y-$Y_2Si_2O_7$ Structure: A7B2C2_mP22_11_3e2f_2e_ab-001

This structure originally had the label `A7B2C2_mP22_11_3e2f_2e_ab`. Calls to that address will be redirected here.

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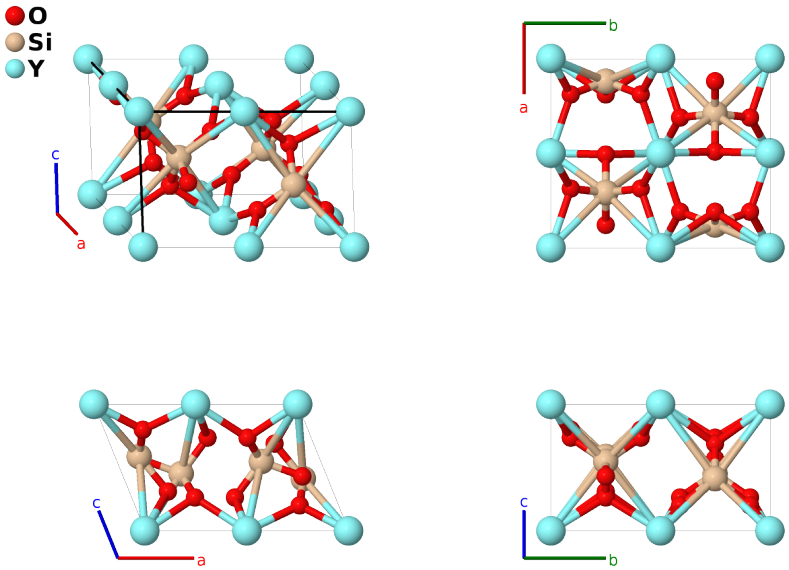
https://aflow.org/p/3RSG

https://aflow.org/p/A7B2C2_mP22_11_3e2f_2e_ab-001

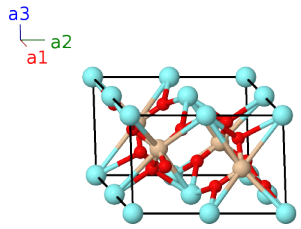


Prototype	$O_7Si_2Y_2$
AFLOW prototype label	A7B2C2_mP22_11_3e2f_2e_ab-001
ICSD	28004
Pearson symbol	mP22
Space group number	11
Space group symbol	$P2_1/m$
AFLOW prototype command	`aflow --proto=A7B2C2_mP22_11_3e2f_2e_ab-001 --params=`$a, b/a, c/a, \beta, x_3, z_3, x_4, z_4, x_5, z_5, x_6, z_6, x_7, z_7, x_8, y_8, z_8, x_9, y_9, z_9$

- (Becerro, 2003) found that the NMR spectrum of y-$Y_2Si_2O_7$ showed only one peak for yttrium. If that is the case, then this crystal structure is incorrect.

Simple Monoclinic primitive vectors

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



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	0	=	0	(2a)	Y I
$\mathbf{B_2}$	=	$\frac{1}{2}\,\mathbf{a}_2$	=	$\frac{1}{2}b\,\hat{\mathbf{y}}$	(2a)	Y I
$\mathbf{B_3}$	=	$\frac{1}{2}\,\mathbf{a}_1$	=	$\frac{1}{2}a\,\hat{\mathbf{x}}$	(2b)	Y II
$\mathbf{B_4}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}b\,\hat{\mathbf{y}}$	(2b)	Y II
$\mathbf{B_5}$	=	$x_3\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 + z_3\,\mathbf{a}_3$	=	$(ax_3 + cz_3\cos\beta)\,\hat{\mathbf{x}} + \frac{1}{4}b\,\hat{\mathbf{y}} + cz_3\sin\beta\,\hat{\mathbf{z}}$	(2e)	O I
$\mathbf{B_6}$	=	$-x_3\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 - z_3\,\mathbf{a}_3$	=	$-(ax_3 + cz_3\cos\beta)\,\hat{\mathbf{x}} + \frac{3}{4}b\,\hat{\mathbf{y}} - cz_3\sin\beta\,\hat{\mathbf{z}}$	(2e)	O I
$\mathbf{B_7}$	=	$x_4\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 + z_4\,\mathbf{a}_3$	=	$(ax_4 + cz_4\cos\beta)\,\hat{\mathbf{x}} + \frac{1}{4}b\,\hat{\mathbf{y}} + cz_4\sin\beta\,\hat{\mathbf{z}}$	(2e)	O II
$\mathbf{B_8}$	=	$-x_4\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 - z_4\,\mathbf{a}_3$	=	$-(ax_4 + cz_4\cos\beta)\,\hat{\mathbf{x}} + \frac{3}{4}b\,\hat{\mathbf{y}} - cz_4\sin\beta\,\hat{\mathbf{z}}$	(2e)	O II
$\mathbf{B_9}$	=	$x_5\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 + z_5\,\mathbf{a}_3$	=	$(ax_5 + cz_5\cos\beta)\,\hat{\mathbf{x}} + \frac{1}{4}b\,\hat{\mathbf{y}} + cz_5\sin\beta\,\hat{\mathbf{z}}$	(2e)	O III
$\mathbf{B_{10}}$	=	$-x_5\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 - z_5\,\mathbf{a}_3$	=	$-(ax_5 + cz_5\cos\beta)\,\hat{\mathbf{x}} + \frac{3}{4}b\,\hat{\mathbf{y}} - cz_5\sin\beta\,\hat{\mathbf{z}}$	(2e)	O III
$\mathbf{B_{11}}$	=	$x_6\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 + z_6\,\mathbf{a}_3$	=	$(ax_6 + cz_6\cos\beta)\,\hat{\mathbf{x}} + \frac{1}{4}b\,\hat{\mathbf{y}} + cz_6\sin\beta\,\hat{\mathbf{z}}$	(2e)	Si I
$\mathbf{B_{12}}$	=	$-x_6\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 - z_6\,\mathbf{a}_3$	=	$-(ax_6 + cz_6\cos\beta)\,\hat{\mathbf{x}} + \frac{3}{4}b\,\hat{\mathbf{y}} - cz_6\sin\beta\,\hat{\mathbf{z}}$	(2e)	Si I
$\mathbf{B_{13}}$	=	$x_7\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 + z_7\,\mathbf{a}_3$	=	$(ax_7 + cz_7\cos\beta)\,\hat{\mathbf{x}} + \frac{1}{4}b\,\hat{\mathbf{y}} + cz_7\sin\beta\,\hat{\mathbf{z}}$	(2e)	Si II
$\mathbf{B_{14}}$	=	$-x_7\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 - z_7\,\mathbf{a}_3$	=	$-(ax_7 + cz_7\cos\beta)\,\hat{\mathbf{x}} + \frac{3}{4}b\,\hat{\mathbf{y}} - cz_7\sin\beta\,\hat{\mathbf{z}}$	(2e)	Si II
$\mathbf{B_{15}}$	=	$x_8\,\mathbf{a}_1 + y_8\,\mathbf{a}_2 + z_8\,\mathbf{a}_3$	=	$(ax_8 + cz_8\cos\beta)\,\hat{\mathbf{x}} + by_8\,\hat{\mathbf{y}} + cz_8\sin\beta\,\hat{\mathbf{z}}$	(4f)	O IV
$\mathbf{B_{16}}$	=	$-x_8\,\mathbf{a}_1 + \left(y_8 + \frac{1}{2}\right)\,\mathbf{a}_2 - z_8\,\mathbf{a}_3$	=	$-(ax_8 + cz_8\cos\beta)\,\hat{\mathbf{x}} + b\left(y_8 + \frac{1}{2}\right)\,\hat{\mathbf{y}} - cz_8\sin\beta\,\hat{\mathbf{z}}$	(4f)	O IV
$\mathbf{B_{17}}$	=	$-x_8\,\mathbf{a}_1 - y_8\,\mathbf{a}_2 - z_8\,\mathbf{a}_3$	=	$-(ax_8 + cz_8\cos\beta)\,\hat{\mathbf{x}} - by_8\,\hat{\mathbf{y}} - cz_8\sin\beta\,\hat{\mathbf{z}}$	(4f)	O IV
$\mathbf{B_{18}}$	=	$x_8\,\mathbf{a}_1 - \left(y_8 - \frac{1}{2}\right)\,\mathbf{a}_2 + z_8\,\mathbf{a}_3$	=	$(ax_8 + cz_8\cos\beta)\,\hat{\mathbf{x}} - b\left(y_8 - \frac{1}{2}\right)\,\hat{\mathbf{y}} + cz_8\sin\beta\,\hat{\mathbf{z}}$	(4f)	O IV
$\mathbf{B_{19}}$	=	$x_9\,\mathbf{a}_1 + y_9\,\mathbf{a}_2 + z_9\,\mathbf{a}_3$	=	$(ax_9 + cz_9\cos\beta)\,\hat{\mathbf{x}} + by_9\,\hat{\mathbf{y}} + cz_9\sin\beta\,\hat{\mathbf{z}}$	(4f)	O V
$\mathbf{B_{20}}$	=	$-x_9\,\mathbf{a}_1 + \left(y_9 + \frac{1}{2}\right)\,\mathbf{a}_2 - z_9\,\mathbf{a}_3$	=	$-(ax_9 + cz_9\cos\beta)\,\hat{\mathbf{x}} + b\left(y_9 + \frac{1}{2}\right)\,\hat{\mathbf{y}} - cz_9\sin\beta\,\hat{\mathbf{z}}$	(4f)	O V
$\mathbf{B_{21}}$	=	$-x_9\,\mathbf{a}_1 - y_9\,\mathbf{a}_2 - z_9\,\mathbf{a}_3$	=	$-(ax_9 + cz_9\cos\beta)\,\hat{\mathbf{x}} - by_9\,\hat{\mathbf{y}} - cz_9\sin\beta\,\hat{\mathbf{z}}$	(4f)	O V
$\mathbf{B_{22}}$	=	$x_9\,\mathbf{a}_1 - \left(y_9 - \frac{1}{2}\right)\,\mathbf{a}_2 + z_9\,\mathbf{a}_3$	=	$(ax_9 + cz_9\cos\beta)\,\hat{\mathbf{x}} - b\left(y_9 - \frac{1}{2}\right)\,\hat{\mathbf{y}} + cz_9\sin\beta\,\hat{\mathbf{z}}$	(4f)	O V

References

[1] N. G. Batalieva and Y. A. Pyatenko, *Artificial yttrialite ("y-phase") - a representative of a new structure type in the rare earth diorthosilicate series*, Sov. Phys. Crystallogr. **16**, 786–789 (1972). Translation of N. G. Batalieva and Yu. A. Pyatenko, Kristallogr. 16, 905 (1971).

[2] A. I. Becerro, A. Escudero, P. Florian, D. Massiot, and M. D. Alba, *Revisiting $Y_2Si_2O_7$ and Y_2SiO_5 polymorphic structures by ^9Y MAS-NMR spectroscopy*, J. Solid State Chem. **177**, 2783–2789 (2004), doi:10.1016/j.jssc.2004.03.047.

Found in

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