Esseneite ($CaFeSi_2O_6$) Structure: ABC6D2_mC40_15_e_e_3f_f-001

This structure originally had the label `ABC6D2_mC40_15_e_e_3f_f`. Calls to that address will be redirected here.

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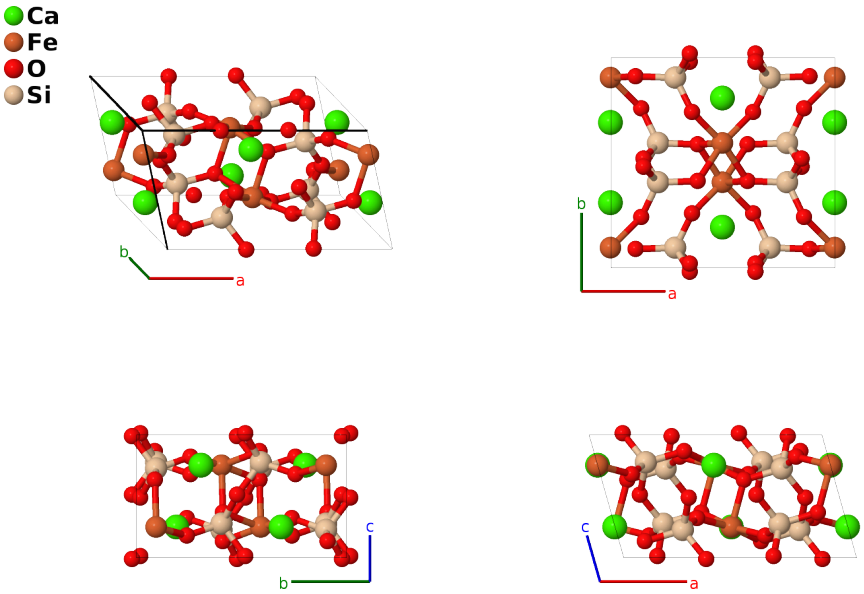
https://aflow.org/p/5WH8

https://aflow.org/p/ABC6D2_mC40_15_e_e_3f_f-001



Prototype	$CaFeO_6Si_2$
AFLOW prototype label	ABC6D2_mC40_15_e_e_3f_f-001
Mineral name	esseneite
ICSD	202160
Pearson symbol	mC40
Space group number	15
Space group symbol	$C2/c$
AFLOW prototype command	`aflow --proto=ABC6D2_mC40_15_e_e_3f_f-001 --params=`$a, b/a, c/a, \beta, y_1, y_2, x_3, y_3, z_3, x_4, y_4, z_4, x_5, y_5, z_5, x_6, y_6, z_6$

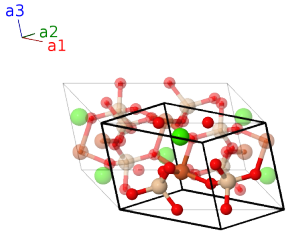
Other compounds with this structure

$CaFeSi_2O_6$ (hedenbergite), $CaMgSi_2O_6$ (diopside), $CaMnGe_2O_6$, $CaMnSi_2O_6$ (johannsenite), $CaMnSi_2O_6$ (johannsenite), $CaNiSi_2O_6$, $CaScSi_2O_6$ (davisite), $CaTiSi_2O_6$ (grossmanite), $CaVSi_2O_6$ (burnettite), $LiAlSi_2O_6$ (spodumene), $NaAlSi_2O_6$ (jadeite), $NaCrSi_2O_6$ (ureyite), $NaFeSi_2O_6$ (acmite/aegirine), $NaFeGe_2O_6$, $NaMnSi_2O_6$ (namansilite), $NaScSi_2O_6$ (jervisite)

- Named for University of Michigan geologist Eric Essene (1939-2010). (Cosca, 1987) gives the composition as $(Ca_{0.97}Fe_{0.03})(Fe_{0.58}Al_{0.42})(Si_{0.54}Al_{0.46})_2O_6$. We will use the majority atom at each site to draw the structure.
- Esseneite is one of the class of "clinopyroxene" materials, composition $XYSi_2O_6$, where in general X is an alkaline or alkaline earth metal and Y is a transition metal. In addition, the silicon may be partially or wholly replaced by another element. Clinopyroxenes are in the space group $C2/c$ #15, distinguishing them from orthopyroxenes, which are in space group *Pbca* #61 and the atoms X and Y are both small radius cations. Most of the structures listed are stable at room temperature and above.
- This structure has the same AFLOW label, ABC6D2_mC40_15_e_e_3f_f, as diopside ($CaMg(SiO_3)_2$, $S4_1$). The structures are generated by the same symmetry operations with different sets of parameters (`--params`) specified in their corresponding CIF files.

Base-centered Monoclinic primitive vectors

$$\begin{aligned}
\mathbf{a_1} &= \tfrac{1}{2}a\,\hat{\mathbf{x}} - \tfrac{1}{2}b\,\hat{\mathbf{y}} \\
\mathbf{a_2} &= \tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{1}{2}b\,\hat{\mathbf{y}} \\
\mathbf{a_3} &= c\cos\beta\,\hat{\mathbf{x}} + c\sin\beta\,\hat{\mathbf{z}}
\end{aligned}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$-y_1\,\mathbf{a}_1 + y_1\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$\frac{1}{4}c\cos\beta\,\hat{\mathbf{x}} + by_1\,\hat{\mathbf{y}} + \frac{1}{4}c\sin\beta\,\hat{\mathbf{z}}$	(4e)	Ca I
$\mathbf{B_2}$	=	$y_1\,\mathbf{a}_1 - y_1\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$\frac{3}{4}c\cos\beta\,\hat{\mathbf{x}} - by_1\,\hat{\mathbf{y}} + \frac{3}{4}c\sin\beta\,\hat{\mathbf{z}}$	(4e)	Ca I
$\mathbf{B_3}$	=	$-y_2\,\mathbf{a}_1 + y_2\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$\frac{1}{4}c\cos\beta\,\hat{\mathbf{x}} + by_2\,\hat{\mathbf{y}} + \frac{1}{4}c\sin\beta\,\hat{\mathbf{z}}$	(4e)	Fe I
$\mathbf{B_4}$	=	$y_2\,\mathbf{a}_1 - y_2\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$\frac{3}{4}c\cos\beta\,\hat{\mathbf{x}} - by_2\,\hat{\mathbf{y}} + \frac{3}{4}c\sin\beta\,\hat{\mathbf{z}}$	(4e)	Fe I
$\mathbf{B_5}$	=	$(x_3 - y_3)\,\mathbf{a}_1 + (x_3 + y_3)\,\mathbf{a}_2 + z_3\,\mathbf{a}_3$	=	$(ax_3 + cz_3\cos\beta)\,\hat{\mathbf{x}} + by_3\,\hat{\mathbf{y}} + cz_3\sin\beta\,\hat{\mathbf{z}}$	(8f)	O I
$\mathbf{B_6}$	=	$-(x_3 + y_3)\,\mathbf{a}_1 - (x_3 - y_3)\,\mathbf{a}_2 - \left(z_3 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-\left(ax_3 + c\left(z_3 - \frac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}} + by_3\,\hat{\mathbf{y}} - c\left(z_3 - \frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(8f)	O I
$\mathbf{B_7}$	=	$-(x_3 - y_3)\,\mathbf{a}_1 - (x_3 + y_3)\,\mathbf{a}_2 - z_3\,\mathbf{a}_3$	=	$-(ax_3 + cz_3\cos\beta)\,\hat{\mathbf{x}} - by_3\,\hat{\mathbf{y}} - cz_3\sin\beta\,\hat{\mathbf{z}}$	(8f)	O I
$\mathbf{B_8}$	=	$(x_3 + y_3)\,\mathbf{a}_1 + (x_3 - y_3)\,\mathbf{a}_2 + \left(z_3 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\left(ax_3 + c\left(z_3 + \frac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}} - by_3\,\hat{\mathbf{y}} + c\left(z_3 + \frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(8f)	O I
$\mathbf{B_9}$	=	$(x_4 - y_4)\,\mathbf{a}_1 + (x_4 + y_4)\,\mathbf{a}_2 + z_4\,\mathbf{a}_3$	=	$(ax_4 + cz_4\cos\beta)\,\hat{\mathbf{x}} + by_4\,\hat{\mathbf{y}} + cz_4\sin\beta\,\hat{\mathbf{z}}$	(8f)	O II
$\mathbf{B_{10}}$	=	$-(x_4 + y_4)\,\mathbf{a}_1 - (x_4 - y_4)\,\mathbf{a}_2 - \left(z_4 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-\left(ax_4 + c\left(z_4 - \frac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}} + by_4\,\hat{\mathbf{y}} - c\left(z_4 - \frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(8f)	O II
$\mathbf{B_{11}}$	=	$-(x_4 - y_4)\,\mathbf{a}_1 - (x_4 + y_4)\,\mathbf{a}_2 - z_4\,\mathbf{a}_3$	=	$-(ax_4 + cz_4\cos\beta)\,\hat{\mathbf{x}} - by_4\,\hat{\mathbf{y}} - cz_4\sin\beta\,\hat{\mathbf{z}}$	(8f)	O II
$\mathbf{B_{12}}$	=	$(x_4 + y_4)\,\mathbf{a}_1 + (x_4 - y_4)\,\mathbf{a}_2 + \left(z_4 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\left(ax_4 + c\left(z_4 + \frac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}} - by_4\,\hat{\mathbf{y}} + c\left(z_4 + \frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(8f)	O II
$\mathbf{B_{13}}$	=	$(x_5 - y_5)\,\mathbf{a}_1 + (x_5 + y_5)\,\mathbf{a}_2 + z_5\,\mathbf{a}_3$	=	$(ax_5 + cz_5\cos\beta)\,\hat{\mathbf{x}} + by_5\,\hat{\mathbf{y}} + cz_5\sin\beta\,\hat{\mathbf{z}}$	(8f)	O III
$\mathbf{B_{14}}$	=	$-(x_5 + y_5)\,\mathbf{a}_1 - (x_5 - y_5)\,\mathbf{a}_2 - \left(z_5 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-\left(ax_5 + c\left(z_5 - \frac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}} + by_5\,\hat{\mathbf{y}} - c\left(z_5 - \frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(8f)	O III

$$\mathbf{B_{15}} = -(x_5 - y_5)\,\mathbf{a}_1 - (x_5 + y_5)\,\mathbf{a}_2 - z_5\,\mathbf{a}_3 = -(ax_5 + cz_5\cos\beta)\,\hat{\mathbf{x}} - by_5\,\hat{\mathbf{y}} - cz_5\sin\beta\,\hat{\mathbf{z}} \quad (8f) \quad \text{O III}$$

$$\mathbf{B_{16}} = (x_5 + y_5)\,\mathbf{a}_1 + (x_5 - y_5)\,\mathbf{a}_2 + \left(z_5 + \tfrac{1}{2}\right)\mathbf{a}_3 = \left(ax_5 + c\left(z_5 + \tfrac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}} - by_5\,\hat{\mathbf{y}} + c\left(z_5 + \tfrac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}} \quad (8f) \quad \text{O III}$$

$$\mathbf{B_{17}} = (x_6 - y_6)\,\mathbf{a}_1 + (x_6 + y_6)\,\mathbf{a}_2 + z_6\,\mathbf{a}_3 = (ax_6 + cz_6\cos\beta)\,\hat{\mathbf{x}} + by_6\,\hat{\mathbf{y}} + cz_6\sin\beta\,\hat{\mathbf{z}} \quad (8f) \quad \text{Si I}$$

$$\mathbf{B_{18}} = -(x_6 + y_6)\,\mathbf{a}_1 - (x_6 - y_6)\,\mathbf{a}_2 - \left(z_6 - \tfrac{1}{2}\right)\mathbf{a}_3 = -\left(ax_6 + c\left(z_6 - \tfrac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}} + by_6\,\hat{\mathbf{y}} - c\left(z_6 - \tfrac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}} \quad (8f) \quad \text{Si I}$$

$$\mathbf{B_{19}} = -(x_6 - y_6)\,\mathbf{a}_1 - (x_6 + y_6)\,\mathbf{a}_2 - z_6\,\mathbf{a}_3 = -(ax_6 + cz_6\cos\beta)\,\hat{\mathbf{x}} - by_6\,\hat{\mathbf{y}} - cz_6\sin\beta\,\hat{\mathbf{z}} \quad (8f) \quad \text{Si I}$$

$$\mathbf{B_{20}} = (x_6 + y_6)\,\mathbf{a}_1 + (x_6 - y_6)\,\mathbf{a}_2 + \left(z_6 + \tfrac{1}{2}\right)\mathbf{a}_3 = \left(ax_6 + c\left(z_6 + \tfrac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}} - by_6\,\hat{\mathbf{y}} + c\left(z_6 + \tfrac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}} \quad (8f) \quad \text{Si I}$$

References

[1] M. A. Cosca and D. R. Peacor, *Chemistry and structure of esseneite ($CaFe^{3+}AlSiO_6$), a new pyroxene produced by pyrometamorphism*, Am. Mineral. **72**, 148–156 (1987).