γ-Y$_2$Si$_2$O$_7$ Structure: A4BC_mP24_14_4e_e_e-001
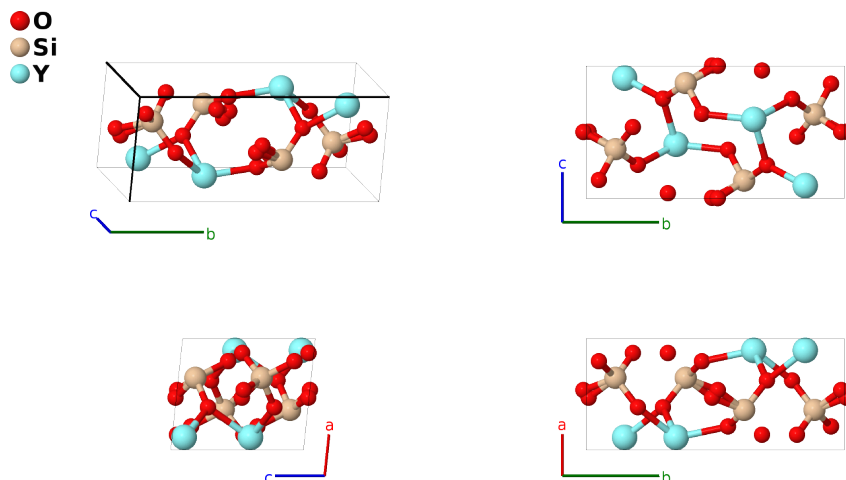
This structure originally had the label `A4BC_mP24_14_4e_e_e`. Calls to that address will be redirected here.

https://aflow.org/p/3TA1

https://aflow.org/p/A4BC_mP24_14_4e_e_e-001

Prototype	O$_7$Si$_2$Y$_2$
AFLOW prototype label	A4BC_mP24_14_4e_e_e-001
ICSD	none
Pearson symbol	mP24
Space group number	14
Space group symbol	$P2_1/c$
AFLOW prototype command	aflow --proto=A4BC_mP24_14_4e_e_e-001 --params=$a, b/a, c/a, \beta, x_1, y_1, z_1, x_2, y_2, z_2, x_3, y_3, z_3, x_4, y_4, z_4, x_5, y_5, z_5, x_6, y_6, z_6$

Other compounds with this structure

γ-Er$_2$Si$_2$O$_7$, γ-Ho$_2$Si$_2$O$_7$
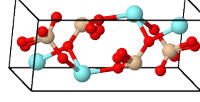
- The O-III site is only 50% occupied. The jmol plot shows the two possible sites as a pair of very closely spaced oxygen atoms.

- (Christensen, 1997) refer to this as D-Y$_2$Si$_2$O$_7$, but we follow the classification of the RE$_2$Si$_2$O$_7$ structures in (Becerro, 2004) and refer to this as γ-Y$_2$Si$_2$O$_7$.

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
$\mathbf{B_1}$	$=$	$x_1\,\mathbf{a_1} + y_1\,\mathbf{a_2} + z_1\,\mathbf{a_3}$	$=$	$(ax_1 + cz_1\cos\beta)\,\hat{\mathbf{x}} + by_1\,\hat{\mathbf{y}} + cz_1\sin\beta\,\hat{\mathbf{z}}$	(4e)	O I
$\mathbf{B_2}$	$=$	$-x_1\,\mathbf{a_1} + \left(y_1 + \tfrac{1}{2}\right)\mathbf{a_2} - \left(z_1 - \tfrac{1}{2}\right)\mathbf{a_3}$	$=$	$-\left(ax_1 + c\left(z_1 - \tfrac{1}{2}\right)\cos\beta\right)\hat{\mathbf{x}} + b\left(y_1 + \tfrac{1}{2}\right)\hat{\mathbf{y}} - c\left(z_1 - \tfrac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(4e)	O I
$\mathbf{B_3}$	$=$	$-x_1\,\mathbf{a_1} - y_1\,\mathbf{a_2} - z_1\,\mathbf{a_3}$	$=$	$-(ax_1 + cz_1\cos\beta)\,\hat{\mathbf{x}} - by_1\,\hat{\mathbf{y}} - cz_1\sin\beta\,\hat{\mathbf{z}}$	(4e)	O I
$\mathbf{B_4}$	$=$	$x_1\,\mathbf{a_1} - \left(y_1 - \tfrac{1}{2}\right)\mathbf{a_2} + \left(z_1 + \tfrac{1}{2}\right)\mathbf{a_3}$	$=$	$\left(ax_1 + c\left(z_1 + \tfrac{1}{2}\right)\cos\beta\right)\hat{\mathbf{x}} - b\left(y_1 - \tfrac{1}{2}\right)\hat{\mathbf{y}} + c\left(z_1 + \tfrac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(4e)	O I
$\mathbf{B_5}$	$=$	$x_2\,\mathbf{a_1} + y_2\,\mathbf{a_2} + z_2\,\mathbf{a_3}$	$=$	$(ax_2 + cz_2\cos\beta)\,\hat{\mathbf{x}} + by_2\,\hat{\mathbf{y}} + cz_2\sin\beta\,\hat{\mathbf{z}}$	(4e)	O II
$\mathbf{B_6}$	$=$	$-x_2\,\mathbf{a_1} + \left(y_2 + \tfrac{1}{2}\right)\mathbf{a_2} - \left(z_2 - \tfrac{1}{2}\right)\mathbf{a_3}$	$=$	$-\left(ax_2 + c\left(z_2 - \tfrac{1}{2}\right)\cos\beta\right)\hat{\mathbf{x}} + b\left(y_2 + \tfrac{1}{2}\right)\hat{\mathbf{y}} - c\left(z_2 - \tfrac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(4e)	O II
$\mathbf{B_7}$	$=$	$-x_2\,\mathbf{a_1} - y_2\,\mathbf{a_2} - z_2\,\mathbf{a_3}$	$=$	$-(ax_2 + cz_2\cos\beta)\,\hat{\mathbf{x}} - by_2\,\hat{\mathbf{y}} - cz_2\sin\beta\,\hat{\mathbf{z}}$	(4e)	O II
$\mathbf{B_8}$	$=$	$x_2\,\mathbf{a_1} - \left(y_2 - \tfrac{1}{2}\right)\mathbf{a_2} + \left(z_2 + \tfrac{1}{2}\right)\mathbf{a_3}$	$=$	$\left(ax_2 + c\left(z_2 + \tfrac{1}{2}\right)\cos\beta\right)\hat{\mathbf{x}} - b\left(y_2 - \tfrac{1}{2}\right)\hat{\mathbf{y}} + c\left(z_2 + \tfrac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(4e)	O II
$\mathbf{B_9}$	$=$	$x_3\,\mathbf{a_1} + y_3\,\mathbf{a_2} + z_3\,\mathbf{a_3}$	$=$	$(ax_3 + cz_3\cos\beta)\,\hat{\mathbf{x}} + by_3\,\hat{\mathbf{y}} + cz_3\sin\beta\,\hat{\mathbf{z}}$	(4e)	O III
$\mathbf{B_{10}}$	$=$	$-x_3\,\mathbf{a_1} + \left(y_3 + \tfrac{1}{2}\right)\mathbf{a_2} - \left(z_3 - \tfrac{1}{2}\right)\mathbf{a_3}$	$=$	$-\left(ax_3 + c\left(z_3 - \tfrac{1}{2}\right)\cos\beta\right)\hat{\mathbf{x}} + b\left(y_3 + \tfrac{1}{2}\right)\hat{\mathbf{y}} - c\left(z_3 - \tfrac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(4e)	O III
$\mathbf{B_{11}}$	$=$	$-x_3\,\mathbf{a_1} - y_3\,\mathbf{a_2} - z_3\,\mathbf{a_3}$	$=$	$-(ax_3 + cz_3\cos\beta)\,\hat{\mathbf{x}} - by_3\,\hat{\mathbf{y}} - cz_3\sin\beta\,\hat{\mathbf{z}}$	(4e)	O III
$\mathbf{B_{12}}$	$=$	$x_3\,\mathbf{a_1} - \left(y_3 - \tfrac{1}{2}\right)\mathbf{a_2} + \left(z_3 + \tfrac{1}{2}\right)\mathbf{a_3}$	$=$	$\left(ax_3 + c\left(z_3 + \tfrac{1}{2}\right)\cos\beta\right)\hat{\mathbf{x}} - b\left(y_3 - \tfrac{1}{2}\right)\hat{\mathbf{y}} + c\left(z_3 + \tfrac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(4e)	O III
$\mathbf{B_{13}}$	$=$	$x_4\,\mathbf{a_1} + y_4\,\mathbf{a_2} + z_4\,\mathbf{a_3}$	$=$	$(ax_4 + cz_4\cos\beta)\,\hat{\mathbf{x}} + by_4\,\hat{\mathbf{y}} + cz_4\sin\beta\,\hat{\mathbf{z}}$	(4e)	O IV
$\mathbf{B_{14}}$	$=$	$-x_4\,\mathbf{a_1} + \left(y_4 + \tfrac{1}{2}\right)\mathbf{a_2} - \left(z_4 - \tfrac{1}{2}\right)\mathbf{a_3}$	$=$	$-\left(ax_4 + c\left(z_4 - \tfrac{1}{2}\right)\cos\beta\right)\hat{\mathbf{x}} + b\left(y_4 + \tfrac{1}{2}\right)\hat{\mathbf{y}} - c\left(z_4 - \tfrac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(4e)	O IV
$\mathbf{B_{15}}$	$=$	$-x_4\,\mathbf{a_1} - y_4\,\mathbf{a_2} - z_4\,\mathbf{a_3}$	$=$	$-(ax_4 + cz_4\cos\beta)\,\hat{\mathbf{x}} - by_4\,\hat{\mathbf{y}} - cz_4\sin\beta\,\hat{\mathbf{z}}$	(4e)	O IV
$\mathbf{B_{16}}$	$=$	$x_4\,\mathbf{a_1} - \left(y_4 - \tfrac{1}{2}\right)\mathbf{a_2} + \left(z_4 + \tfrac{1}{2}\right)\mathbf{a_3}$	$=$	$\left(ax_4 + c\left(z_4 + \tfrac{1}{2}\right)\cos\beta\right)\hat{\mathbf{x}} - b\left(y_4 - \tfrac{1}{2}\right)\hat{\mathbf{y}} + c\left(z_4 + \tfrac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(4e)	O IV
$\mathbf{B_{17}}$	$=$	$x_5\,\mathbf{a_1} + y_5\,\mathbf{a_2} + z_5\,\mathbf{a_3}$	$=$	$(ax_5 + cz_5\cos\beta)\,\hat{\mathbf{x}} + by_5\,\hat{\mathbf{y}} + cz_5\sin\beta\,\hat{\mathbf{z}}$	(4e)	Si I
$\mathbf{B_{18}}$	$=$	$-x_5\,\mathbf{a_1} + \left(y_5 + \tfrac{1}{2}\right)\mathbf{a_2} - \left(z_5 - \tfrac{1}{2}\right)\mathbf{a_3}$	$=$	$-\left(ax_5 + c\left(z_5 - \tfrac{1}{2}\right)\cos\beta\right)\hat{\mathbf{x}} + b\left(y_5 + \tfrac{1}{2}\right)\hat{\mathbf{y}} - c\left(z_5 - \tfrac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(4e)	Si I
$\mathbf{B_{19}}$	$=$	$-x_5\,\mathbf{a_1} - y_5\,\mathbf{a_2} - z_5\,\mathbf{a_3}$	$=$	$-(ax_5 + cz_5\cos\beta)\,\hat{\mathbf{x}} - by_5\,\hat{\mathbf{y}} - cz_5\sin\beta\,\hat{\mathbf{z}}$	(4e)	Si I
$\mathbf{B_{20}}$	$=$	$x_5\,\mathbf{a_1} - \left(y_5 - \tfrac{1}{2}\right)\mathbf{a_2} + \left(z_5 + \tfrac{1}{2}\right)\mathbf{a_3}$	$=$	$\left(ax_5 + c\left(z_5 + \tfrac{1}{2}\right)\cos\beta\right)\hat{\mathbf{x}} - b\left(y_5 - \tfrac{1}{2}\right)\hat{\mathbf{y}} + c\left(z_5 + \tfrac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(4e)	Si I
$\mathbf{B_{21}}$	$=$	$x_6\,\mathbf{a_1} + y_6\,\mathbf{a_2} + z_6\,\mathbf{a_3}$	$=$	$(ax_6 + cz_6\cos\beta)\,\hat{\mathbf{x}} + by_6\,\hat{\mathbf{y}} + cz_6\sin\beta\,\hat{\mathbf{z}}$	(4e)	Y I
$\mathbf{B_{22}}$	$=$	$-x_6\,\mathbf{a_1} + \left(y_6 + \tfrac{1}{2}\right)\mathbf{a_2} - \left(z_6 - \tfrac{1}{2}\right)\mathbf{a_3}$	$=$	$-\left(ax_6 + c\left(z_6 - \tfrac{1}{2}\right)\cos\beta\right)\hat{\mathbf{x}} + b\left(y_6 + \tfrac{1}{2}\right)\hat{\mathbf{y}} - c\left(z_6 - \tfrac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(4e)	Y I
$\mathbf{B_{23}}$	$=$	$-x_6\,\mathbf{a_1} - y_6\,\mathbf{a_2} - z_6\,\mathbf{a_3}$	$=$	$-(ax_6 + cz_6\cos\beta)\,\hat{\mathbf{x}} - by_6\,\hat{\mathbf{y}} - cz_6\sin\beta\,\hat{\mathbf{z}}$	(4e)	Y I

$$\mathbf{B_{24}} \quad = \quad x_6\,\mathbf{a}_1 - \left(y_6 - \tfrac{1}{2}\right)\mathbf{a}_2 + \left(z_6 + \tfrac{1}{2}\right)\mathbf{a}_3 \quad = \quad \left(ax_6 + c\left(z_6 + \tfrac{1}{2}\right)\cos\beta\right)\hat{\mathbf{x}} - \qquad\qquad \text{(4e)} \qquad \text{Y I}$$
$$b\left(y_6 - \tfrac{1}{2}\right)\hat{\mathbf{y}} + c\left(z_6 + \tfrac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$$

References

[1] A. N. Christensen, R. G. Hazell, and A. W. Hewat, *Synthesis, Crystal Growth and Structure Investigations of Rare-Earth Disilicates and Rare-Earth Oxyapatites*, Acta Chem. Scand. **51**, 37–41 (1997), doi:10.3891/acta.chem.scand.51-0037.

Found in

[1] A. I. Becerro and A. Escudero, *Revision of the crystallographic data of polymorphic $Y_2Si_2O_7$ and Y_2SiO_5 compounds*, Phase Transit. **77**, 1093–1102 (2004), doi:10.1080/01411590412331282814.