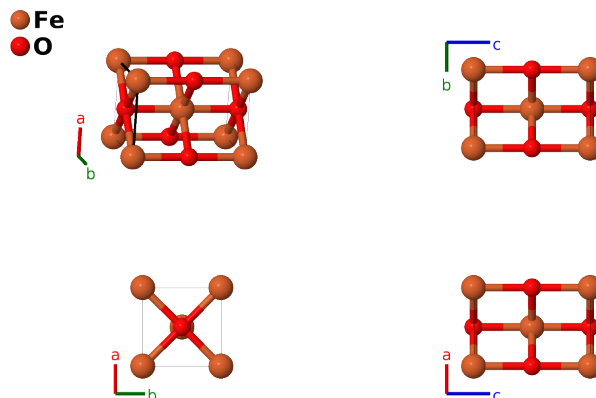


# $\beta$ -LiFeO<sub>2</sub> Structure: AB\_tI4\_139\_a\_b-003

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/G0K3>

[https://aflow.org/p/AB\\_tI4\\_139\\_a\\_b-003](https://aflow.org/p/AB_tI4_139_a_b-003)



<b>Prototype</b>	FeLiO <sub>2</sub>
<b>AFLOW prototype label</b>	AB_tI4_139_a_b-003
<b>ICSD</b>	28366
<b>Pearson symbol</b>	tI4
<b>Space group number</b>	139
<b>Space group symbol</b>	<i>I4/mmm</i>
<b>AFLOW prototype command</b>	<code>aflow --proto=AB_tI4_139_a_b-003 --params=a, c/a</code>

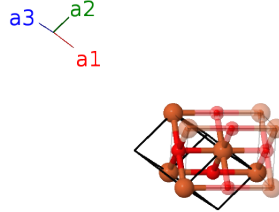
- FeLiO<sub>2</sub> exhibits a wide variety of structures, with the exact structure present depends on thermodynamic effects, preparation methods, and charge/discharge history.
- We follow the nomenclature of (Kanno, 1996), where appropriate, with modifications found in (Tabuchi, 1995) and (Abdel-Ghany, 2012). The following list of structures is no doubt incomplete:
  - $\alpha$ -LiFeO<sub>2</sub> 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<sub>2</sub> (this structure) is a tetragonal distortion of  $\alpha$ -LiFeO<sub>2</sub> with the lithium and iron atoms still randomly placed on their sublattice (we denote this site as Fe).
  - $\beta'$ -LiFeO<sub>2</sub> is monoclinic and transforms to  $\gamma$ -LiFeO<sub>2</sub> near room temperature. This is likely the phase (Kanno, 1996) refers to as  $\beta$ -LiFeO<sub>2</sub>.
  - $\gamma$ -LiFeO<sub>2</sub> is created by low-temperature synthesis below 500°C and can be considered as an ordered version of  $\alpha$ -LiFeO<sub>2</sub>, with a doubled unit cell.
  - $\delta$ -LiFeO<sub>2</sub> is orthorhombic, produced by an ion exchange interaction. It is (meta)-stable below 400°C, transforming to  $\alpha$ -LiFeO<sub>2</sub> above 600°C.

- In  $\beta$ -LiFeO<sub>2</sub> the iron and lithium atoms occupy the (1a) Wyckoff position equally (Anderson, 1964). We arbitrarily label these as iron here.
- (Anderson, 1964) place this in space group  $I4/m$  #87, but the atomic positions are consistent with the higher symmetry  $I4/mmm$  #139, so we place it there.
- $L'2_0$  FeC<sub>x</sub> and  $\beta$ -LiFeO<sub>2</sub> have the same AFLOW prototype label, AB.tI4\_139\_a.b. They are generated by the same symmetry operations with different sets of parameters (`--params`) specified in their corresponding CIF files.

---

### Body-centered Tetragonal primitive vectors

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




---

### Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	=	0	=	0	(2a) Fe I
$\mathbf{B}_2$	=	$\frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2$	=	$\frac{1}{2} c \hat{\mathbf{z}}$	(2b) O I

### References

- [1] J. C. Anderson and M. Schieber, *Order-disorder transitions in heat-treated rock-salt Lithium Ferrite*, J. Phys. Chem. Solids **25**, 961–968 (1964), doi:10.1016/0022-3697(64)90033-2.
- [2] R. Kanno, T. Shirane, Y. Kawamoto, Y. Takeda, M. Takano, M. Ohashi, and Y. Yamaguchi, *Synthesis, Structure, and Electrochemical Properties of a New Lithium Iron Oxide, LiFeO<sub>2</sub>, with a Corrugated Layer Structure*, J. Electrochem. Soc. **143**, 2435–2442 (1996), doi:10.1149/1.1837027.
- [3] A. E. Abdel-Ghany, A. Mauger, H. Groult, K. Zaghbi, and C. M. Julien, *Structural properties and electrochemistry of  $\alpha$ -LiFeO<sub>2</sub>*, J. Power Sources **197**, 285–291 (2012), doi:10.1016/j.jpowsour.2011.09.054.
- [4] Y. S. Lee, S. Sato, Y. K. Sun, K. Kobayakawa, and Y. Sato, *A new type of orthorhombic LiFeO<sub>2</sub> with advanced battery performance and its structural change during cycling*, J. Power Sources **119-121**, 285–289 (2003), doi:10.1016/S0378-7753(03)00152-6.
- [5] M. Tabuchi, K. Ado, H. Sakaebe, C. Masquelier, H. Kageyama, and O. Nakamura, *Preparation of AFeO<sub>2</sub> (A = Li, Na) by hydrothermal method*, Solid State Ionics **79**, 220–226 (1995), doi:10.1016/0167-2738(95)00065-E.

### Found in

- [1] M. Barré and M. Catti, *Neutron diffraction study of the  $\beta'$  and  $\gamma$  phases of LiFeO<sub>2</sub>*, J. Solid State Chem. **182**, 2549–2554 (2009), doi:10.1016/j.jssc.2009.06.029.