

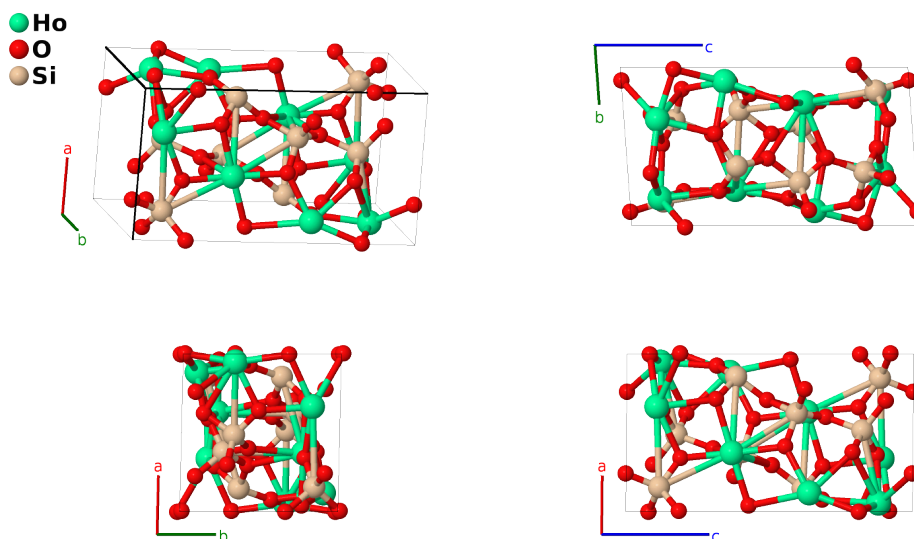
α -Ho₂Si₂O₇ Structure: A2B7C2_aP44_2_4i_14i_4i-001

This structure originally had the label A2B7C2_aP44_2_4i_14i_4i. Calls to that address will be redirected here.

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<https://aflow.org/p/VN5Q>

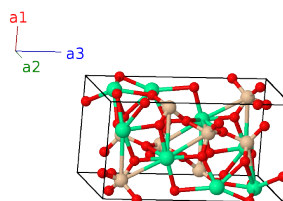
https://aflow.org/p/A2B7C2_aP44_2_4i_14i_4i-001



Prototype	Ho ₂ O ₇ Si ₂
AFLOW prototype label	A2B7C2_aP44_2_4i_14i_4i-001
ICSD	23619
Pearson symbol	aP44
Space group number	2
Space group symbol	$P\bar{1}$
AFLOW prototype command	aflow --proto=A2B7C2_aP44_2_4i_14i_4i-001 --params=a, b/a, c/a, α , β , γ , $x_1, y_1, z_1, x_2, y_2, z_2, x_3, y_3, z_3, x_4, y_4, z_4, x_5, y_5, z_5, x_6, y_6, z_6, x_7, y_7, z_7, x_8, y_8, z_8, x_9, y_9, z_9, x_{10}, y_{10}, z_{10}, x_{11}, y_{11}, z_{11}, x_{12}, y_{12}, z_{12}, x_{13}, y_{13}, z_{13}, x_{14}, y_{14}, z_{14}, x_{15}, y_{15}, z_{15}, x_{16}, y_{16}, z_{16}, x_{17}, y_{17}, z_{17}, x_{18}, y_{18}, z_{18}, x_{19}, y_{19}, z_{19}, x_{20}, y_{20}, z_{20}, x_{21}, y_{21}, z_{21}, x_{22}, y_{22}, z_{22}$

Triclinic primitive vectors

$$\begin{aligned} \mathbf{a}_1 &= a \hat{\mathbf{x}} \\ \mathbf{a}_2 &= b \cos \gamma \hat{\mathbf{x}} + b \sin \gamma \hat{\mathbf{y}} \\ \mathbf{a}_3 &= c_x \hat{\mathbf{x}} + c_y \hat{\mathbf{y}} + c_z \hat{\mathbf{z}} \\ c_x &= c \cos \beta \\ c_y &= c(\cos \alpha - \cos \beta \cos \gamma) / \sin \gamma \\ c_z &= \sqrt{c^2 - c_x^2 - c_y^2} \end{aligned}$$



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
\mathbf{B}_1	$= x_1 \mathbf{a}_1 + y_1 \mathbf{a}_2 + z_1 \mathbf{a}_3$	$=$	$(ax_1 + by_1 \cos \gamma + c_x z_1) \hat{\mathbf{x}} + (by_1 \sin \gamma + c_y z_1) \hat{\mathbf{y}} + c_z z_1 \hat{\mathbf{z}}$	(2i)	Ho I
\mathbf{B}_2	$= -x_1 \mathbf{a}_1 - y_1 \mathbf{a}_2 - z_1 \mathbf{a}_3$	$=$	$-(ax_1 + by_1 \cos \gamma + c_x z_1) \hat{\mathbf{x}} - (by_1 \sin \gamma + c_y z_1) \hat{\mathbf{y}} - c_z z_1 \hat{\mathbf{z}}$	(2i)	Ho I
\mathbf{B}_3	$= x_2 \mathbf{a}_1 + y_2 \mathbf{a}_2 + z_2 \mathbf{a}_3$	$=$	$(ax_2 + by_2 \cos \gamma + c_x z_2) \hat{\mathbf{x}} + (by_2 \sin \gamma + c_y z_2) \hat{\mathbf{y}} + c_z z_2 \hat{\mathbf{z}}$	(2i)	Ho II
\mathbf{B}_4	$= -x_2 \mathbf{a}_1 - y_2 \mathbf{a}_2 - z_2 \mathbf{a}_3$	$=$	$-(ax_2 + by_2 \cos \gamma + c_x z_2) \hat{\mathbf{x}} - (by_2 \sin \gamma + c_y z_2) \hat{\mathbf{y}} - c_z z_2 \hat{\mathbf{z}}$	(2i)	Ho II
\mathbf{B}_5	$= x_3 \mathbf{a}_1 + y_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$(ax_3 + by_3 \cos \gamma + c_x z_3) \hat{\mathbf{x}} + (by_3 \sin \gamma + c_y z_3) \hat{\mathbf{y}} + c_z z_3 \hat{\mathbf{z}}$	(2i)	Ho III
\mathbf{B}_6	$= -x_3 \mathbf{a}_1 - y_3 \mathbf{a}_2 - z_3 \mathbf{a}_3$	$=$	$-(ax_3 + by_3 \cos \gamma + c_x z_3) \hat{\mathbf{x}} - (by_3 \sin \gamma + c_y z_3) \hat{\mathbf{y}} - c_z z_3 \hat{\mathbf{z}}$	(2i)	Ho III
\mathbf{B}_7	$= x_4 \mathbf{a}_1 + y_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$(ax_4 + by_4 \cos \gamma + c_x z_4) \hat{\mathbf{x}} + (by_4 \sin \gamma + c_y z_4) \hat{\mathbf{y}} + c_z z_4 \hat{\mathbf{z}}$	(2i)	Ho IV
\mathbf{B}_8	$= -x_4 \mathbf{a}_1 - y_4 \mathbf{a}_2 - z_4 \mathbf{a}_3$	$=$	$-(ax_4 + by_4 \cos \gamma + c_x z_4) \hat{\mathbf{x}} - (by_4 \sin \gamma + c_y z_4) \hat{\mathbf{y}} - c_z z_4 \hat{\mathbf{z}}$	(2i)	Ho IV
\mathbf{B}_9	$= x_5 \mathbf{a}_1 + y_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$(ax_5 + by_5 \cos \gamma + c_x z_5) \hat{\mathbf{x}} + (by_5 \sin \gamma + c_y z_5) \hat{\mathbf{y}} + c_z z_5 \hat{\mathbf{z}}$	(2i)	O I
\mathbf{B}_{10}	$= -x_5 \mathbf{a}_1 - y_5 \mathbf{a}_2 - z_5 \mathbf{a}_3$	$=$	$-(ax_5 + by_5 \cos \gamma + c_x z_5) \hat{\mathbf{x}} - (by_5 \sin \gamma + c_y z_5) \hat{\mathbf{y}} - c_z z_5 \hat{\mathbf{z}}$	(2i)	O I
\mathbf{B}_{11}	$= x_6 \mathbf{a}_1 + y_6 \mathbf{a}_2 + z_6 \mathbf{a}_3$	$=$	$(ax_6 + by_6 \cos \gamma + c_x z_6) \hat{\mathbf{x}} + (by_6 \sin \gamma + c_y z_6) \hat{\mathbf{y}} + c_z z_6 \hat{\mathbf{z}}$	(2i)	O II
\mathbf{B}_{12}	$= -x_6 \mathbf{a}_1 - y_6 \mathbf{a}_2 - z_6 \mathbf{a}_3$	$=$	$-(ax_6 + by_6 \cos \gamma + c_x z_6) \hat{\mathbf{x}} - (by_6 \sin \gamma + c_y z_6) \hat{\mathbf{y}} - c_z z_6 \hat{\mathbf{z}}$	(2i)	O II
\mathbf{B}_{13}	$= x_7 \mathbf{a}_1 + y_7 \mathbf{a}_2 + z_7 \mathbf{a}_3$	$=$	$(ax_7 + by_7 \cos \gamma + c_x z_7) \hat{\mathbf{x}} + (by_7 \sin \gamma + c_y z_7) \hat{\mathbf{y}} + c_z z_7 \hat{\mathbf{z}}$	(2i)	O III
\mathbf{B}_{14}	$= -x_7 \mathbf{a}_1 - y_7 \mathbf{a}_2 - z_7 \mathbf{a}_3$	$=$	$-(ax_7 + by_7 \cos \gamma + c_x z_7) \hat{\mathbf{x}} - (by_7 \sin \gamma + c_y z_7) \hat{\mathbf{y}} - c_z z_7 \hat{\mathbf{z}}$	(2i)	O III
\mathbf{B}_{15}	$= x_8 \mathbf{a}_1 + y_8 \mathbf{a}_2 + z_8 \mathbf{a}_3$	$=$	$(ax_8 + by_8 \cos \gamma + c_x z_8) \hat{\mathbf{x}} + (by_8 \sin \gamma + c_y z_8) \hat{\mathbf{y}} + c_z z_8 \hat{\mathbf{z}}$	(2i)	O IV
\mathbf{B}_{16}	$= -x_8 \mathbf{a}_1 - y_8 \mathbf{a}_2 - z_8 \mathbf{a}_3$	$=$	$-(ax_8 + by_8 \cos \gamma + c_x z_8) \hat{\mathbf{x}} - (by_8 \sin \gamma + c_y z_8) \hat{\mathbf{y}} - c_z z_8 \hat{\mathbf{z}}$	(2i)	O IV
\mathbf{B}_{17}	$= x_9 \mathbf{a}_1 + y_9 \mathbf{a}_2 + z_9 \mathbf{a}_3$	$=$	$(ax_9 + by_9 \cos \gamma + c_x z_9) \hat{\mathbf{x}} + (by_9 \sin \gamma + c_y z_9) \hat{\mathbf{y}} + c_z z_9 \hat{\mathbf{z}}$	(2i)	O V
\mathbf{B}_{18}	$= -x_9 \mathbf{a}_1 - y_9 \mathbf{a}_2 - z_9 \mathbf{a}_3$	$=$	$-(ax_9 + by_9 \cos \gamma + c_x z_9) \hat{\mathbf{x}} - (by_9 \sin \gamma + c_y z_9) \hat{\mathbf{y}} - c_z z_9 \hat{\mathbf{z}}$	(2i)	O V
\mathbf{B}_{19}	$= x_{10} \mathbf{a}_1 + y_{10} \mathbf{a}_2 + z_{10} \mathbf{a}_3$	$=$	$(ax_{10} + by_{10} \cos \gamma + c_x z_{10}) \hat{\mathbf{x}} + (by_{10} \sin \gamma + c_y z_{10}) \hat{\mathbf{y}} + c_z z_{10} \hat{\mathbf{z}}$	(2i)	O VI
\mathbf{B}_{20}	$= -x_{10} \mathbf{a}_1 - y_{10} \mathbf{a}_2 - z_{10} \mathbf{a}_3$	$=$	$-(ax_{10} + by_{10} \cos \gamma + c_x z_{10}) \hat{\mathbf{x}} - (by_{10} \sin \gamma + c_y z_{10}) \hat{\mathbf{y}} - c_z z_{10} \hat{\mathbf{z}}$	(2i)	O VI
\mathbf{B}_{21}	$= x_{11} \mathbf{a}_1 + y_{11} \mathbf{a}_2 + z_{11} \mathbf{a}_3$	$=$	$(ax_{11} + by_{11} \cos \gamma + c_x z_{11}) \hat{\mathbf{x}} + (by_{11} \sin \gamma + c_y z_{11}) \hat{\mathbf{y}} + c_z z_{11} \hat{\mathbf{z}}$	(2i)	O VII
\mathbf{B}_{22}	$= -x_{11} \mathbf{a}_1 - y_{11} \mathbf{a}_2 - z_{11} \mathbf{a}_3$	$=$	$-(ax_{11} + by_{11} \cos \gamma + c_x z_{11}) \hat{\mathbf{x}} - (by_{11} \sin \gamma + c_y z_{11}) \hat{\mathbf{y}} - c_z z_{11} \hat{\mathbf{z}}$	(2i)	O VII

\mathbf{B}_{23}	$=$	$x_{12} \mathbf{a}_1 + y_{12} \mathbf{a}_2 + z_{12} \mathbf{a}_3$	$=$	$(ax_{12} + by_{12} \cos \gamma + c_x z_{12}) \hat{\mathbf{x}} +$ $(by_{12} \sin \gamma + c_y z_{12}) \hat{\mathbf{y}} + c_z z_{12} \hat{\mathbf{z}}$	(2i)	O VIII
\mathbf{B}_{24}	$=$	$-x_{12} \mathbf{a}_1 - y_{12} \mathbf{a}_2 - z_{12} \mathbf{a}_3$	$=$	$-(ax_{12} + by_{12} \cos \gamma + c_x z_{12}) \hat{\mathbf{x}} -$ $(by_{12} \sin \gamma + c_y z_{12}) \hat{\mathbf{y}} - c_z z_{12} \hat{\mathbf{z}}$	(2i)	O VIII
\mathbf{B}_{25}	$=$	$x_{13} \mathbf{a}_1 + y_{13} \mathbf{a}_2 + z_{13} \mathbf{a}_3$	$=$	$(ax_{13} + by_{13} \cos \gamma + c_x z_{13}) \hat{\mathbf{x}} +$ $(by_{13} \sin \gamma + c_y z_{13}) \hat{\mathbf{y}} + c_z z_{13} \hat{\mathbf{z}}$	(2i)	O IX
\mathbf{B}_{26}	$=$	$-x_{13} \mathbf{a}_1 - y_{13} \mathbf{a}_2 - z_{13} \mathbf{a}_3$	$=$	$-(ax_{13} + by_{13} \cos \gamma + c_x z_{13}) \hat{\mathbf{x}} -$ $(by_{13} \sin \gamma + c_y z_{13}) \hat{\mathbf{y}} - c_z z_{13} \hat{\mathbf{z}}$	(2i)	O IX
\mathbf{B}_{27}	$=$	$x_{14} \mathbf{a}_1 + y_{14} \mathbf{a}_2 + z_{14} \mathbf{a}_3$	$=$	$(ax_{14} + by_{14} \cos \gamma + c_x z_{14}) \hat{\mathbf{x}} +$ $(by_{14} \sin \gamma + c_y z_{14}) \hat{\mathbf{y}} + c_z z_{14} \hat{\mathbf{z}}$	(2i)	O X
\mathbf{B}_{28}	$=$	$-x_{14} \mathbf{a}_1 - y_{14} \mathbf{a}_2 - z_{14} \mathbf{a}_3$	$=$	$-(ax_{14} + by_{14} \cos \gamma + c_x z_{14}) \hat{\mathbf{x}} -$ $(by_{14} \sin \gamma + c_y z_{14}) \hat{\mathbf{y}} - c_z z_{14} \hat{\mathbf{z}}$	(2i)	O X
\mathbf{B}_{29}	$=$	$x_{15} \mathbf{a}_1 + y_{15} \mathbf{a}_2 + z_{15} \mathbf{a}_3$	$=$	$(ax_{15} + by_{15} \cos \gamma + c_x z_{15}) \hat{\mathbf{x}} +$ $(by_{15} \sin \gamma + c_y z_{15}) \hat{\mathbf{y}} + c_z z_{15} \hat{\mathbf{z}}$	(2i)	O XI
\mathbf{B}_{30}	$=$	$-x_{15} \mathbf{a}_1 - y_{15} \mathbf{a}_2 - z_{15} \mathbf{a}_3$	$=$	$-(ax_{15} + by_{15} \cos \gamma + c_x z_{15}) \hat{\mathbf{x}} -$ $(by_{15} \sin \gamma + c_y z_{15}) \hat{\mathbf{y}} - c_z z_{15} \hat{\mathbf{z}}$	(2i)	O XI
\mathbf{B}_{31}	$=$	$x_{16} \mathbf{a}_1 + y_{16} \mathbf{a}_2 + z_{16} \mathbf{a}_3$	$=$	$(ax_{16} + by_{16} \cos \gamma + c_x z_{16}) \hat{\mathbf{x}} +$ $(by_{16} \sin \gamma + c_y z_{16}) \hat{\mathbf{y}} + c_z z_{16} \hat{\mathbf{z}}$	(2i)	O XII
\mathbf{B}_{32}	$=$	$-x_{16} \mathbf{a}_1 - y_{16} \mathbf{a}_2 - z_{16} \mathbf{a}_3$	$=$	$-(ax_{16} + by_{16} \cos \gamma + c_x z_{16}) \hat{\mathbf{x}} -$ $(by_{16} \sin \gamma + c_y z_{16}) \hat{\mathbf{y}} - c_z z_{16} \hat{\mathbf{z}}$	(2i)	O XII
\mathbf{B}_{33}	$=$	$x_{17} \mathbf{a}_1 + y_{17} \mathbf{a}_2 + z_{17} \mathbf{a}_3$	$=$	$(ax_{17} + by_{17} \cos \gamma + c_x z_{17}) \hat{\mathbf{x}} +$ $(by_{17} \sin \gamma + c_y z_{17}) \hat{\mathbf{y}} + c_z z_{17} \hat{\mathbf{z}}$	(2i)	O XIII
\mathbf{B}_{34}	$=$	$-x_{17} \mathbf{a}_1 - y_{17} \mathbf{a}_2 - z_{17} \mathbf{a}_3$	$=$	$-(ax_{17} + by_{17} \cos \gamma + c_x z_{17}) \hat{\mathbf{x}} -$ $(by_{17} \sin \gamma + c_y z_{17}) \hat{\mathbf{y}} - c_z z_{17} \hat{\mathbf{z}}$	(2i)	O XIII
\mathbf{B}_{35}	$=$	$x_{18} \mathbf{a}_1 + y_{18} \mathbf{a}_2 + z_{18} \mathbf{a}_3$	$=$	$(ax_{18} + by_{18} \cos \gamma + c_x z_{18}) \hat{\mathbf{x}} +$ $(by_{18} \sin \gamma + c_y z_{18}) \hat{\mathbf{y}} + c_z z_{18} \hat{\mathbf{z}}$	(2i)	O XIV
\mathbf{B}_{36}	$=$	$-x_{18} \mathbf{a}_1 - y_{18} \mathbf{a}_2 - z_{18} \mathbf{a}_3$	$=$	$-(ax_{18} + by_{18} \cos \gamma + c_x z_{18}) \hat{\mathbf{x}} -$ $(by_{18} \sin \gamma + c_y z_{18}) \hat{\mathbf{y}} - c_z z_{18} \hat{\mathbf{z}}$	(2i)	O XIV
\mathbf{B}_{37}	$=$	$x_{19} \mathbf{a}_1 + y_{19} \mathbf{a}_2 + z_{19} \mathbf{a}_3$	$=$	$(ax_{19} + by_{19} \cos \gamma + c_x z_{19}) \hat{\mathbf{x}} +$ $(by_{19} \sin \gamma + c_y z_{19}) \hat{\mathbf{y}} + c_z z_{19} \hat{\mathbf{z}}$	(2i)	Si I
\mathbf{B}_{38}	$=$	$-x_{19} \mathbf{a}_1 - y_{19} \mathbf{a}_2 - z_{19} \mathbf{a}_3$	$=$	$-(ax_{19} + by_{19} \cos \gamma + c_x z_{19}) \hat{\mathbf{x}} -$ $(by_{19} \sin \gamma + c_y z_{19}) \hat{\mathbf{y}} - c_z z_{19} \hat{\mathbf{z}}$	(2i)	Si I
\mathbf{B}_{39}	$=$	$x_{20} \mathbf{a}_1 + y_{20} \mathbf{a}_2 + z_{20} \mathbf{a}_3$	$=$	$(ax_{20} + by_{20} \cos \gamma + c_x z_{20}) \hat{\mathbf{x}} +$ $(by_{20} \sin \gamma + c_y z_{20}) \hat{\mathbf{y}} + c_z z_{20} \hat{\mathbf{z}}$	(2i)	Si II
\mathbf{B}_{40}	$=$	$-x_{20} \mathbf{a}_1 - y_{20} \mathbf{a}_2 - z_{20} \mathbf{a}_3$	$=$	$-(ax_{20} + by_{20} \cos \gamma + c_x z_{20}) \hat{\mathbf{x}} -$ $(by_{20} \sin \gamma + c_y z_{20}) \hat{\mathbf{y}} - c_z z_{20} \hat{\mathbf{z}}$	(2i)	Si II
\mathbf{B}_{41}	$=$	$x_{21} \mathbf{a}_1 + y_{21} \mathbf{a}_2 + z_{21} \mathbf{a}_3$	$=$	$(ax_{21} + by_{21} \cos \gamma + c_x z_{21}) \hat{\mathbf{x}} +$ $(by_{21} \sin \gamma + c_y z_{21}) \hat{\mathbf{y}} + c_z z_{21} \hat{\mathbf{z}}$	(2i)	Si III
\mathbf{B}_{42}	$=$	$-x_{21} \mathbf{a}_1 - y_{21} \mathbf{a}_2 - z_{21} \mathbf{a}_3$	$=$	$-(ax_{21} + by_{21} \cos \gamma + c_x z_{21}) \hat{\mathbf{x}} -$ $(by_{21} \sin \gamma + c_y z_{21}) \hat{\mathbf{y}} - c_z z_{21} \hat{\mathbf{z}}$	(2i)	Si III
\mathbf{B}_{43}	$=$	$x_{22} \mathbf{a}_1 + y_{22} \mathbf{a}_2 + z_{22} \mathbf{a}_3$	$=$	$(ax_{22} + by_{22} \cos \gamma + c_x z_{22}) \hat{\mathbf{x}} +$ $(by_{22} \sin \gamma + c_y z_{22}) \hat{\mathbf{y}} + c_z z_{22} \hat{\mathbf{z}}$	(2i)	Si IV
\mathbf{B}_{44}	$=$	$-x_{22} \mathbf{a}_1 - y_{22} \mathbf{a}_2 - z_{22} \mathbf{a}_3$	$=$	$-(ax_{22} + by_{22} \cos \gamma + c_x z_{22}) \hat{\mathbf{x}} -$ $(by_{22} \sin \gamma + c_y z_{22}) \hat{\mathbf{y}} - c_z z_{22} \hat{\mathbf{z}}$	(2i)	Si IV

References

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Found in

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