

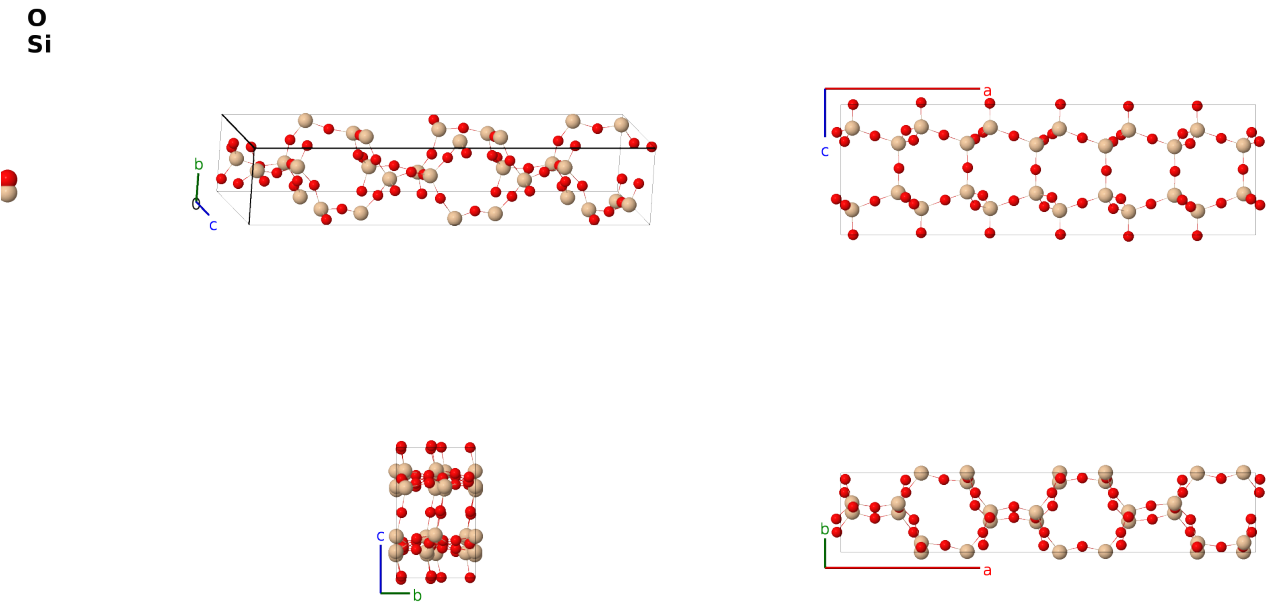
Orthorhombic Tridymite (SiO₂) Structure: A2B_oP72_19_12a_6a-001

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

https://aflow.org/prototype-encyclopedia/A2B_oP72_19_12a_6a-001

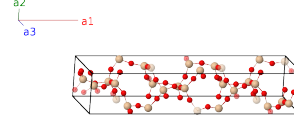


Prototype	O ₂ Si
AFLOW prototype label	A2B_oP72_19_12a_6a-001
Mineral name	tridymite
ICSD	153470
CCDC	1670161
Pearson symbol	oP72
Space group number	19
Space group symbol	$P2_12_12_1$
AFLOW prototype command	<pre>aflow --proto=A2B_oP72_19_12a_6a-001 --params=a,b/a,c/a,x₁,y₁,z₁,x₂,y₂,z₂,x₃,y₃,z₃,x₄,y₄,z₄,x₅,y₅,z₅,x₆,y₆,z₆,x₇, y₇,z₇,x₈,y₈,z₈,x₉,y₉,z₉,x₁₀,y₁₀,z₁₀,x₁₁,y₁₁,z₁₁,x₁₂,y₁₂,z₁₂,x₁₃,y₁₃,z₁₃,x₁₄,y₁₄,z₁₄,x₁₅, y₁₅,z₁₅,x₁₆,y₁₆,z₁₆,x₁₇,y₁₇,z₁₇,x₁₈,y₁₈,z₁₈</pre>

- This is an orthorhombic form of tridymite which appears at temperatures above 115°C. It is distinguished from what we call orthorhombic high tridymite by its origin.
- At temperatures below 115°C both structures transform into monoclinic “low” tridymite,” and at temperatures above 420°C they transform into hexagonal β (“high”) tridymite, *Strukturbericht C10*.
- Data for this structure was obtained from ICSD Entry 153470.
- This is a chiral structure, Sohncke Class III. The mirror image of this structure has the same bond distances and angles as the original, and so has the same formation energy. Either structure can form depending on the boundary conditions.
- More information about other SiO_2 and related structures can be found in our article on SiO_2 and AlPO_4 .

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
$\mathbf{B}_1$	$= x_1 \mathbf{a}_1 + y_1 \mathbf{a}_2 + z_1 \mathbf{a}_3$	$=$	$ax_1 \hat{\mathbf{x}} + by_1 \hat{\mathbf{y}} + cz_1 \hat{\mathbf{z}}$		(4a)	O I
$\mathbf{B}_2$	$= -\left(x_1 - \frac{1}{2}\right) \mathbf{a}_1 - y_1 \mathbf{a}_2 + \left(z_1 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-a\left(x_1 - \frac{1}{2}\right) \hat{\mathbf{x}} - by_1 \hat{\mathbf{y}} + c\left(z_1 + \frac{1}{2}\right) \hat{\mathbf{z}}$		(4a)	O I
$\mathbf{B}_3$	$= -x_1 \mathbf{a}_1 + \left(y_1 + \frac{1}{2}\right) \mathbf{a}_2 - \left(z_1 - \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-ax_1 \hat{\mathbf{x}} + b\left(y_1 + \frac{1}{2}\right) \hat{\mathbf{y}} - c\left(z_1 - \frac{1}{2}\right) \hat{\mathbf{z}}$		(4a)	O I
$\mathbf{B}_4$	$= \left(x_1 + \frac{1}{2}\right) \mathbf{a}_1 - \left(y_1 - \frac{1}{2}\right) \mathbf{a}_2 - z_1 \mathbf{a}_3$	$=$	$a\left(x_1 + \frac{1}{2}\right) \hat{\mathbf{x}} - b\left(y_1 - \frac{1}{2}\right) \hat{\mathbf{y}} - cz_1 \hat{\mathbf{z}}$		(4a)	O I
$\mathbf{B}_5$	$= x_2 \mathbf{a}_1 + y_2 \mathbf{a}_2 + z_2 \mathbf{a}_3$	$=$	$ax_2 \hat{\mathbf{x}} + by_2 \hat{\mathbf{y}} + cz_2 \hat{\mathbf{z}}$		(4a)	O II
$\mathbf{B}_6$	$= -\left(x_2 - \frac{1}{2}\right) \mathbf{a}_1 - y_2 \mathbf{a}_2 + \left(z_2 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-a\left(x_2 - \frac{1}{2}\right) \hat{\mathbf{x}} - by_2 \hat{\mathbf{y}} + c\left(z_2 + \frac{1}{2}\right) \hat{\mathbf{z}}$		(4a)	O II
$\mathbf{B}_7$	$= -x_2 \mathbf{a}_1 + \left(y_2 + \frac{1}{2}\right) \mathbf{a}_2 - \left(z_2 - \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-ax_2 \hat{\mathbf{x}} + b\left(y_2 + \frac{1}{2}\right) \hat{\mathbf{y}} - c\left(z_2 - \frac{1}{2}\right) \hat{\mathbf{z}}$		(4a)	O II
$\mathbf{B}_8$	$= \left(x_2 + \frac{1}{2}\right) \mathbf{a}_1 - \left(y_2 - \frac{1}{2}\right) \mathbf{a}_2 - z_2 \mathbf{a}_3$	$=$	$a\left(x_2 + \frac{1}{2}\right) \hat{\mathbf{x}} - b\left(y_2 - \frac{1}{2}\right) \hat{\mathbf{y}} - cz_2 \hat{\mathbf{z}}$		(4a)	O II
$\mathbf{B}_9$	$= x_3 \mathbf{a}_1 + y_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$ax_3 \hat{\mathbf{x}} + by_3 \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}}$		(4a)	O III
$\mathbf{B}_{10}$	$= -\left(x_3 - \frac{1}{2}\right) \mathbf{a}_1 - y_3 \mathbf{a}_2 + \left(z_3 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-a\left(x_3 - \frac{1}{2}\right) \hat{\mathbf{x}} - by_3 \hat{\mathbf{y}} + c\left(z_3 + \frac{1}{2}\right) \hat{\mathbf{z}}$		(4a)	O III
$\mathbf{B}_{11}$	$= -x_3 \mathbf{a}_1 + \left(y_3 + \frac{1}{2}\right) \mathbf{a}_2 - \left(z_3 - \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-ax_3 \hat{\mathbf{x}} + b\left(y_3 + \frac{1}{2}\right) \hat{\mathbf{y}} - c\left(z_3 - \frac{1}{2}\right) \hat{\mathbf{z}}$		(4a)	O III
$\mathbf{B}_{12}$	$= \left(x_3 + \frac{1}{2}\right) \mathbf{a}_1 - \left(y_3 - \frac{1}{2}\right) \mathbf{a}_2 - z_3 \mathbf{a}_3$	$=$	$a\left(x_3 + \frac{1}{2}\right) \hat{\mathbf{x}} - b\left(y_3 - \frac{1}{2}\right) \hat{\mathbf{y}} - cz_3 \hat{\mathbf{z}}$		(4a)	O III
$\mathbf{B}_{13}$	$= x_4 \mathbf{a}_1 + y_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$ax_4 \hat{\mathbf{x}} + by_4 \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}}$		(4a)	O IV
$\mathbf{B}_{14}$	$= -\left(x_4 - \frac{1}{2}\right) \mathbf{a}_1 - y_4 \mathbf{a}_2 + \left(z_4 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-a\left(x_4 - \frac{1}{2}\right) \hat{\mathbf{x}} - by_4 \hat{\mathbf{y}} + c\left(z_4 + \frac{1}{2}\right) \hat{\mathbf{z}}$		(4a)	O IV
$\mathbf{B}_{15}$	$= -x_4 \mathbf{a}_1 + \left(y_4 + \frac{1}{2}\right) \mathbf{a}_2 - \left(z_4 - \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-ax_4 \hat{\mathbf{x}} + b\left(y_4 + \frac{1}{2}\right) \hat{\mathbf{y}} - c\left(z_4 - \frac{1}{2}\right) \hat{\mathbf{z}}$		(4a)	O IV
$\mathbf{B}_{16}$	$= \left(x_4 + \frac{1}{2}\right) \mathbf{a}_1 - \left(y_4 - \frac{1}{2}\right) \mathbf{a}_2 - z_4 \mathbf{a}_3$	$=$	$a\left(x_4 + \frac{1}{2}\right) \hat{\mathbf{x}} - b\left(y_4 - \frac{1}{2}\right) \hat{\mathbf{y}} - cz_4 \hat{\mathbf{z}}$		(4a)	O IV
$\mathbf{B}_{17}$	$= x_5 \mathbf{a}_1 + y_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$ax_5 \hat{\mathbf{x}} + by_5 \hat{\mathbf{y}} + cz_5 \hat{\mathbf{z}}$		(4a)	O V

$\mathbf{B}_{18} =$	$-(x_5 - \frac{1}{2}) \mathbf{a}_1 - y_5 \mathbf{a}_2 +$	$=$	$-a(x_5 - \frac{1}{2}) \hat{\mathbf{x}} - by_5 \hat{\mathbf{y}} + c(z_5 + \frac{1}{2}) \hat{\mathbf{z}}$	(4a)	O V
	$(z_5 + \frac{1}{2}) \mathbf{a}_3$				
$\mathbf{B}_{19} =$	$-x_5 \mathbf{a}_1 + (y_5 + \frac{1}{2}) \mathbf{a}_2 -$	$=$	$-ax_5 \hat{\mathbf{x}} + b(y_5 + \frac{1}{2}) \hat{\mathbf{y}} - c(z_5 - \frac{1}{2}) \hat{\mathbf{z}}$	(4a)	O V
	$(z_5 - \frac{1}{2}) \mathbf{a}_3$				
$\mathbf{B}_{20} =$	$(x_5 + \frac{1}{2}) \mathbf{a}_1 - (y_5 - \frac{1}{2}) \mathbf{a}_2 - z_5 \mathbf{a}_3$	$=$	$a(x_5 + \frac{1}{2}) \hat{\mathbf{x}} - b(y_5 - \frac{1}{2}) \hat{\mathbf{y}} - cz_5 \hat{\mathbf{z}}$	(4a)	O V
$\mathbf{B}_{21} =$	$x_6 \mathbf{a}_1 + y_6 \mathbf{a}_2 + z_6 \mathbf{a}_3$	$=$	$ax_6 \hat{\mathbf{x}} + by_6 \hat{\mathbf{y}} + cz_6 \hat{\mathbf{z}}$	(4a)	O VI
$\mathbf{B}_{22} =$	$-(x_6 - \frac{1}{2}) \mathbf{a}_1 - y_6 \mathbf{a}_2 +$	$=$	$-a(x_6 - \frac{1}{2}) \hat{\mathbf{x}} - by_6 \hat{\mathbf{y}} + c(z_6 + \frac{1}{2}) \hat{\mathbf{z}}$	(4a)	O VI
	$(z_6 + \frac{1}{2}) \mathbf{a}_3$				
$\mathbf{B}_{23} =$	$-x_6 \mathbf{a}_1 + (y_6 + \frac{1}{2}) \mathbf{a}_2 -$	$=$	$-ax_6 \hat{\mathbf{x}} + b(y_6 + \frac{1}{2}) \hat{\mathbf{y}} - c(z_6 - \frac{1}{2}) \hat{\mathbf{z}}$	(4a)	O VI
	$(z_6 - \frac{1}{2}) \mathbf{a}_3$				
$\mathbf{B}_{24} =$	$(x_6 + \frac{1}{2}) \mathbf{a}_1 - (y_6 - \frac{1}{2}) \mathbf{a}_2 - z_6 \mathbf{a}_3$	$=$	$a(x_6 + \frac{1}{2}) \hat{\mathbf{x}} - b(y_6 - \frac{1}{2}) \hat{\mathbf{y}} - cz_6 \hat{\mathbf{z}}$	(4a)	O VI
$\mathbf{B}_{25} =$	$x_7 \mathbf{a}_1 + y_7 \mathbf{a}_2 + z_7 \mathbf{a}_3$	$=$	$ax_7 \hat{\mathbf{x}} + by_7 \hat{\mathbf{y}} + cz_7 \hat{\mathbf{z}}$	(4a)	O VII
$\mathbf{B}_{26} =$	$-(x_7 - \frac{1}{2}) \mathbf{a}_1 - y_7 \mathbf{a}_2 +$	$=$	$-a(x_7 - \frac{1}{2}) \hat{\mathbf{x}} - by_7 \hat{\mathbf{y}} + c(z_7 + \frac{1}{2}) \hat{\mathbf{z}}$	(4a)	O VII
	$(z_7 + \frac{1}{2}) \mathbf{a}_3$				
$\mathbf{B}_{27} =$	$-x_7 \mathbf{a}_1 + (y_7 + \frac{1}{2}) \mathbf{a}_2 -$	$=$	$-ax_7 \hat{\mathbf{x}} + b(y_7 + \frac{1}{2}) \hat{\mathbf{y}} - c(z_7 - \frac{1}{2}) \hat{\mathbf{z}}$	(4a)	O VII
	$(z_7 - \frac{1}{2}) \mathbf{a}_3$				
$\mathbf{B}_{28} =$	$(x_7 + \frac{1}{2}) \mathbf{a}_1 - (y_7 - \frac{1}{2}) \mathbf{a}_2 - z_7 \mathbf{a}_3$	$=$	$a(x_7 + \frac{1}{2}) \hat{\mathbf{x}} - b(y_7 - \frac{1}{2}) \hat{\mathbf{y}} - cz_7 \hat{\mathbf{z}}$	(4a)	O VII
$\mathbf{B}_{29} =$	$x_8 \mathbf{a}_1 + y_8 \mathbf{a}_2 + z_8 \mathbf{a}_3$	$=$	$ax_8 \hat{\mathbf{x}} + by_8 \hat{\mathbf{y}} + cz_8 \hat{\mathbf{z}}$	(4a)	O VIII
$\mathbf{B}_{30} =$	$-(x_8 - \frac{1}{2}) \mathbf{a}_1 - y_8 \mathbf{a}_2 +$	$=$	$-a(x_8 - \frac{1}{2}) \hat{\mathbf{x}} - by_8 \hat{\mathbf{y}} + c(z_8 + \frac{1}{2}) \hat{\mathbf{z}}$	(4a)	O VIII
	$(z_8 + \frac{1}{2}) \mathbf{a}_3$				
$\mathbf{B}_{31} =$	$-x_8 \mathbf{a}_1 + (y_8 + \frac{1}{2}) \mathbf{a}_2 -$	$=$	$-ax_8 \hat{\mathbf{x}} + b(y_8 + \frac{1}{2}) \hat{\mathbf{y}} - c(z_8 - \frac{1}{2}) \hat{\mathbf{z}}$	(4a)	O VIII
	$(z_8 - \frac{1}{2}) \mathbf{a}_3$				
$\mathbf{B}_{32} =$	$(x_8 + \frac{1}{2}) \mathbf{a}_1 - (y_8 - \frac{1}{2}) \mathbf{a}_2 - z_8 \mathbf{a}_3$	$=$	$a(x_8 + \frac{1}{2}) \hat{\mathbf{x}} - b(y_8 - \frac{1}{2}) \hat{\mathbf{y}} - cz_8 \hat{\mathbf{z}}$	(4a)	O VIII
$\mathbf{B}_{33} =$	$x_9 \mathbf{a}_1 + y_9 \mathbf{a}_2 + z_9 \mathbf{a}_3$	$=$	$ax_9 \hat{\mathbf{x}} + by_9 \hat{\mathbf{y}} + cz_9 \hat{\mathbf{z}}$	(4a)	O IX
$\mathbf{B}_{34} =$	$-(x_9 - \frac{1}{2}) \mathbf{a}_1 - y_9 \mathbf{a}_2 +$	$=$	$-a(x_9 - \frac{1}{2}) \hat{\mathbf{x}} - by_9 \hat{\mathbf{y}} + c(z_9 + \frac{1}{2}) \hat{\mathbf{z}}$	(4a)	O IX
	$(z_9 + \frac{1}{2}) \mathbf{a}_3$				
$\mathbf{B}_{35} =$	$-x_9 \mathbf{a}_1 + (y_9 + \frac{1}{2}) \mathbf{a}_2 -$	$=$	$-ax_9 \hat{\mathbf{x}} + b(y_9 + \frac{1}{2}) \hat{\mathbf{y}} - c(z_9 - \frac{1}{2}) \hat{\mathbf{z}}$	(4a)	O IX
	$(z_9 - \frac{1}{2}) \mathbf{a}_3$				
$\mathbf{B}_{36} =$	$(x_9 + \frac{1}{2}) \mathbf{a}_1 - (y_9 - \frac{1}{2}) \mathbf{a}_2 - z_9 \mathbf{a}_3$	$=$	$a(x_9 + \frac{1}{2}) \hat{\mathbf{x}} - b(y_9 - \frac{1}{2}) \hat{\mathbf{y}} - cz_9 \hat{\mathbf{z}}$	(4a)	O IX
$\mathbf{B}_{37} =$	$x_{10} \mathbf{a}_1 + y_{10} \mathbf{a}_2 + z_{10} \mathbf{a}_3$	$=$	$ax_{10} \hat{\mathbf{x}} + by_{10} \hat{\mathbf{y}} + cz_{10} \hat{\mathbf{z}}$	(4a)	O X
$\mathbf{B}_{38} =$	$-(x_{10} - \frac{1}{2}) \mathbf{a}_1 - y_{10} \mathbf{a}_2 +$	$=$	$-a(x_{10} - \frac{1}{2}) \hat{\mathbf{x}} - by_{10} \hat{\mathbf{y}} + c(z_{10} + \frac{1}{2}) \hat{\mathbf{z}}$	(4a)	O X
	$(z_{10} + \frac{1}{2}) \mathbf{a}_3$				
$\mathbf{B}_{39} =$	$-x_{10} \mathbf{a}_1 + (y_{10} + \frac{1}{2}) \mathbf{a}_2 -$	$=$	$-ax_{10} \hat{\mathbf{x}} + b(y_{10} + \frac{1}{2}) \hat{\mathbf{y}} - c(z_{10} - \frac{1}{2}) \hat{\mathbf{z}}$	(4a)	O X
	$(z_{10} - \frac{1}{2}) \mathbf{a}_3$				
$\mathbf{B}_{40} =$	$(x_{10} + \frac{1}{2}) \mathbf{a}_1 - (y_{10} - \frac{1}{2}) \mathbf{a}_2 -$	$=$	$a(x_{10} + \frac{1}{2}) \hat{\mathbf{x}} - b(y_{10} - \frac{1}{2}) \hat{\mathbf{y}} - cz_{10} \hat{\mathbf{z}}$	(4a)	O X
	$z_{10} \mathbf{a}_3$				
$\mathbf{B}_{41} =$	$x_{11} \mathbf{a}_1 + y_{11} \mathbf{a}_2 + z_{11} \mathbf{a}_3$	$=$	$ax_{11} \hat{\mathbf{x}} + by_{11} \hat{\mathbf{y}} + cz_{11} \hat{\mathbf{z}}$	(4a)	O XI
$\mathbf{B}_{42} =$	$-(x_{11} - \frac{1}{2}) \mathbf{a}_1 - y_{11} \mathbf{a}_2 +$	$=$	$-a(x_{11} - \frac{1}{2}) \hat{\mathbf{x}} - by_{11} \hat{\mathbf{y}} + c(z_{11} + \frac{1}{2}) \hat{\mathbf{z}}$	(4a)	O XI
	$(z_{11} + \frac{1}{2}) \mathbf{a}_3$				
$\mathbf{B}_{43} =$	$-x_{11} \mathbf{a}_1 + (y_{11} + \frac{1}{2}) \mathbf{a}_2 -$	$=$	$-ax_{11} \hat{\mathbf{x}} + b(y_{11} + \frac{1}{2}) \hat{\mathbf{y}} - c(z_{11} - \frac{1}{2}) \hat{\mathbf{z}}$	(4a)	O XI
	$(z_{11} - \frac{1}{2}) \mathbf{a}_3$				
$\mathbf{B}_{44} =$	$(x_{11} + \frac{1}{2}) \mathbf{a}_1 - (y_{11} - \frac{1}{2}) \mathbf{a}_2 -$	$=$	$a(x_{11} + \frac{1}{2}) \hat{\mathbf{x}} - b(y_{11} - \frac{1}{2}) \hat{\mathbf{y}} - cz_{11} \hat{\mathbf{z}}$	(4a)	O XI
	$z_{11} \mathbf{a}_3$				
$\mathbf{B}_{45} =$	$x_{12} \mathbf{a}_1 + y_{12} \mathbf{a}_2 + z_{12} \mathbf{a}_3$	$=$	$ax_{12} \hat{\mathbf{x}} + by_{12} \hat{\mathbf{y}} + cz_{12} \hat{\mathbf{z}}$	(4a)	O XII

$$\mathbf{B}_{72} = \begin{pmatrix} x_{18} + \frac{1}{2} \\ y_{18} - \frac{1}{2} \\ z_{18} \end{pmatrix} \mathbf{a}_1 - \begin{pmatrix} x_{18} + \frac{1}{2} \\ y_{18} - \frac{1}{2} \\ z_{18} \end{pmatrix} \mathbf{a}_2 - \begin{pmatrix} x_{18} + \frac{1}{2} \\ y_{18} - \frac{1}{2} \\ z_{18} \end{pmatrix} \mathbf{a}_3 = a \left(x_{18} + \frac{1}{2} \right) \hat{\mathbf{x}} - b \left(y_{18} - \frac{1}{2} \right) \hat{\mathbf{y}} - cz_{18} \hat{\mathbf{z}} \quad (4a) \quad \text{Si VI}$$

References

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Found in

- [1] ICSD, Inorganic Crystal Structure Database. ID 1534705.

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