Predicted SiO_2 ($P2$) Structure: A2B_mP12_3_ab3e_2e-001

This structure originally had the label `A2B_mP12_3_bc3e_2e`. Calls to that address will be redirected here.

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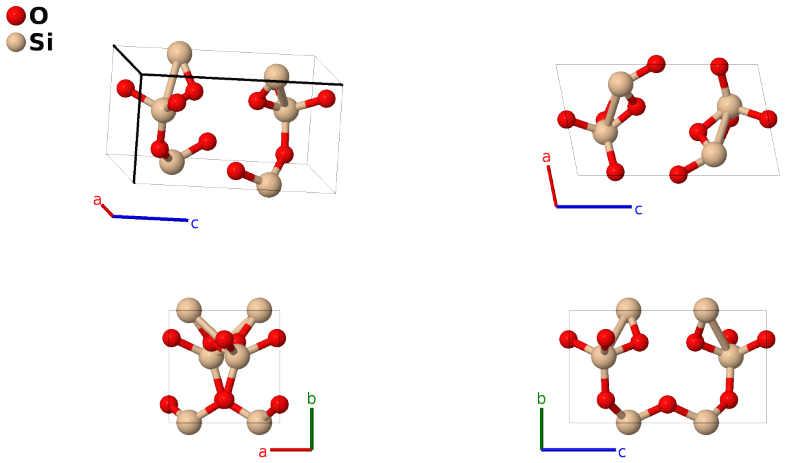
https://aflow.org/p/QAF3

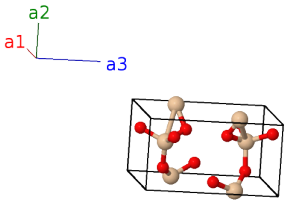
https://aflow.org/p/A2B_mP12_3_ab3e_2e-001



Prototype	O_2Si
AFLOW prototype label	A2B_mP12_3_ab3e_2e-001
ICSD	75669
Pearson symbol	mP12
Space group number	3
Space group symbol	$P2$
AFLOW prototype command	`aflow --proto=A2B_mP12_3_ab3e_2e-001 --params=`$a, b/a, c/a, \beta, y_1, y_2, x_3, y_3, z_3, x_4, y_4, z_4, x_5, y_5, z_5, x_6, y_6, z_6, x_7, y_7, z_7$

- This structure is the result of simulations of SiO_2 structures from a potential fitted to the $H_6Si_2O_7$ molecule. As such we do not believe it has been seen in nature. It does, however, describe a structure in space group $P2$ #3.

Simple Monoclinic primitive vectors



$$\mathbf{a_1} = a\,\hat{\mathbf{x}}$$
$$\mathbf{a_2} = b\,\hat{\mathbf{y}}$$
$$\mathbf{a_3} = c\cos\beta\,\hat{\mathbf{x}} + c\sin\beta\,\hat{\mathbf{z}}$$

Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$y_1\,\mathbf{a}_2$	=	$by_1\,\hat{\mathbf{y}}$	(1a)	O I
$\mathbf{B_2}$	=	$y_2\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}c\cos\beta\,\hat{\mathbf{x}} + by_2\,\hat{\mathbf{y}} + \frac{1}{2}c\sin\beta\,\hat{\mathbf{z}}$	(1b)	O II
$\mathbf{B_3}$	=	$x_3\,\mathbf{a}_1 + y_3\,\mathbf{a}_2 + z_3\,\mathbf{a}_3$	=	$(ax_3 + cz_3\cos\beta)\,\hat{\mathbf{x}} + by_3\,\hat{\mathbf{y}} + cz_3\sin\beta\,\hat{\mathbf{z}}$	(2e)	O III
$\mathbf{B_4}$	=	$-x_3\,\mathbf{a}_1 + y_3\,\mathbf{a}_2 - z_3\,\mathbf{a}_3$	=	$-(ax_3 + cz_3\cos\beta)\,\hat{\mathbf{x}} + by_3\,\hat{\mathbf{y}} - cz_3\sin\beta\,\hat{\mathbf{z}}$	(2e)	O III
$\mathbf{B_5}$	=	$x_4\,\mathbf{a}_1 + y_4\,\mathbf{a}_2 + z_4\,\mathbf{a}_3$	=	$(ax_4 + cz_4\cos\beta)\,\hat{\mathbf{x}} + by_4\,\hat{\mathbf{y}} + cz_4\sin\beta\,\hat{\mathbf{z}}$	(2e)	O IV
$\mathbf{B_6}$	=	$-x_4\,\mathbf{a}_1 + y_4\,\mathbf{a}_2 - z_4\,\mathbf{a}_3$	=	$-(ax_4 + cz_4\cos\beta)\,\hat{\mathbf{x}} + by_4\,\hat{\mathbf{y}} - cz_4\sin\beta\,\hat{\mathbf{z}}$	(2e)	O IV
$\mathbf{B_7}$	=	$x_5\,\mathbf{a}_1 + y_5\,\mathbf{a}_2 + z_5\,\mathbf{a}_3$	=	$(ax_5 + cz_5\cos\beta)\,\hat{\mathbf{x}} + by_5\,\hat{\mathbf{y}} + cz_5\sin\beta\,\hat{\mathbf{z}}$	(2e)	O V
$\mathbf{B_8}$	=	$-x_5\,\mathbf{a}_1 + y_5\,\mathbf{a}_2 - z_5\,\mathbf{a}_3$	=	$-(ax_5 + cz_5\cos\beta)\,\hat{\mathbf{x}} + by_5\,\hat{\mathbf{y}} - cz_5\sin\beta\,\hat{\mathbf{z}}$	(2e)	O V
$\mathbf{B_9}$	=	$x_6\,\mathbf{a}_1 + y_6\,\mathbf{a}_2 + z_6\,\mathbf{a}_3$	=	$(ax_6 + cz_6\cos\beta)\,\hat{\mathbf{x}} + by_6\,\hat{\mathbf{y}} + cz_6\sin\beta\,\hat{\mathbf{z}}$	(2e)	Si I
$\mathbf{B_{10}}$	=	$-x_6\,\mathbf{a}_1 + y_6\,\mathbf{a}_2 - z_6\,\mathbf{a}_3$	=	$-(ax_6 + cz_6\cos\beta)\,\hat{\mathbf{x}} + by_6\,\hat{\mathbf{y}} - cz_6\sin\beta\,\hat{\mathbf{z}}$	(2e)	Si I
$\mathbf{B_{11}}$	=	$x_7\,\mathbf{a}_1 + y_7\,\mathbf{a}_2 + z_7\,\mathbf{a}_3$	=	$(ax_7 + cz_7\cos\beta)\,\hat{\mathbf{x}} + by_7\,\hat{\mathbf{y}} + cz_7\sin\beta\,\hat{\mathbf{z}}$	(2e)	Si II
$\mathbf{B_{12}}$	=	$-x_7\,\mathbf{a}_1 + y_7\,\mathbf{a}_2 - z_7\,\mathbf{a}_3$	=	$-(ax_7 + cz_7\cos\beta)\,\hat{\mathbf{x}} + by_7\,\hat{\mathbf{y}} - cz_7\sin\beta\,\hat{\mathbf{z}}$	(2e)	Si II

References

[1] J. M. B. Boisen, G. V. Gibbs, and M. S. T. Bukowinski, *Framework silica structures generated using simulated annealing with a potential energy function based on an $H_6Si_2O_7$ molecule*, Phys. Chem. Miner. **21**, 269–284 (1994), doi:10.1007/BF00202091.