$-ax_9 \hat{\mathbf{x}} + \frac{3}{4} b \hat{\mathbf{y}} - cz_9 \hat{\mathbf{z}}$	(4c)	O III
$\mathbf{B}_{36} =$	$(x_9 + \frac{1}{2}) \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 - (z_9 - \frac{1}{2}) \mathbf{a}_3$	$=$	$a(x_9 + \frac{1}{2}) \hat{\mathbf{x}} + \frac{1}{4} b \hat{\mathbf{y}} - c(z_9 - \frac{1}{2}) \hat{\mathbf{z}}$	(4c)	O III
$\mathbf{B}_{37} =$	$x_{10} \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_{10} \mathbf{a}_3$	$=$	$ax_{10} \hat{\mathbf{x}} + \frac{1}{4} b \hat{\mathbf{y}} + cz_{10} \hat{\mathbf{z}}$	(4c)	O IV
$\mathbf{B}_{38} =$	$-(x_{10} - \frac{1}{2}) \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + (z_{10} + \frac{1}{2}) \mathbf{a}_3$	$=$	$-a(x_{10} - \frac{1}{2}) \hat{\mathbf{x}} + \frac{3}{4} b \hat{\mathbf{y}} + c(z_{10} + \frac{1}{2}) \hat{\mathbf{z}}$	(4c)	O IV
$\mathbf{B}_{39} =$	$-x_{10} \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_{10} \mathbf{a}_3$	$=$	$-ax_{10} \hat{\mathbf{x}} + \frac{3}{4} b \hat{\mathbf{y}} - cz_{10} \hat{\mathbf{z}}$	(4c)	O IV
$\mathbf{B}_{40} =$	$(x_{10} + \frac{1}{2}) \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 - (z_{10} - \frac{1}{2}) \mathbf{a}_3$	$=$	$a(x_{10} + \frac{1}{2}) \hat{\mathbf{x}} + \frac{1}{4} b \hat{\mathbf{y}} - c(z_{10} - \frac{1}{2}) \hat{\mathbf{z}}$	(4c)	O IV
$\mathbf{B}_{41} =$	$x_{11} \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_{11} \mathbf{a}_3$	$=$	$ax_{11} \hat{\mathbf{x}} + \frac{1}{4} b \hat{\mathbf{y}} + cz_{11} \hat{\mathbf{z}}$	(4c)	O V
$\mathbf{B}_{42} =$	$-(x_{11} - \frac{1}{2}) \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + (z_{11} + \frac{1}{2}) \mathbf{a}_3$	$=$	$-a(x_{11} - \frac{1}{2}) \hat{\mathbf{x}} + \frac{3}{4} b \hat{\mathbf{y}} + c(z_{11} + \frac{1}{2}) \hat{\mathbf{z}}$	(4c)	O V
$\mathbf{B}_{43} =$	$-x_{11} \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_{11} \mathbf{a}_3$	$=$	$-ax_{11} \hat{\mathbf{x}} + \frac{3}{4} b \hat{\mathbf{y}} - cz_{11} \hat{\mathbf{z}}$	(4c)	O V
$\mathbf{B}_{44} =$	$(x_{11} + \frac{1}{2}) \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 - (z_{11} - \frac{1}{2}) \mathbf{a}_3$	$=$	$a(x_{11} + \frac{1}{2}) \hat{\mathbf{x}} + \frac{1}{4} b \hat{\mathbf{y}} - c(z_{11} - \frac{1}{2}) \hat{\mathbf{z}}$	(4c)	O V
$\mathbf{B}_{45} =$	$x_{12} \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_{12} \mathbf{a}_3$	$=$	$ax_{12} \hat{\mathbf{x}} + \frac{1}{4} b \hat{\mathbf{y}} + cz_{12} \hat{\mathbf{z}}$	(4c)	O VI
$\mathbf{B}_{46} =$	$-(x_{12} - \frac{1}{2}) \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + (z_{12} + \frac{1}{2}) \mathbf{a}_3$	$=$	$-a(x_{12} - \frac{1}{2}) \hat{\mathbf{x}} + \frac{3}{4} b \hat{\mathbf{y}} + c(z_{12} + \frac{1}{2}) \hat{\mathbf{z}}$	(4c)	O VI
$\mathbf{B}_{47} =$	$-x_{12} \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_{12} \mathbf{a}_3$	$=$	$-ax_{12} \hat{\mathbf{x}} + \frac{3}{4} b \hat{\mathbf{y}} - cz_{12} \hat{\mathbf{z}}$	(4c)	O VI
$\mathbf{B}_{48} =$	$(x_{12} + \frac{1}{2}) \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 - (z_{12} - \frac{1}{2}) \mathbf{a}_3$	$=$	$a(x_{12} + \frac{1}{2}) \hat{\mathbf{x}} + \frac{1}{4} b \hat{\mathbf{y}} - c(z_{12} - \frac{1}{2}) \hat{\mathbf{z}}$	(4c)	O VI

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