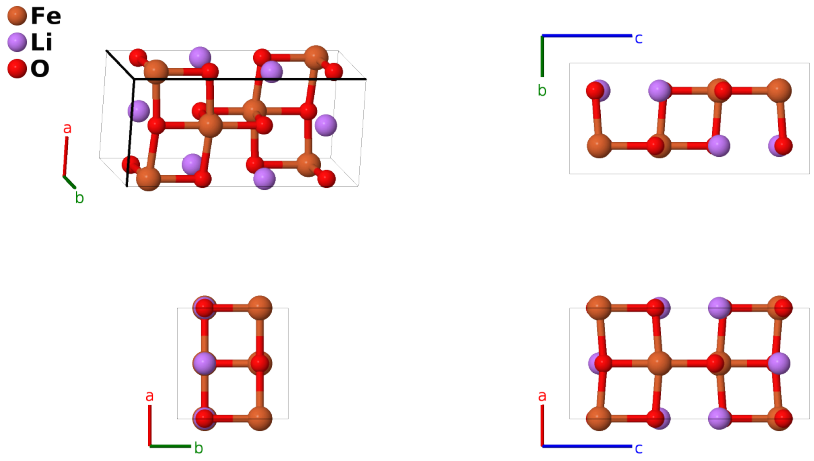
# $\gamma$-$LiFeO_2$ Structure: ABC2_tI16_141_a_b_e-003

Cite this page as: H. Eckert, S. Divilov, A. Zettel, M. J. Mehl, D. Hicks, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 4*. In preparation.

https://aflow.org/p/XJE5

https://aflow.org/p/ABC2_tI16_141_a_b_e-003




| | |
|---|---|
| **Prototype** | $FeLiO_2$ |
| **AFLOW prototype label** | ABC2_tI16_141_a_b_e-003 |
| **ICSD** | 174085 |
| **Pearson symbol** | tI16 |
| **Space group number** | 141 |
| **Space group symbol** | $I4_1/amd$ |
| **AFLOW prototype command** | `aflow --proto=ABC2_tI16_141_a_b_e-003 --params=`$a, c/a, z_3$ |

**Other compounds with this structure**
$ErLiO_2$, $\delta$-$LiAlO_2$, $NaGdO_2$, $NdNaO_2$, $InLiO_2$

- $FeLiO_2$ 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:
  - $\alpha$-$LiFeO_2$ 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.
  - $\beta$-$LiFeO_2$ is a tetragonal distortion of $\alpha$-$LiFeO_2$ with the lithium and iron atoms still randomly placed on their sublattice (we denote this site as Fe).
  - $\beta'$-$LiFeO_2$ is monoclinic and transforms to $\gamma$-$LiFeO_2$ near room temperature. This is likely the phase (Kanno, 1996) refers to as $\beta$-$LiFeO_2$.

  - $\gamma$-$LiFeO_2$ (this structure) is created by low-temperature synthesis below 500°C and can be considered as an ordered version of $\alpha$-$LiFeO_2$, with a doubled unit cell.
  - o-$LiFeO_2$ is orthorhombic, produced by an ion exchange interaction. It is (meta)-stable below 400°C, transforming to $\alpha$-$LiFeO_2$ above 600°C.

- For $\gamma$-$FeLiO_2$ we use the data taken by (Barré, 2009) at 25°.

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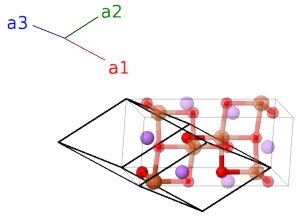
**Body-centered Tetragonal primitive vectors**

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

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**Basis vectors**

| | | Lattice coordinates | | Cartesian coordinates | Wyckoff position | Atom type |
|---|---|---|---|---|---|---|
| $\mathbf{B_1}$ | = | $\frac{7}{8}\,\mathbf{a}_1 + \frac{1}{8}\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$ | = | $\frac{3}{4}a\,\hat{\mathbf{y}} + \frac{1}{8}c\,\hat{\mathbf{z}}$ | (4a) | Fe I |
| $\mathbf{B_2}$ | = | $\frac{1}{8}\,\mathbf{a}_1 + \frac{7}{8}\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$ | = | $\frac{1}{2}a\,\hat{\mathbf{x}} - \frac{1}{4}a\,\hat{\mathbf{y}} + \frac{3}{8}c\,\hat{\mathbf{z}}$ | (4a) | Fe I |
| $\mathbf{B_3}$ | = | $\frac{5}{8}\,\mathbf{a}_1 + \frac{3}{8}\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$ | = | $\frac{1}{4}a\,\hat{\mathbf{y}} + \frac{3}{8}c\,\hat{\mathbf{z}}$ | (4b) | Li I |
| $\mathbf{B_4}$ | = | $\frac{3}{8}\,\mathbf{a}_1 + \frac{5}{8}\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$ | = | $\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{4}a\,\hat{\mathbf{y}} + \frac{1}{8}c\,\hat{\mathbf{z}}$ | (4b) | Li I |
| $\mathbf{B_5}$ | = | $\left(z_3 + \frac{1}{4}\right)\,\mathbf{a}_1 + z_3\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$ | = | $\frac{1}{4}a\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$ | (8e) | O I |
| $\mathbf{B_6}$ | = | $z_3\,\mathbf{a}_1 + \left(z_3 + \frac{1}{4}\right)\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$ | = | $\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{4}a\,\hat{\mathbf{y}} + c\left(z_3 - \frac{1}{4}\right)\,\hat{\mathbf{z}}$ | (8e) | O I |
| $\mathbf{B_7}$ | = | $-\left(z_3 - \frac{3}{4}\right)\,\mathbf{a}_1 - z_3\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$ | = | $\frac{3}{4}a\,\hat{\mathbf{y}} - cz_3\,\hat{\mathbf{z}}$ | (8e) | O I |
| $\mathbf{B_8}$ | = | $-z_3\,\mathbf{a}_1 - \left(z_3 - \frac{3}{4}\right)\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$ | = | $\frac{1}{2}a\,\hat{\mathbf{x}} - \frac{1}{4}a\,\hat{\mathbf{y}} - c\left(z_3 - \frac{1}{4}\right)\,\hat{\mathbf{z}}$ | (8e) | O I |

**References**


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[3] M. Tabuchi, K. Ado, H. Sakaebe, C. Masquelier, H. Kageyama, and O. Nakamura, *Preparation of $AFeO_2$ (A = Li, Na) by hydrothermal method*, Solid State Ionics **79**, 220–226 (1995), doi:10.1016/0167-2738(95)00065-E.

[4] A. E. Abdel-Ghany, A. Mauger, H. Groult, K. Zaghib, and C. M. Julien, *Structural properties and electrochemistry of α-$LiFeO_2$*, J. Power Sources **197**, 285–291 (2012), doi:10.1016/j.jpowsour.2011.09.054.