

β' -LiFeO₂ Structure:

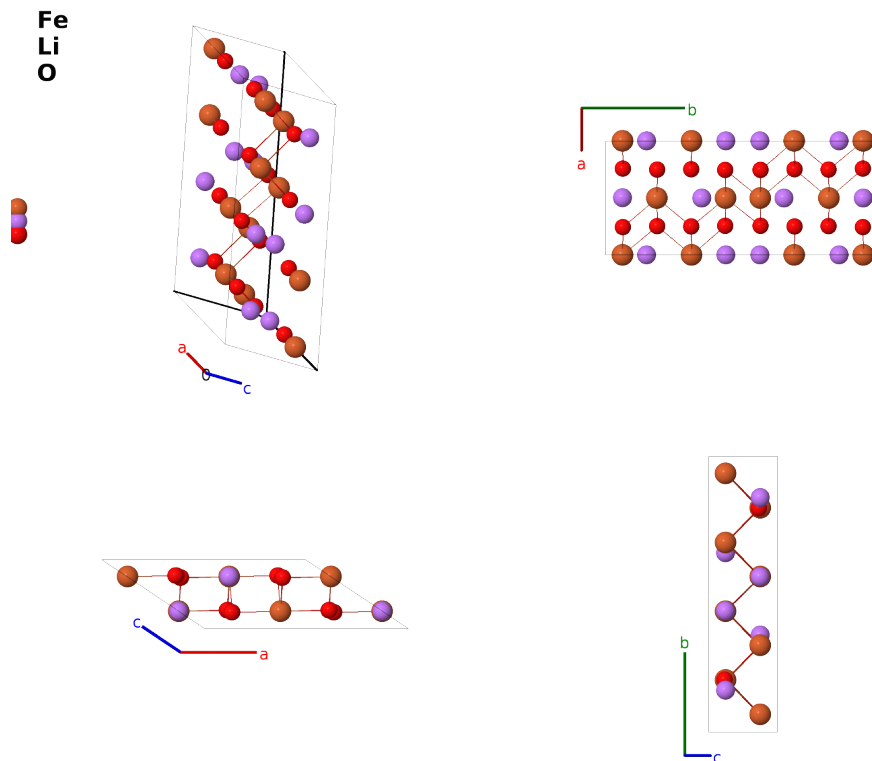
ABC2_mC32_15_2e_2e_2f-002

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<https://aflow.org/prototype-encyclopedia/VG40>

https://aflow.org/prototype-encyclopedia/ABC2_mC32_15_2e_2e_2f-002



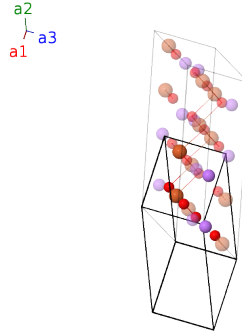
Prototype	FeLiO ₂
AFLOW prototype label	ABC2_mC32_15_2e_2e_2f-002
ICSD	174084
CCDC	1688976
Pearson symbol	mC32
Space group number	15
Space group symbol	$C2/c$
AFLOW prototype command	<pre>aflow --proto=ABC2_mC32_15_2e_2e_2f-002 --params=a,b/a,c/a,β,y₁,y₂,y₃,y₄,x₅,y₅,z₅,x₆,y₆,z₆</pre>

Other compounds with this structure

ErLiO₂, ErNaO₂

- FeLiO₂ exhibits a wide variety of structures, with the exact structure present depends on thermodynamic effects, preparation methods, and charge/discharge history.
- We follow the nomenclature of (Kanno, 1996), where appropriate, with modifications found in (Tabuchi, 1995) and (Abdel-Ghany, 2012). The following list of structures is no doubt incomplete:
 - α -LiFeO₂ is in the cubic rock salt (*B1*) structure, with lithium and iron randomly placed on the sodium site and oxygen on the chlorine site. It is synthesized at temperatures above 600°C.
 - β -LiFeO₂ is a tetragonal distortion of α -LiFeO₂ with the lithium and iron atoms still randomly placed on their sublattice.
 - β' -LiFeO₂ (this structure) is monoclinic and transforms to γ -LiFeO₂ near room temperature. This is likely the phase (Kanno, 1996) refers to as β -LiFeO₂.
 - γ -LiFeO₂ is created by low-temperature synthesis below 500°C and can be considered as an ordered version of α -LiFeO₂, with a doubled unit cell.
 - o-LiFeO₂ is orthorhombic, produced by an ion exchange interaction. It is (meta)-stable below 400°C, transforming to α -LiFeO₂ above 600°C.
- As with α - and β -LiFeO₂, so of the iron and lithium atoms in β' -LiFeO₂ are partially disordered. The Fe-I site is 56% iron and 46% lithium, while the Li-I site is 46% iron and 54% lithium. The Fe-II and Li-II sites are fully ordered.
- Some other sources use ErNaO₂ as the prototype. We choose β' -LiFeO₂ to highlight the connection with the other LiFeO₂ structures.

Base-centered Monoclinic primitive vectors

$$\begin{aligned}
 \mathbf{a}_1 &= \frac{1}{2}a \hat{\mathbf{x}} - \frac{1}{2}b \hat{\mathbf{y}} \\
 \mathbf{a}_2 &= \frac{1}{2}a \hat{\mathbf{x}} + \frac{1}{2}b \hat{\mathbf{y}} \\
 \mathbf{a}_3 &= c \cos \beta \hat{\mathbf{x}} + c \sin \beta \hat{\mathbf{z}}
 \end{aligned}$$


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)	Fe 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)	Fe 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 II
$\mathbf{B}_4$	$= y_2 \mathbf{a}_1 - y_2 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$\frac{3}{4}c \cos \beta \hat{\mathbf{x}} - by_2 \hat{\mathbf{y}} + \frac{3}{4}c \sin \beta \hat{\mathbf{z}}$	(4e)	Fe II
$\mathbf{B}_5$	$= -y_3 \mathbf{a}_1 + y_3 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$\frac{1}{4}c \cos \beta \hat{\mathbf{x}} + by_3 \hat{\mathbf{y}} + \frac{1}{4}c \sin \beta \hat{\mathbf{z}}$	(4e)	Li I
$\mathbf{B}_6$	$= y_3 \mathbf{a}_1 - y_3 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$\frac{3}{4}c \cos \beta \hat{\mathbf{x}} - by_3 \hat{\mathbf{y}} + \frac{3}{4}c \sin \beta \hat{\mathbf{z}}$	(4e)	Li I
$\mathbf{B}_7$	$= -y_4 \mathbf{a}_1 + y_4 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$\frac{1}{4}c \cos \beta \hat{\mathbf{x}} + by_4 \hat{\mathbf{y}} + \frac{1}{4}c \sin \beta \hat{\mathbf{z}}$	(4e)	Li II
$\mathbf{B}_8$	$= y_4 \mathbf{a}_1 - y_4 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$\frac{3}{4}c \cos \beta \hat{\mathbf{x}} - by_4 \hat{\mathbf{y}} + \frac{3}{4}c \sin \beta \hat{\mathbf{z}}$	(4e)	Li II
$\mathbf{B}_9$	$= (x_5 - y_5) \mathbf{a}_1 + (x_5 + y_5) \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$(ax_5 + cz_5 \cos \beta) \hat{\mathbf{x}} + by_5 \hat{\mathbf{y}} + cz_5 \sin \beta \hat{\mathbf{z}}$	(8f)	O I
$\mathbf{B}_{10}$	$= -(x_5 + y_5) \mathbf{a}_1 - (x_5 - y_5) \mathbf{a}_2 - (z_5 - \frac{1}{2}) \mathbf{a}_3$	$=$	$-(ax_5 + c(z_5 - \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} + by_5 \hat{\mathbf{y}} - c(z_5 - \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$	(8f)	O I

$$\begin{aligned}
\mathbf{B}_{11} &= \begin{matrix} -(x_5 - y_5) \mathbf{a}_1 - (x_5 + y_5) \mathbf{a}_2 - \\ z_5 \mathbf{a}_3 \end{matrix} = -(ax_5 + cz_5 \cos \beta) \hat{\mathbf{x}} - by_5 \hat{\mathbf{y}} - cz_5 \sin \beta \hat{\mathbf{z}} & (8f) & \text{O I} \\
\mathbf{B}_{12} &= \begin{matrix} (x_5 + y_5) \mathbf{a}_1 + (x_5 - y_5) \mathbf{a}_2 + \\ (z_5 + \frac{1}{2}) \mathbf{a}_3 \end{matrix} = \begin{matrix} (ax_5 + c(z_5 + \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} - by_5 \hat{\mathbf{y}} + \\ c(z_5 + \frac{1}{2}) \sin \beta \hat{\mathbf{z}} \end{matrix} & (8f) & \text{O I} \\
\mathbf{B}_{13} &= \begin{matrix} (x_6 - y_6) \mathbf{a}_1 + (x_6 + y_6) \mathbf{a}_2 + \\ z_6 \mathbf{a}_3 \end{matrix} = (ax_6 + cz_6 \cos \beta) \hat{\mathbf{x}} + by_6 \hat{\mathbf{y}} + cz_6 \sin \beta \hat{\mathbf{z}} & (8f) & \text{O II} \\
\mathbf{B}_{14} &= \begin{matrix} -(x_6 + y_6) \mathbf{a}_1 - (x_6 - y_6) \mathbf{a}_2 - \\ (z_6 - \frac{1}{2}) \mathbf{a}_3 \end{matrix} = \begin{matrix} -(ax_6 + c(z_6 - \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} + by_6 \hat{\mathbf{y}} - \\ c(z_6 - \frac{1}{2}) \sin \beta \hat{\mathbf{z}} \end{matrix} & (8f) & \text{O II} \\
\mathbf{B}_{15} &= \begin{matrix} -(x_6 - y_6) \mathbf{a}_1 - (x_6 + y_6) \mathbf{a}_2 - \\ z_6 \mathbf{a}_3 \end{matrix} = -(ax_6 + cz_6 \cos \beta) \hat{\mathbf{x}} - by_6 \hat{\mathbf{y}} - cz_6 \sin \beta \hat{\mathbf{z}} & (8f) & \text{O II} \\
\mathbf{B}_{16} &= \begin{matrix} (x_6 + y_6) \mathbf{a}_1 + (x_6 - y_6) \mathbf{a}_2 + \\ (z_6 + \frac{1}{2}) \mathbf{a}_3 \end{matrix} = \begin{matrix} (ax_6 + c(z_6 + \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} - by_6 \hat{\mathbf{y}} + \\ c(z_6 + \frac{1}{2}) \sin \beta \hat{\mathbf{z}} \end{matrix} & (8f) & \text{O II}
\end{aligned}$$

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