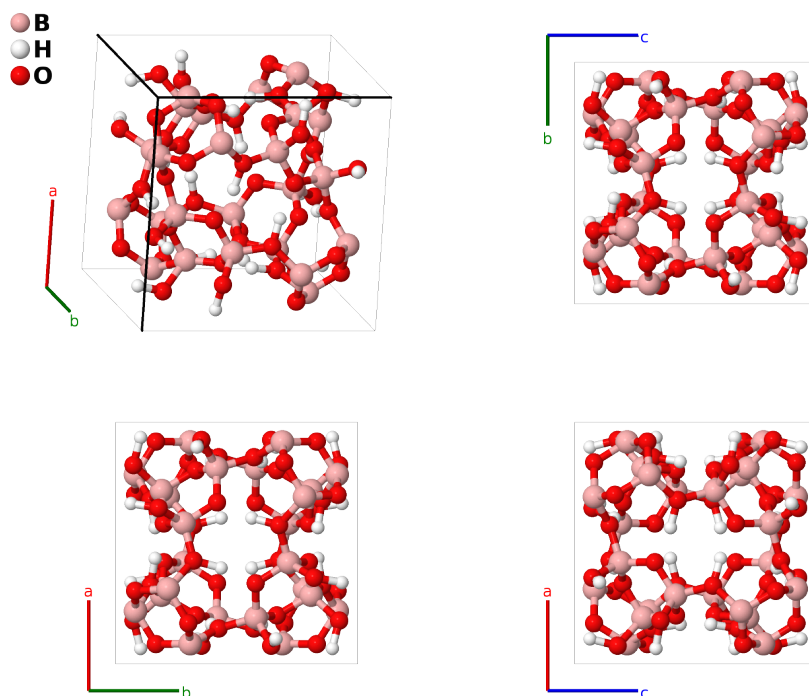


γ -HBO₂ (cubic) Structure: ABC2_cP96_218_i_i_2i-001

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<https://aflow.org/p/W9M1>

https://aflow.org/p/ABC2_cP96_218_i_i_2i-001

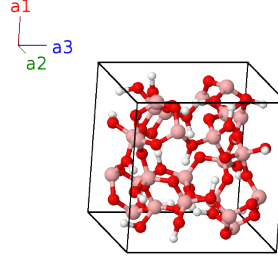


Prototype	BHO ₂
AFLOW prototype label	ABC2_cP96_218_i_i_2i-001
ICSD	34639
Pearson symbol	cP96
Space group number	218
Space group symbol	$P\bar{4}3n$
AFLOW prototype command	<code>aflow --proto=ABC2_cP96_218_i_i_2i-001</code> <code>--params=a, x₁, y₁, z₁, x₂, y₂, z₂, x₃, y₃, z₃, x₄, y₄, z₄</code>

- Metaboric acid, HBO₂, is found in three forms (Kracke, 1938):
 - orthorhombic α -HBO₂, also known as HBO₂ I,
 - monoclinic β -HBO₂, also known as HBO₂ II, and
 - cubic γ -HBO₂, also known as HBO₂ III (this structure).
- The structures are named in order of stability, although all can exist at room temperature.

Simple Cubic primitive vectors

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



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
\mathbf{B}_1	$x_1 \mathbf{a}_1 + y_1 \mathbf{a}_2 + z_1 \mathbf{a}_3$	=	$ax_1 \hat{\mathbf{x}} + ay_1 \hat{\mathbf{y}} + az_1 \hat{\mathbf{z}}$	(24i)	B I
\mathbf{B}_2	$-x_1 \mathbf{a}_1 - y_1 \mathbf{a}_2 + z_1 \mathbf{a}_3$	=	$-ax_1 \hat{\mathbf{x}} - ay_1 \hat{\mathbf{y}} + az_1 \hat{\mathbf{z}}$	(24i)	B I
\mathbf{B}_3	$-x_1 \mathbf{a}_1 + y_1 \mathbf{a}_2 - z_1 \mathbf{a}_3$	=	$-ax_1 \hat{\mathbf{x}} + ay_1 \hat{\mathbf{y}} - az_1 \hat{\mathbf{z}}$	(24i)	B I
\mathbf{B}_4	$x_1 \mathbf{a}_1 - y_1 \mathbf{a}_2 - z_1 \mathbf{a}_3$	=	$ax_1 \hat{\mathbf{x}} - ay_1 \hat{\mathbf{y}} - az_1 \hat{\mathbf{z}}$	(24i)	B I
\mathbf{B}_5	$z_1 \mathbf{a}_1 + x_1 \mathbf{a}_2 + y_1 \mathbf{a}_3$	=	$az_1 \hat{\mathbf{x}} + ax_1 \hat{\mathbf{y}} + ay_1 \hat{\mathbf{z}}$	(24i)	B I
\mathbf{B}_6	$z_1 \mathbf{a}_1 - x_1 \mathbf{a}_2 - y_1 \mathbf{a}_3$	=	$az_1 \hat{\mathbf{x}} - ax_1 \hat{\mathbf{y}} - ay_1 \hat{\mathbf{z}}$	(24i)	B I
\mathbf{B}_7	$-z_1 \mathbf{a}_1 - x_1 \mathbf{a}_2 + y_1 \mathbf{a}_3$	=	$-az_1 \hat{\mathbf{x}} - ax_1 \hat{\mathbf{y}} + ay_1 \hat{\mathbf{z}}$	(24i)	B I
\mathbf{B}_8	$-z_1 \mathbf{a}_1 + x_1 \mathbf{a}_2 - y_1 \mathbf{a}_3$	=	$-az_1 \hat{\mathbf{x}} + ax_1 \hat{\mathbf{y}} - ay_1 \hat{\mathbf{z}}$	(24i)	B I
\mathbf{B}_9	$y_1 \mathbf{a}_1 + z_1 \mathbf{a}_2 + x_1 \mathbf{a}_3$	=	$ay_1 \hat{\mathbf{x}} + az_1 \hat{\mathbf{y}} + ax_1 \hat{\mathbf{z}}$	(24i)	B I
\mathbf{B}_{10}	$-y_1 \mathbf{a}_1 + z_1 \mathbf{a}_2 - x_1 \mathbf{a}_3$	=	$-ay_1 \hat{\mathbf{x}} + az_1 \hat{\mathbf{y}} - ax_1 \hat{\mathbf{z}}$	(24i)	B I
\mathbf{B}_{11}	$y_1 \mathbf{a}_1 - z_1 \mathbf{a}_2 - x_1 \mathbf{a}_3$	=	$ay_1 \hat{\mathbf{x}} - az_1 \hat{\mathbf{y}} - ax_1 \hat{\mathbf{z}}$	(24i)	B I
\mathbf{B}_{12}	$-y_1 \mathbf{a}_1 - z_1 \mathbf{a}_2 + x_1 \mathbf{a}_3$	=	$-ay_1 \hat{\mathbf{x}} - az_1 \hat{\mathbf{y}} + ax_1 \hat{\mathbf{z}}$	(24i)	B I
\mathbf{B}_{13}	$(y_1 + \frac{1}{2}) \mathbf{a}_1 + (x_1 + \frac{1}{2}) \mathbf{a}_2 + (z_1 + \frac{1}{2}) \mathbf{a}_3$	=	$a(y_1 + \frac{1}{2}) \hat{\mathbf{x}} + a(x_1 + \frac{1}{2}) \hat{\mathbf{y}} + a(z_1 + \frac{1}{2}) \hat{\mathbf{z}}$	(24i)	B I
\mathbf{B}_{14}	$-(y_1 - \frac{1}{2}) \mathbf{a}_1 - (x_1 - \frac{1}{2}) \mathbf{a}_2 + (z_1 + \frac{1}{2}) \mathbf{a}_3$	=	$-a(y_1 - \frac{1}{2}) \hat{\mathbf{x}} - a(x_1 - \frac{1}{2}) \hat{\mathbf{y}} + a(z_1 + \frac{1}{2}) \hat{\mathbf{z}}$	(24i)	B I
\mathbf{B}_{15}	$(y_1 + \frac{1}{2}) \mathbf{a}_1 - (x_1 - \frac{1}{2}) \mathbf{a}_2 - (z_1 - \frac{1}{2}) \mathbf{a}_3$	=	$a(y_1 + \frac{1}{2}) \hat{\mathbf{x}} - a(x_1 - \frac{1}{2}) \hat{\mathbf{y}} - a(z_1 - \frac{1}{2}) \hat{\mathbf{z}}$	(24i)	B I
\mathbf{B}_{16}	$-(y_1 - \frac{1}{2}) \mathbf{a}_1 + (x_1 + \frac{1}{2}) \mathbf{a}_2 - (z_1 - \frac{1}{2}) \mathbf{a}_3$	=	$-a(y_1 - \frac{1}{2}) \hat{\mathbf{x}} + a(x_1 + \frac{1}{2}) \hat{\mathbf{y}} - a(z_1 - \frac{1}{2}) \hat{\mathbf{z}}$	(24i)	B I
\mathbf{B}_{17}	$(x_1 + \frac{1}{2}) \mathbf{a}_1 + (z_1 + \frac{1}{2}) \mathbf{a}_2 + (y_1 + \frac{1}{2}) \mathbf{a}_3$	=	$a(x_1 + \frac{1}{2}) \hat{\mathbf{x}} + a(z_1 + \frac{1}{2}) \hat{\mathbf{y}} + a(y_1 + \frac{1}{2}) \hat{\mathbf{z}}$	(24i)	B I
\mathbf{B}_{18}	$-(x_1 - \frac{1}{2}) \mathbf{a}_1 + (z_1 + \frac{1}{2}) \mathbf{a}_2 - (y_1 - \frac{1}{2}) \mathbf{a}_3$	=	$-a(x_1 - \frac{1}{2}) \hat{\mathbf{x}} + a(z_1 + \frac{1}{2}) \hat{\mathbf{y}} - a(y_1 - \frac{1}{2}) \hat{\mathbf{z}}$	(24i)	B I
\mathbf{B}_{19}	$-(x_1 - \frac{1}{2}) \mathbf{a}_1 - (z_1 - \frac{1}{2}) \mathbf{a}_2 + (y_1 + \frac{1}{2}) \mathbf{a}_3$	=	$-a(x_1 - \frac{1}{2}) \hat{\mathbf{x}} - a(z_1 - \frac{1}{2}) \hat{\mathbf{y}} + a(y_1 + \frac{1}{2}) \hat{\mathbf{z}}$	(24i)	B I
\mathbf{B}_{20}	$(x_1 + \frac{1}{2}) \mathbf{a}_1 - (z_1 - \frac{1}{2}) \mathbf{a}_2 - (y_1 - \frac{1}{2}) \mathbf{a}_3$	=	$a(x_1 + \frac{1}{2}) \hat{\mathbf{x}} - a(z_1 - \frac{1}{2}) \hat{\mathbf{y}} - a(y_1 - \frac{1}{2}) \hat{\mathbf{z}}$	(24i)	B I
\mathbf{B}_{21}	$(z_1 + \frac{1}{2}) \mathbf{a}_1 + (y_1 + \frac{1}{2}) \mathbf{a}_2 + (x_1 + \frac{1}{2}) \mathbf{a}_3$	=	$a(z_1 + \frac{1}{2}) \hat{\mathbf{x}} + a(y_1 + \frac{1}{2}) \hat{\mathbf{y}} + a(x_1 + \frac{1}{2}) \hat{\mathbf{z}}$	(24i)	B I

$$\begin{aligned}
\mathbf{B}_{84} &= -y_4 \mathbf{a}_1 - z_4 \mathbf{a}_2 + x_4 \mathbf{a}_3 &= -ay_4 \hat{\mathbf{x}} - az_4 \hat{\mathbf{y}} + ax_4 \hat{\mathbf{z}} & (24i) & \text{O II} \\
\mathbf{B}_{85} &= \begin{pmatrix} y_4 + \frac{1}{2} \\ z_4 + \frac{1}{2} \end{pmatrix} \mathbf{a}_1 + \begin{pmatrix} x_4 + \frac{1}{2} \\ z_4 + \frac{1}{2} \end{pmatrix} \mathbf{a}_2 + \begin{pmatrix} x_4 + \frac{1}{2} \\ z_4 + \frac{1}{2} \end{pmatrix} \mathbf{a}_3 &= a \begin{pmatrix} y_4 + \frac{1}{2} \\ z_4 + \frac{1}{2} \end{pmatrix} \hat{\mathbf{x}} + a \begin{pmatrix} x_4 + \frac{1}{2} \\ z_4 + \frac{1}{2} \end{pmatrix} \hat{\mathbf{y}} + a \begin{pmatrix} x_4 + \frac{1}{2} \\ z_4 + \frac{1}{2} \end{pmatrix} \hat{\mathbf{z}} & (24i) & \text{O II} \\
\mathbf{B}_{86} &= -\begin{pmatrix} y_4 - \frac{1}{2} \\ z_4 + \frac{1}{2} \end{pmatrix} \mathbf{a}_1 - \begin{pmatrix} x_4 - \frac{1}{2} \\ z_4 + \frac{1}{2} \end{pmatrix} \mathbf{a}_2 + \begin{pmatrix} x_4 - \frac{1}{2} \\ z_4 + \frac{1}{2} \end{pmatrix} \mathbf{a}_3 &= -a \begin{pmatrix} y_4 - \frac{1}{2} \\ z_4 + \frac{1}{2} \end{pmatrix} \hat{\mathbf{x}} - a \begin{pmatrix} x_4 - \frac{1}{2} \\ z_4 + \frac{1}{2} \end{pmatrix} \hat{\mathbf{y}} + a \begin{pmatrix} x_4 - \frac{1}{2} \\ z_4 + \frac{1}{2} \end{pmatrix} \hat{\mathbf{z}} & (24i) & \text{O II} \\
\mathbf{B}_{87} &= \begin{pmatrix} y_4 + \frac{1}{2} \\ z_4 - \frac{1}{2} \end{pmatrix} \mathbf{a}_1 - \begin{pmatrix} x_4 - \frac{1}{2} \\ z_4 - \frac{1}{2} \end{pmatrix} \mathbf{a}_2 - \begin{pmatrix} x_4 - \frac{1}{2} \\ z_4 - \frac{1}{2} \end{pmatrix} \mathbf{a}_3 &= a \begin{pmatrix} y_4 + \frac{1}{2} \\ z_4 - \frac{1}{2} \end{pmatrix} \hat{\mathbf{x}} - a \begin{pmatrix} x_4 - \frac{1}{2} \\ z_4 - \frac{1}{2} \end{pmatrix} \hat{\mathbf{y}} - a \begin{pmatrix} x_4 - \frac{1}{2} \\ z_4 - \frac{1}{2} \end{pmatrix} \hat{\mathbf{z}} & (24i) & \text{O II} \\
\mathbf{B}_{88} &= -\begin{pmatrix} y_4 - \frac{1}{2} \\ z_4 - \frac{1}{2} \end{pmatrix} \mathbf{a}_1 + \begin{pmatrix} x_4 + \frac{1}{2} \\ z_4 - \frac{1}{2} \end{pmatrix} \mathbf{a}_2 - \begin{pmatrix} x_4 + \frac{1}{2} \\ z_4 - \frac{1}{2} \end{pmatrix} \mathbf{a}_3 &= -a \begin{pmatrix} y_4 - \frac{1}{2} \\ z_4 - \frac{1}{2} \end{pmatrix} \hat{\mathbf{x}} + a \begin{pmatrix} x_4 + \frac{1}{2} \\ z_4 - \frac{1}{2} \end{pmatrix} \hat{\mathbf{y}} - a \begin{pmatrix} x_4 + \frac{1}{2} \\ z_4 - \frac{1}{2} \end{pmatrix} \hat{\mathbf{z}} & (24i) & \text{O II} \\
\mathbf{B}_{89} &= \begin{pmatrix} x_4 + \frac{1}{2} \\ y_4 + \frac{1}{2} \end{pmatrix} \mathbf{a}_1 + \begin{pmatrix} z_4 + \frac{1}{2} \\ y_4 + \frac{1}{2} \end{pmatrix} \mathbf{a}_2 + \begin{pmatrix} x_4 + \frac{1}{2} \\ y_4 + \frac{1}{2} \end{pmatrix} \mathbf{a}_3 &= a \begin{pmatrix} x_4 + \frac{1}{2} \\ y_4 + \frac{1}{2} \end{pmatrix} \hat{\mathbf{x}} + a \begin{pmatrix} z_4 + \frac{1}{2} \\ y_4 + \frac{1}{2} \end{pmatrix} \hat{\mathbf{y}} + a \begin{pmatrix} x_4 + \frac{1}{2} \\ y_4 + \frac{1}{2} \end{pmatrix} \hat{\mathbf{z}} & (24i) & \text{O II} \\
\mathbf{B}_{90} &= -\begin{pmatrix} x_4 - \frac{1}{2} \\ y_4 - \frac{1}{2} \end{pmatrix} \mathbf{a}_1 + \begin{pmatrix} z_4 + \frac{1}{2} \\ y_4 - \frac{1}{2} \end{pmatrix} \mathbf{a}_2 - \begin{pmatrix} x_4 - \frac{1}{2} \\ y_4 - \frac{1}{2} \end{pmatrix} \mathbf{a}_3 &= -a \begin{pmatrix} x_4 - \frac{1}{2} \\ y_4 - \frac{1}{2} \end{pmatrix} \hat{\mathbf{x}} + a \begin{pmatrix} z_4 + \frac{1}{2} \\ y_4 - \frac{1}{2} \end{pmatrix} \hat{\mathbf{y}} - a \begin{pmatrix} x_4 - \frac{1}{2} \\ y_4 - \frac{1}{2} \end{pmatrix} \hat{\mathbf{z}} & (24i) & \text{O II} \\
\mathbf{B}_{91} &= -\begin{pmatrix} x_4 - \frac{1}{2} \\ y_4 + \frac{1}{2} \end{pmatrix} \mathbf{a}_1 - \begin{pmatrix} z_4 - \frac{1}{2} \\ y_4 + \frac{1}{2} \end{pmatrix} \mathbf{a}_2 + \begin{pmatrix} x_4 - \frac{1}{2} \\ y_4 + \frac{1}{2} \end{pmatrix} \mathbf{a}_3 &= -a \begin{pmatrix} x_4 - \frac{1}{2} \\ y_4 + \frac{1}{2} \end{pmatrix} \hat{\mathbf{x}} - a \begin{pmatrix} z_4 - \frac{1}{2} \\ y_4 + \frac{1}{2} \end{pmatrix} \hat{\mathbf{y}} + a \begin{pmatrix} x_4 - \frac{1}{2} \\ y_4 + \frac{1}{2} \end{pmatrix} \hat{\mathbf{z}} & (24i) & \text{O II} \\
\mathbf{B}_{92} &= \begin{pmatrix} x_4 + \frac{1}{2} \\ y_4 - \frac{1}{2} \end{pmatrix} \mathbf{a}_1 - \begin{pmatrix} z_4 - \frac{1}{2} \\ y_4 - \frac{1}{2} \end{pmatrix} \mathbf{a}_2 - \begin{pmatrix} x_4 + \frac{1}{2} \\ y_4 - \frac{1}{2} \end{pmatrix} \mathbf{a}_3 &= a \begin{pmatrix} x_4 + \frac{1}{2} \\ y_4 - \frac{1}{2} \end{pmatrix} \hat{\mathbf{x}} - a \begin{pmatrix} z_4 - \frac{1}{2} \\ y_4 - \frac{1}{2} \end{pmatrix} \hat{\mathbf{y}} - a \begin{pmatrix} x_4 + \frac{1}{2} \\ y_4 - \frac{1}{2} \end{pmatrix} \hat{\mathbf{z}} & (24i) & \text{O II} \\
\mathbf{B}_{93} &= \begin{pmatrix} z_4 + \frac{1}{2} \\ x_4 + \frac{1}{2} \end{pmatrix} \mathbf{a}_1 + \begin{pmatrix} y_4 + \frac{1}{2} \\ x_4 + \frac{1}{2} \end{pmatrix} \mathbf{a}_2 + \begin{pmatrix} z_4 + \frac{1}{2} \\ x_4 + \frac{1}{2} \end{pmatrix} \mathbf{a}_3 &= a \begin{pmatrix} z_4 + \frac{1}{2} \\ x_4 + \frac{1}{2} \end{pmatrix} \hat{\mathbf{x}} + a \begin{pmatrix} y_4 + \frac{1}{2} \\ x_4 + \frac{1}{2} \end{pmatrix} \hat{\mathbf{y}} + a \begin{pmatrix} z_4 + \frac{1}{2} \\ x_4 + \frac{1}{2} \end{pmatrix} \hat{\mathbf{z}} & (24i) & \text{O II} \\
\mathbf{B}_{94} &= \begin{pmatrix} z_4 + \frac{1}{2} \\ x_4 - \frac{1}{2} \end{pmatrix} \mathbf{a}_1 - \begin{pmatrix} y_4 - \frac{1}{2} \\ x_4 - \frac{1}{2} \end{pmatrix} \mathbf{a}_2 - \begin{pmatrix} z_4 + \frac{1}{2} \\ x_4 - \frac{1}{2} \end{pmatrix} \mathbf{a}_3 &= a \begin{pmatrix} z_4 + \frac{1}{2} \\ x_4 - \frac{1}{2} \end{pmatrix} \hat{\mathbf{x}} - a \begin{pmatrix} y_4 - \frac{1}{2} \\ x_4 - \frac{1}{2} \end{pmatrix} \hat{\mathbf{y}} - a \begin{pmatrix} z_4 + \frac{1}{2} \\ x_4 - \frac{1}{2} \end{pmatrix} \hat{\mathbf{z}} & (24i) & \text{O II} \\
\mathbf{B}_{95} &= -\begin{pmatrix} z_4 - \frac{1}{2} \\ x_4 - \frac{1}{2} \end{pmatrix} \mathbf{a}_1 + \begin{pmatrix} y_4 + \frac{1}{2} \\ x_4 - \frac{1}{2} \end{pmatrix} \mathbf{a}_2 - \begin{pmatrix} z_4 - \frac{1}{2} \\ x_4 - \frac{1}{2} \end{pmatrix} \mathbf{a}_3 &= -a \begin{pmatrix} z_4 - \frac{1}{2} \\ x_4 - \frac{1}{2} \end{pmatrix} \hat{\mathbf{x}} + a \begin{pmatrix} y_4 + \frac{1}{2} \\ x_4 - \frac{1}{2} \end{pmatrix} \hat{\mathbf{y}} - a \begin{pmatrix} z_4 - \frac{1}{2} \\ x_4 - \frac{1}{2} \end{pmatrix} \hat{\mathbf{z}} & (24i) & \text{O II} \\
\mathbf{B}_{96} &= -\begin{pmatrix} z_4 - \frac{1}{2} \\ x_4 + \frac{1}{2} \end{pmatrix} \mathbf{a}_1 - \begin{pmatrix} y_4 - \frac{1}{2} \\ x_4 + \frac{1}{2} \end{pmatrix} \mathbf{a}_2 + \begin{pmatrix} z_4 - \frac{1}{2} \\ x_4 + \frac{1}{2} \end{pmatrix} \mathbf{a}_3 &= -a \begin{pmatrix} z_4 - \frac{1}{2} \\ x_4 + \frac{1}{2} \end{pmatrix} \hat{\mathbf{x}} - a \begin{pmatrix} y_4 - \frac{1}{2} \\ x_4 + \frac{1}{2} \end{pmatrix} \hat{\mathbf{y}} + a \begin{pmatrix} z_4 - \frac{1}{2} \\ x_4 + \frac{1}{2} \end{pmatrix} \hat{\mathbf{z}} & (24i) & \text{O II}
\end{aligned}$$

References

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