Monoclinic (I) Li_2FeSiO_4 Structure: AB2C4D_mP32_4_2a_4a_8a_2a-001

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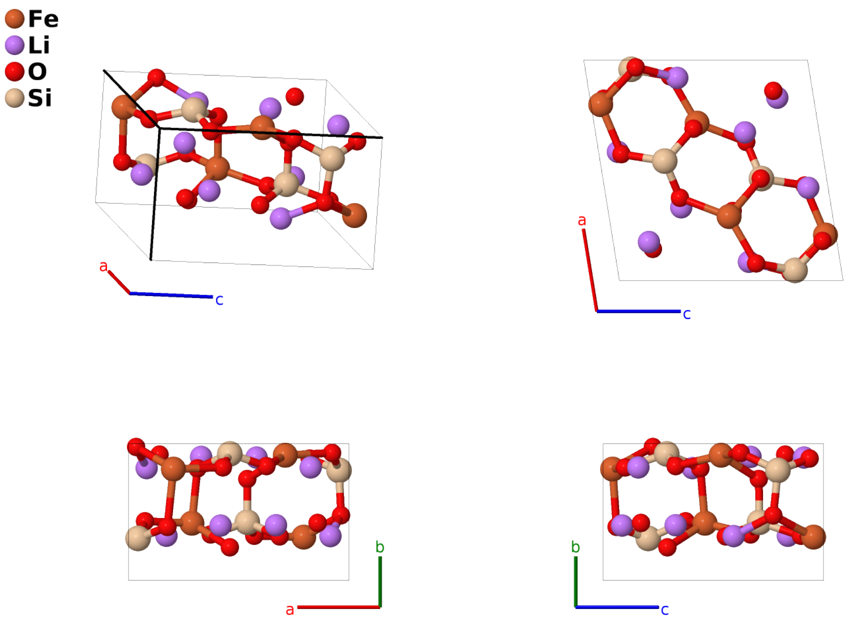
https://aflow.org/p/TK4X

https://aflow.org/p/AB2C4D_mP32_4_2a_4a_8a_2a-001



Prototype $FeLi_2O_4Si$

AFLOW prototype label AB2C4D_mP32_4_2a_4a_8a_2a-001

ICSD 246132

Pearson symbol mP32

Space group number 4

Space group symbol $P2_1$

AFLOW prototype command `aflow --proto=AB2C4D_mP32_4_2a_4a_8a_2a-001`
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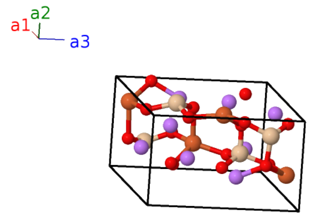
- This is the monoclinic structure of (Nishimura, 2008). (Masese, 2015) find an alternative structure in space group $P2_1/c$ #14, a structure that was explicitly rejected by (Nishimura, 2008).
- Li_2FeSiO_4 is also known to exist in the orthorhombic β-Li_3PO_4 and Li_2CdSiO_4 structures. (Boulineau, 2010).

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
$\mathbf{B_1}$	=	$x_1\,\mathbf{a}_1 + y_1\,\mathbf{a}_2 + z_1\,\mathbf{a}_3$	=	$\left(ax_1 + cz_1\cos\beta\right)\,\hat{\mathbf{x}} + by_1\,\hat{\mathbf{y}} + cz_1\sin\beta\,\hat{\mathbf{z}}$	(2a)	Fe I
$\mathbf{B_2}$	=	$-x_1\,\mathbf{a}_1 + \left(y_1 + \frac{1}{2}\right)\,\mathbf{a}_2 - z_1\,\mathbf{a}_3$	=	$-\left(ax_1 + cz_1\cos\beta\right)\,\hat{\mathbf{x}} + b\left(y_1 + \frac{1}{2}\right)\,\hat{\mathbf{y}} - cz_1\sin\beta\,\hat{\mathbf{z}}$	(2a)	Fe I
$\mathbf{B_3}$	=	$x_2\,\mathbf{a}_1 + y_2\,\mathbf{a}_2 + z_2\,\mathbf{a}_3$	=	$\left(ax_2 + cz_2\cos\beta\right)\,\hat{\mathbf{x}} + by_2\,\hat{\mathbf{y}} + cz_2\sin\beta\,\hat{\mathbf{z}}$	(2a)	Fe II
$\mathbf{B_4}$	=	$-x_2\,\mathbf{a}_1 + \left(y_2 + \frac{1}{2}\right)\,\mathbf{a}_2 - z_2\,\mathbf{a}_3$	=	$-\left(ax_2 + cz_2\cos\beta\right)\,\hat{\mathbf{x}} + b\left(y_2 + \frac{1}{2}\right)\,\hat{\mathbf{y}} - cz_2\sin\beta\,\hat{\mathbf{z}}$	(2a)	Fe II
$\mathbf{B_5}$	=	$x_3\,\mathbf{a}_1 + y_3\,\mathbf{a}_2 + z_3\,\mathbf{a}_3$	=	$\left(ax_3 + cz_3\cos\beta\right)\,\hat{\mathbf{x}} + by_3\,\hat{\mathbf{y}} + cz_3\sin\beta\,\hat{\mathbf{z}}$	(2a)	Li I
$\mathbf{B_6}$	=	$-x_3\,\mathbf{a}_1 + \left(y_3 + \frac{1}{2}\right)\,\mathbf{a}_2 - z_3\,\mathbf{a}_3$	=	$-\left(ax_3 + cz_3\cos\beta\right)\,\hat{\mathbf{x}} + b\left(y_3 + \frac{1}{2}\right)\,\hat{\mathbf{y}} - cz_3\sin\beta\,\hat{\mathbf{z}}$	(2a)	Li I
$\mathbf{B_7}$	=	$x_4\,\mathbf{a}_1 + y_4\,\mathbf{a}_2 + z_4\,\mathbf{a}_3$	=	$\left(ax_4 + cz_4\cos\beta\right)\,\hat{\mathbf{x}} + by_4\,\hat{\mathbf{y}} + cz_4\sin\beta\,\hat{\mathbf{z}}$	(2a)	Li II
$\mathbf{B_8}$	=	$-x_4\,\mathbf{a}_1 + \left(y_4 + \frac{1}{2}\right)\,\mathbf{a}_2 - z_4\,\mathbf{a}_3$	=	$-\left(ax_4 + cz_4\cos\beta\right)\,\hat{\mathbf{x}} + b\left(y_4 + \frac{1}{2}\right)\,\hat{\mathbf{y}} - cz_4\sin\beta\,\hat{\mathbf{z}}$	(2a)	Li II
$\mathbf{B_9}$	=	$x_5\,\mathbf{a}_1 + y_5\,\mathbf{a}_2 + z_5\,\mathbf{a}_3$	=	$\left(ax_5 + cz_5\cos\beta\right)\,\hat{\mathbf{x}} + by_5\,\hat{\mathbf{y}} + cz_5\sin\beta\,\hat{\mathbf{z}}$	(2a)	Li III
$\mathbf{B_{10}}$	=	$-x_5\,\mathbf{a}_1 + \left(y_5 + \frac{1}{2}\right)\,\mathbf{a}_2 - z_5\,\mathbf{a}_3$	=	$-\left(ax_5 + cz_5\cos\beta\right)\,\hat{\mathbf{x}} + b\left(y_5 + \frac{1}{2}\right)\,\hat{\mathbf{y}} - cz_5\sin\beta\,\hat{\mathbf{z}}$	(2a)	Li III
$\mathbf{B_{11}}$	=	$x_6\,\mathbf{a}_1 + y_6\,\mathbf{a}_2 + z_6\,\mathbf{a}_3$	=	$\left(ax_6 + cz_6\cos\beta\right)\,\hat{\mathbf{x}} + by_6\,\hat{\mathbf{y}} + cz_6\sin\beta\,\hat{\mathbf{z}}$	(2a)	Li IV
$\mathbf{B_{12}}$	=	$-x_6\,\mathbf{a}_1 + \left(y_6 + \frac{1}{2}\right)\,\mathbf{a}_2 - z_6\,\mathbf{a}_3$	=	$-\left(ax_6 + cz_6\cos\beta\right)\,\hat{\mathbf{x}} + b\left(y_6 + \frac{1}{2}\right)\,\hat{\mathbf{y}} - cz_6\sin\beta\,\hat{\mathbf{z}}$	(2a)	Li IV
$\mathbf{B_{13}}$	=	$x_7\,\mathbf{a}_1 + y_7\,\mathbf{a}_2 + z_7\,\mathbf{a}_3$	=	$\left(ax_7 + cz_7\cos\beta\right)\,\hat{\mathbf{x}} + by_7\,\hat{\mathbf{y}} + cz_7\sin\beta\,\hat{\mathbf{z}}$	(2a)	O I
$\mathbf{B_{14}}$	=	$-x_7\,\mathbf{a}_1 + \left(y_7 + \frac{1}{2}\right)\,\mathbf{a}_2 - z_7\,\mathbf{a}_3$	=	$-\left(ax_7 + cz_7\cos\beta\right)\,\hat{\mathbf{x}} + b\left(y_7 + \frac{1}{2}\right)\,\hat{\mathbf{y}} - cz_7\sin\beta\,\hat{\mathbf{z}}$	(2a)	O I
$\mathbf{B_{15}}$	=	$x_8\,\mathbf{a}_1 + y_8\,\mathbf{a}_2 + z_8\,\mathbf{a}_3$	=	$\left(ax_8 + cz_8\cos\beta\right)\,\hat{\mathbf{x}} + by_8\,\hat{\mathbf{y}} + cz_8\sin\beta\,\hat{\mathbf{z}}$	(2a)	O II
$\mathbf{B_{16}}$	=	$-x_8\,\mathbf{a}_1 + \left(y_8 + \frac{1}{2}\right)\,\mathbf{a}_2 - z_8\,\mathbf{a}_3$	=	$-\left(ax_8 + cz_8\cos\beta\right)\,\hat{\mathbf{x}} + b\left(y_8 + \frac{1}{2}\right)\,\hat{\mathbf{y}} - cz_8\sin\beta\,\hat{\mathbf{z}}$	(2a)	O II
$\mathbf{B_{17}}$	=	$x_9\,\mathbf{a}_1 + y_9\,\mathbf{a}_2 + z_9\,\mathbf{a}_3$	=	$\left(ax_9 + cz_9\cos\beta\right)\,\hat{\mathbf{x}} + by_9\,\hat{\mathbf{y}} + cz_9\sin\beta\,\hat{\mathbf{z}}$	(2a)	O III
$\mathbf{B_{18}}$	=	$-x_9\,\mathbf{a}_1 + \left(y_9 + \frac{1}{2}\right)\,\mathbf{a}_2 - z_9\,\mathbf{a}_3$	=	$-\left(ax_9 + cz_9\cos\beta\right)\,\hat{\mathbf{x}} + b\left(y_9 + \frac{1}{2}\right)\,\hat{\mathbf{y}} - cz_9\sin\beta\,\hat{\mathbf{z}}$	(2a)	O III
$\mathbf{B_{19}}$	=	$x_{10}\,\mathbf{a}_1 + y_{10}\,\mathbf{a}_2 + z_{10}\,\mathbf{a}_3$	=	$\left(ax_{10} + cz_{10}\cos\beta\right)\,\hat{\mathbf{x}} + by_{10}\,\hat{\mathbf{y}} + cz_{10}\sin\beta\,\hat{\mathbf{z}}$	(2a)	O IV
$\mathbf{B_{20}}$	=	$-x_{10}\,\mathbf{a}_1 + \left(y_{10} + \frac{1}{2}\right)\,\mathbf{a}_2 - z_{10}\,\mathbf{a}_3$	=	$-\left(ax_{10} + cz_{10}\cos\beta\right)\,\hat{\mathbf{x}} + b\left(y_{10} + \frac{1}{2}\right)\,\hat{\mathbf{y}} - cz_{10}\sin\beta\,\hat{\mathbf{z}}$	(2a)	O IV
$\mathbf{B_{21}}$	=	$x_{11}\,\mathbf{a}_1 + y_{11}\,\mathbf{a}_2 + z_{11}\,\mathbf{a}_3$	=	$\left(ax_{11} + cz_{11}\cos\beta\right)\,\hat{\mathbf{x}} + by_{11}\,\hat{\mathbf{y}} + cz_{11}\sin\beta\,\hat{\mathbf{z}}$	(2a)	O V

$\mathbf{B_{22}}$	=	$-x_{11}\,\mathbf{a}_1 + \left(y_{11} + \frac{1}{2}\right)\,\mathbf{a}_2 - z_{11}\,\mathbf{a}_3$	=	$-\left(ax_{11} + cz_{11}\cos\beta\right)\,\hat{\mathbf{x}} + b\left(y_{11} + \frac{1}{2}\right)\,\hat{\mathbf{y}} - cz_{11}\sin\beta\,\hat{\mathbf{z}}$	(2a)	O V
$\mathbf{B_{23}}$	=	$x_{12}\,\mathbf{a}_1 + y_{12}\,\mathbf{a}_2 + z_{12}\,\mathbf{a}_3$	=	$\left(ax_{12} + cz_{12}\cos\beta\right)\,\hat{\mathbf{x}} + by_{12}\,\hat{\mathbf{y}} + cz_{12}\sin\beta\,\hat{\mathbf{z}}$	(2a)	O VI
$\mathbf{B_{24}}$	=	$-x_{12}\,\mathbf{a}_1 + \left(y_{12} + \frac{1}{2}\right)\,\mathbf{a}_2 - z_{12}\,\mathbf{a}_3$	=	$-\left(ax_{12} + cz_{12}\cos\beta\right)\,\hat{\mathbf{x}} + b\left(y_{12} + \frac{1}{2}\right)\,\hat{\mathbf{y}} - cz_{12}\sin\beta\,\hat{\mathbf{z}}$	(2a)	O VI
$\mathbf{B_{25}}$	=	$x_{13}\,\mathbf{a}_1 + y_{13}\,\mathbf{a}_2 + z_{13}\,\mathbf{a}_3$	=	$\left(ax_{13} + cz_{13}\cos\beta\right)\,\hat{\mathbf{x}} + by_{13}\,\hat{\mathbf{y}} + cz_{13}\sin\beta\,\hat{\mathbf{z}}$	(2a)	O VII
$\mathbf{B_{26}}$	=	$-x_{13}\,\mathbf{a}_1 + \left(y_{13} + \frac{1}{2}\right)\,\mathbf{a}_2 - z_{13}\,\mathbf{a}_3$	=	$-\left(ax_{13} + cz_{13}\cos\beta\right)\,\hat{\mathbf{x}} + b\left(y_{13} + \frac{1}{2}\right)\,\hat{\mathbf{y}} - cz_{13}\sin\beta\,\hat{\mathbf{z}}$	(2a)	O VII
$\mathbf{B_{27}}$	=	$x_{14}\,\mathbf{a}_1 + y_{14}\,\mathbf{a}_2 + z_{14}\,\mathbf{a}_3$	=	$\left(ax_{14} + cz_{14}\cos\beta\right)\,\hat{\mathbf{x}} + by_{14}\,\hat{\mathbf{y}} + cz_{14}\sin\beta\,\hat{\mathbf{z}}$	(2a)	O VIII
$\mathbf{B_{28}}$	=	$-x_{14}\,\mathbf{a}_1 + \left(y_{14} + \frac{1}{2}\right)\,\mathbf{a}_2 - z_{14}\,\mathbf{a}_3$	=	$-\left(ax_{14} + cz_{14}\cos\beta\right)\,\hat{\mathbf{x}} + b\left(y_{14} + \frac{1}{2}\right)\,\hat{\mathbf{y}} - cz_{14}\sin\beta\,\hat{\mathbf{z}}$	(2a)	O VIII
$\mathbf{B_{29}}$	=	$x_{15}\,\mathbf{a}_1 + y_{15}\,\mathbf{a}_2 + z_{15}\,\mathbf{a}_3$	=	$\left(ax_{15} + cz_{15}\cos\beta\right)\,\hat{\mathbf{x}} + by_{15}\,\hat{\mathbf{y}} + cz_{15}\sin\beta\,\hat{\mathbf{z}}$	(2a)	Si I
$\mathbf{B_{30}}$	=	$-x_{15}\,\mathbf{a}_1 + \left(y_{15} + \frac{1}{2}\right)\,\mathbf{a}_2 - z_{15}\,\mathbf{a}_3$	=	$-\left(ax_{15} + cz_{15}\cos\beta\right)\,\hat{\mathbf{x}} + b\left(y_{15} + \frac{1}{2}\right)\,\hat{\mathbf{y}} - cz_{15}\sin\beta\,\hat{\mathbf{z}}$	(2a)	Si I
$\mathbf{B_{31}}$	=	$x_{16}\,\mathbf{a}_1 + y_{16}\,\mathbf{a}_2 + z_{16}\,\mathbf{a}_3$	=	$\left(ax_{16} + cz_{16}\cos\beta\right)\,\hat{\mathbf{x}} + by_{16}\,\hat{\mathbf{y}} + cz_{16}\sin\beta\,\hat{\mathbf{z}}$	(2a)	Si II
$\mathbf{B_{32}}$	=	$-x_{16}\,\mathbf{a}_1 + \left(y_{16} + \frac{1}{2}\right)\,\mathbf{a}_2 - z_{16}\,\mathbf{a}_3$	=	$-\left(ax_{16} + cz_{16}\cos\beta\right)\,\hat{\mathbf{x}} + b\left(y_{16} + \frac{1}{2}\right)\,\hat{\mathbf{y}} - cz_{16}\sin\beta\,\hat{\mathbf{z}}$	(2a)	Si II

References

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