Er$_2$Si$_2$O$_7$ Structure: A2B7C2_mP22_14_e_a3e_e-001
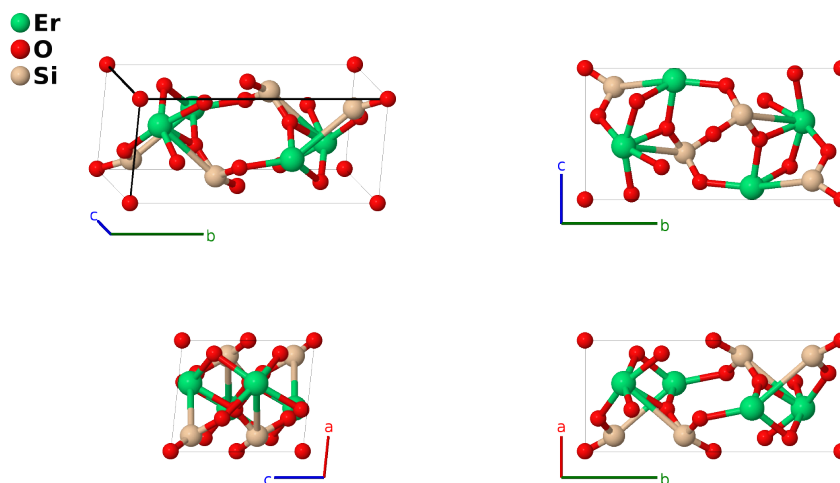
Prototype	Er$_2$O$_7$Si$_2$
AFLOW prototype label	A2B7C2_mP22_14_e_a3e_e-001
ICSD	16049
Pearson symbol	mP22
Space group number	14
Space group symbol	$P2_1/c$
AFLOW prototype command	aflow --proto=A2B7C2_mP22_14_e_a3e_e-001
	--params=$a, b/a, c/a, \beta, x_2, y_2, z_2, x_3, y_3, z_3, x_4, y_4, z_4, x_5, y_5, z_5, x_6, y_6, z_6$

Other compounds with this structure
Ho$_2$Si$_2$O$_7$, Y$_2$Si$_2$O$_7$

- (Felsche, 1970) refers to this as the "D-RE$_2$Si$_2$O$_7$ structure, where "RE" is a rare-earth element.

- Some authors use Ho$_2$Si$_2$O$_7$ as the prototype structure, but (Smolin, 1970) only gives lattice parameters for that compound, while giving full structural information for Er$_2$Si$_2$O$_7$, so we use this as the prototype.

- (Smolin, 1970) give the structure in the $P2_1/b$ setting of space group #14 with a unique c-axis. We used FINDSYM to transform this to the standard $P2_1/c$ setting with unique axis b.

Simple Monoclinic primitive vectors

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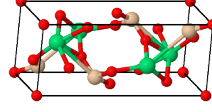
Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	$=$	0	$=$	0	(2a)	O I
$\mathbf{B_2}$	$=$	$\frac{1}{2}\mathbf{a_2} + \frac{1}{2}\mathbf{a_3}$	$=$	$\frac{1}{2}c\cos\beta\,\hat{\mathbf{x}} + \frac{1}{2}b\,\hat{\mathbf{y}} + \frac{1}{2}c\sin\beta\,\hat{\mathbf{z}}$	(2a)	O I
$\mathbf{B_3}$	$=$	$x_2\,\mathbf{a_1} + y_2\,\mathbf{a_2} + z_2\,\mathbf{a_3}$	$=$	$(ax_2 + cz_2\cos\beta)\,\hat{\mathbf{x}} + by_2\,\hat{\mathbf{y}} + cz_2\sin\beta\,\hat{\mathbf{z}}$	(4e)	Er I
$\mathbf{B_4}$	$=$	$-x_2\,\mathbf{a_1} + \left(y_2 + \frac{1}{2}\right)\mathbf{a_2} - \left(z_2 - \frac{1}{2}\right)\mathbf{a_3}$	$=$	$-\left(ax_2 + c\left(z_2 - \frac{1}{2}\right)\cos\beta\right)\hat{\mathbf{x}} + b\left(y_2 + \frac{1}{2}\right)\hat{\mathbf{y}} - c\left(z_2 - \frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(4e)	Er I
$\mathbf{B_5}$	$=$	$-x_2\,\mathbf{a_1} - y_2\,\mathbf{a_2} - z_2\,\mathbf{a_3}$	$=$	$-\left(ax_2 + cz_2\cos\beta\right)\hat{\mathbf{x}} - by_2\,\hat{\mathbf{y}} - cz_2\sin\beta\,\hat{\mathbf{z}}$	(4e)	Er I
$\mathbf{B_6}$	$=$	$x_2\,\mathbf{a_1} - \left(y_2 - \frac{1}{2}\right)\mathbf{a_2} + \left(z_2 + \frac{1}{2}\right)\mathbf{a_3}$	$=$	$\left(ax_2 + c\left(z_2 + \frac{1}{2}\right)\cos\beta\right)\hat{\mathbf{x}} - b\left(y_2 - \frac{1}{2}\right)\hat{\mathbf{y}} + c\left(z_2 + \frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(4e)	Er I
$\mathbf{B_7}$	$=$	$x_3\,\mathbf{a_1} + y_3\,\mathbf{a_2} + z_3\,\mathbf{a_3}$	$=$	$(ax_3 + cz_3\cos\beta)\,\hat{\mathbf{x}} + by_3\,\hat{\mathbf{y}} + cz_3\sin\beta\,\hat{\mathbf{z}}$	(4e)	O II
$\mathbf{B_8}$	$=$	$-x_3\,\mathbf{a_1} + \left(y_3 + \frac{1}{2}\right)\mathbf{a_2} - \left(z_3 - \frac{1}{2}\right)\mathbf{a_3}$	$=$	$-\left(ax_3 + c\left(z_3 - \frac{1}{2}\right)\cos\beta\right)\hat{\mathbf{x}} + b\left(y_3 + \frac{1}{2}\right)\hat{\mathbf{y}} - c\left(z_3 - \frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(4e)	O II
$\mathbf{B_9}$	$=$	$-x_3\,\mathbf{a_1} - y_3\,\mathbf{a_2} - z_3\,\mathbf{a_3}$	$=$	$-\left(ax_3 + cz_3\cos\beta\right)\hat{\mathbf{x}} - by_3\,\hat{\mathbf{y}} - cz_3\sin\beta\,\hat{\mathbf{z}}$	(4e)	O II
$\mathbf{B_{10}}$	$=$	$x_3\,\mathbf{a_1} - \left(y_3 - \frac{1}{2}\right)\mathbf{a_2} + \left(z_3 + \frac{1}{2}\right)\mathbf{a_3}$	$=$	$\left(ax_3 + c\left(z_3 + \frac{1}{2}\right)\cos\beta\right)\hat{\mathbf{x}} - b\left(y_3 - \frac{1}{2}\right)\hat{\mathbf{y}} + c\left(z_3 + \frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(4e)	O II
$\mathbf{B_{11}}$	$=$	$x_4\,\mathbf{a_1} + y_4\,\mathbf{a_2} + z_4\,\mathbf{a_3}$	$=$	$(ax_4 + cz_4\cos\beta)\,\hat{\mathbf{x}} + by_4\,\hat{\mathbf{y}} + cz_4\sin\beta\,\hat{\mathbf{z}}$	(4e)	O III
$\mathbf{B_{12}}$	$=$	$-x_4\,\mathbf{a_1} + \left(y_4 + \frac{1}{2}\right)\mathbf{a_2} - \left(z_4 - \frac{1}{2}\right)\mathbf{a_3}$	$=$	$-\left(ax_4 + c\left(z_4 - \frac{1}{2}\right)\cos\beta\right)\hat{\mathbf{x}} + b\left(y_4 + \frac{1}{2}\right)\hat{\mathbf{y}} - c\left(z_4 - \frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(4e)	O III
$\mathbf{B_{13}}$	$=$	$-x_4\,\mathbf{a_1} - y_4\,\mathbf{a_2} - z_4\,\mathbf{a_3}$	$=$	$-\left(ax_4 + cz_4\cos\beta\right)\hat{\mathbf{x}} - by_4\,\hat{\mathbf{y}} - cz_4\sin\beta\,\hat{\mathbf{z}}$	(4e)	O III
$\mathbf{B_{14}}$	$=$	$x_4\,\mathbf{a_1} - \left(y_4 - \frac{1}{2}\right)\mathbf{a_2} + \left(z_4 + \frac{1}{2}\right)\mathbf{a_3}$	$=$	$\left(ax_4 + c\left(z_4 + \frac{1}{2}\right)\cos\beta\right)\hat{\mathbf{x}} - b\left(y_4 - \frac{1}{2}\right)\hat{\mathbf{y}} + c\left(z_4 + \frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(4e)	O III
$\mathbf{B_{15}}$	$=$	$x_5\,\mathbf{a_1} + y_5\,\mathbf{a_2} + z_5\,\mathbf{a_3}$	$=$	$(ax_5 + cz_5\cos\beta)\,\hat{\mathbf{x}} + by_5\,\hat{\mathbf{y}} + cz_5\sin\beta\,\hat{\mathbf{z}}$	(4e)	O IV
$\mathbf{B_{16}}$	$=$	$-x_5\,\mathbf{a_1} + \left(y_5 + \frac{1}{2}\right)\mathbf{a_2} - \left(z_5 - \frac{1}{2}\right)\mathbf{a_3}$	$=$	$-\left(ax_5 + c\left(z_5 - \frac{1}{2}\right)\cos\beta\right)\hat{\mathbf{x}} + b\left(y_5 + \frac{1}{2}\right)\hat{\mathbf{y}} - c\left(z_5 - \frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(4e)	O IV
$\mathbf{B_{17}}$	$=$	$-x_5\,\mathbf{a_1} - y_5\,\mathbf{a_2} - z_5\,\mathbf{a_3}$	$=$	$-\left(ax_5 + cz_5\cos\beta\right)\hat{\mathbf{x}} - by_5\,\hat{\mathbf{y}} - cz_5\sin\beta\,\hat{\mathbf{z}}$	(4e)	O IV
$\mathbf{B_{18}}$	$=$	$x_5\,\mathbf{a_1} - \left(y_5 - \frac{1}{2}\right)\mathbf{a_2} + \left(z_5 + \frac{1}{2}\right)\mathbf{a_3}$	$=$	$\left(ax_5 + c\left(z_5 + \frac{1}{2}\right)\cos\beta\right)\hat{\mathbf{x}} - b\left(y_5 - \frac{1}{2}\right)\hat{\mathbf{y}} + c\left(z_5 + \frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(4e)	O IV
$\mathbf{B_{19}}$	$=$	$x_6\,\mathbf{a_1} + y_6\,\mathbf{a_2} + z_6\,\mathbf{a_3}$	$=$	$(ax_6 + cz_6\cos\beta)\,\hat{\mathbf{x}} + by_6\,\hat{\mathbf{y}} + cz_6\sin\beta\,\hat{\mathbf{z}}$	(4e)	Si I
$\mathbf{B_{20}}$	$=$	$-x_6\,\mathbf{a_1} + \left(y_6 + \frac{1}{2}\right)\mathbf{a_2} - \left(z_6 - \frac{1}{2}\right)\mathbf{a_3}$	$=$	$-\left(ax_6 + c\left(z_6 - \frac{1}{2}\right)\cos\beta\right)\hat{\mathbf{x}} + b\left(y_6 + \frac{1}{2}\right)\hat{\mathbf{y}} - c\left(z_6 - \frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(4e)	Si I
$\mathbf{B_{21}}$	$=$	$-x_6\,\mathbf{a_1} - y_6\,\mathbf{a_2} - z_6\,\mathbf{a_3}$	$=$	$-\left(ax_6 + cz_6\cos\beta\right)\hat{\mathbf{x}} - by_6\,\hat{\mathbf{y}} - cz_6\sin\beta\,\hat{\mathbf{z}}$	(4e)	Si I
$\mathbf{B_{22}}$	$=$	$x_6\,\mathbf{a_1} - \left(y_6 - \frac{1}{2}\right)\mathbf{a_2} + \left(z_6 + \frac{1}{2}\right)\mathbf{a_3}$	$=$	$\left(ax_6 + c\left(z_6 + \frac{1}{2}\right)\cos\beta\right)\hat{\mathbf{x}} - b\left(y_6 - \frac{1}{2}\right)\hat{\mathbf{y}} + c\left(z_6 + \frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(4e)	Si I

References

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[2] J. Felsche, *Polymorphism and crystal data of the rare-earth disilicates of type $R.E._2Si_2O_7$*, J. Less-Common Met. **21**, 1–14 (1970), doi:10.1016/0022-5088(70)90159-1.