

α -Ho₂Si₂O₇ Structure:

A2B7C2_aP44_2_4i_14i_4i-001

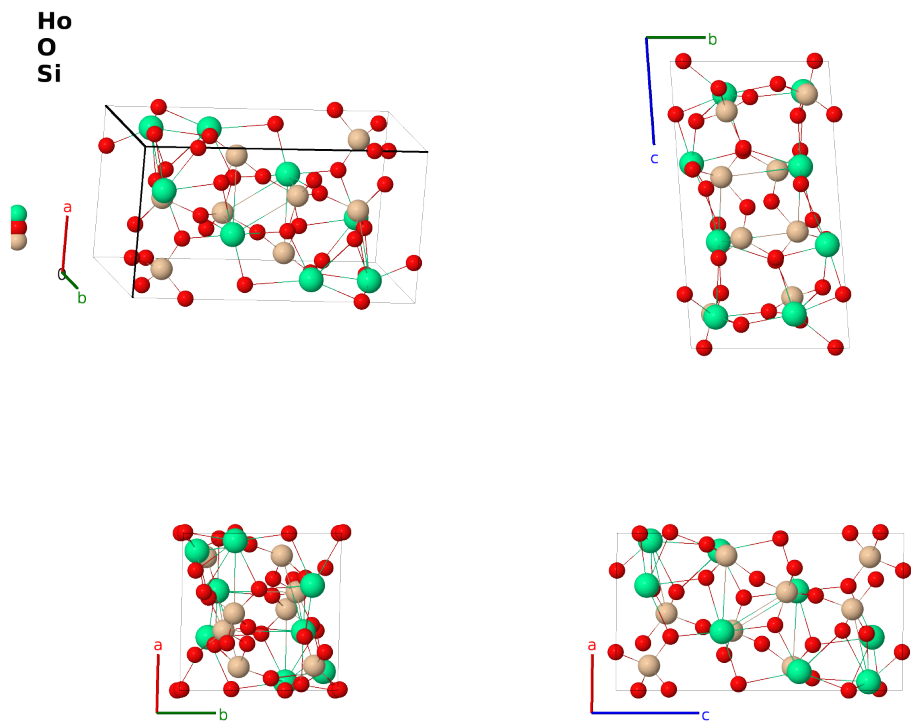
This structure previously used the label(s) **A2B7C2_aP44_2_4i_14i_4i**. Calls to these addresses will be redirected here.

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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/VN5Q>

https://aflow.org/prototype-encyclopedia/A2B7C2_aP44_2_4i_14i_4i-001

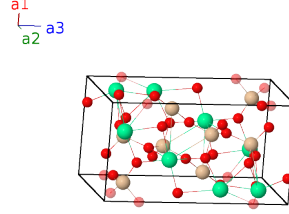


Prototype	Ho ₂ O ₇ Si ₂
AFLOW prototype label	A2B7C2_aP44_2_4i_14i_4i-001
ICSD	23619
CCDC	1599718
Pearson symbol	aP44
Space group number	2
Space group symbol	$P\bar{1}$

AFLOW prototype command `aflow --proto=A2B7C2_aP44_2_4i_14i_4i-001`
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 `$z_6, x_7, y_7, z_7, x_8, y_8, z_8, x_9, y_9, z_9, x_{10}, y_{10}, z_{10}, x_{11}, y_{11}, z_{11}, x_{12}, y_{12}, z_{12}, x_{13}, y_{13}, z_{13}, x_{14}, y_{14}, z_{14},$`
 `$x_{15}, y_{15}, z_{15}, x_{16}, y_{16}, z_{16}, x_{17}, y_{17}, z_{17}, x_{18}, y_{18}, z_{18}, x_{19}, y_{19}, z_{19}, x_{20}, y_{20}, z_{20}, x_{21}, y_{21}, z_{21}, x_{22},$`
 `$y_{22}, z_{22}$`

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

$$\begin{aligned}
\mathbf{B}_{39} &= x_{20} \mathbf{a}_1 + y_{20} \mathbf{a}_2 + z_{20} \mathbf{a}_3 &= (ax_{20} + by_{20} \cos \gamma + c_x z_{20}) \hat{\mathbf{x}} + (by_{20} \sin \gamma + c_y z_{20}) \hat{\mathbf{y}} + c_z z_{20} \hat{\mathbf{z}} &(2i) &\text{Si II} \\
\mathbf{B}_{40} &= -x_{20} \mathbf{a}_1 - y_{20} \mathbf{a}_2 - z_{20} \mathbf{a}_3 &= -(ax_{20} + by_{20} \cos \gamma + c_x z_{20}) \hat{\mathbf{x}} - (by_{20} \sin \gamma + c_y z_{20}) \hat{\mathbf{y}} - c_z z_{20} \hat{\mathbf{z}} &(2i) &\text{Si II} \\
\mathbf{B}_{41} &= x_{21} \mathbf{a}_1 + y_{21} \mathbf{a}_2 + z_{21} \mathbf{a}_3 &= (ax_{21} + by_{21} \cos \gamma + c_x z_{21}) \hat{\mathbf{x}} + (by_{21} \sin \gamma + c_y z_{21}) \hat{\mathbf{y}} + c_z z_{21} \hat{\mathbf{z}} &(2i) &\text{Si III} \\
\mathbf{B}_{42} &= -x_{21} \mathbf{a}_1 - y_{21} \mathbf{a}_2 - z_{21} \mathbf{a}_3 &= -(ax_{21} + by_{21} \cos \gamma + c_x z_{21}) \hat{\mathbf{x}} - (by_{21} \sin \gamma + c_y z_{21}) \hat{\mathbf{y}} - c_z z_{21} \hat{\mathbf{z}} &(2i) &\text{Si III} \\
\mathbf{B}_{43} &= x_{22} \mathbf{a}_1 + y_{22} \mathbf{a}_2 + z_{22} \mathbf{a}_3 &= (ax_{22} + by_{22} \cos \gamma + c_x z_{22}) \hat{\mathbf{x}} + (by_{22} \sin \gamma + c_y z_{22}) \hat{\mathbf{y}} + c_z z_{22} \hat{\mathbf{z}} &(2i) &\text{Si IV} \\
\mathbf{B}_{44} &= -x_{22} \mathbf{a}_1 - y_{22} \mathbf{a}_2 - z_{22} \mathbf{a}_3 &= -(ax_{22} + by_{22} \cos \gamma + c_x z_{22}) \hat{\mathbf{x}} - (by_{22} \sin \gamma + c_y z_{22}) \hat{\mathbf{y}} - c_z z_{22} \hat{\mathbf{z}} &(2i) &\text{Si IV}
\end{aligned}$$

References

- [1] J. Felsche, *A new silicate structure containing linear $[\text{Si}_3\text{O}_{10}]$ groups*, *Naturwissenschaften* **59**, 35–36 (1972), doi:10.1007/BF00594623.

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- [1] A. I. Becerro and A. Escudero, *Revision of the crystallographic data of polymorphic $\text{Y}_2\text{Si}_2\text{O}_7$ and Y_2SiO_5 compounds*, *Phase Transit.* **77**, 1093–1102 (2004), doi:10.1080/01411590412331282814.

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