β-$LiFeO_2$ Structure: AB_tI4_139_a_b-003

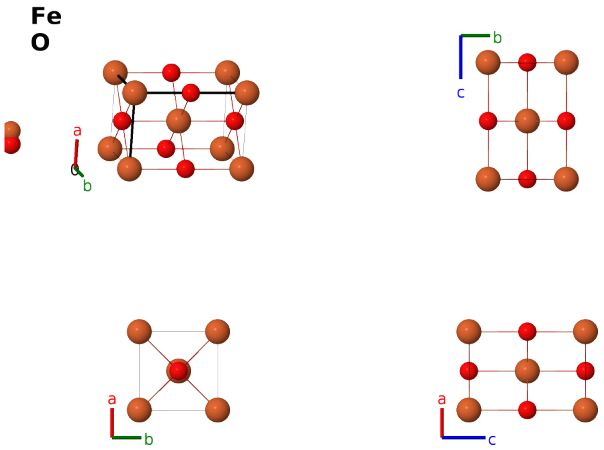
Cite this page as:

- H. Eckert, S. Divilov, M. J. Mehl, D. Hicks, A. C. Zettel, M. Esters, X. Campilongo, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 4*, Comput. Mater. Sci. **240**, 112988 (2024), doi: 10.1016/j.commatsci.2024.112988.
- D. Hicks, M. J. Mehl, M. Esters, C. Oses, O. Levy, G. L. W. Hart, C. Toher, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 3*, Comput. Mater. Sci. **199**, 110450 (2021), doi: 10.1016/j.commatsci.2021.110450.

---

https://aflow.org/prototype-encyclopedia/G0K3

https://aflow.org/prototype-encyclopedia/AB_tI4_139_a_b-003



Prototype	$FeLiO_2$
AFLOW prototype label	AB_tI4_139_a_b-003
ICSD	28366
CCDC	1603449
Pearson symbol	tI4
Space group number	139
Space group symbol	$I4/mmm$
AFLOW prototype command	`aflow --proto=AB_tI4_139_a_b-003 --params=`$a, c/a$

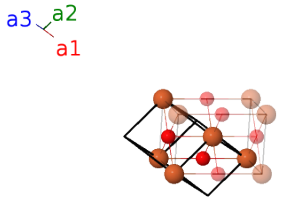
- $FeLiO_2$ exhibits a wide variety of structures, with the exact structure present depends on thermodynamic effects, preparation methods, and charge/discharge history.
- We follow the nomenclature of (Kanno, 1996), where appropriate, with modifications found in (Tabuchi, 1995) and (Abdel-Ghany, 2012). The following list of structures is no doubt incomplete:
  - α-$LiFeO_2$ 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.
  - β-$LiFeO_2$ (this structure) is a tetragonal distortion of α-$LiFeO_2$ with the lithium and iron atoms still randomly placed on their sublattice (we denote this site as Fe).

  - β'-$LiFeO_2$ is monoclinic and transforms to γ-$LiFeO_2$ near room temperature. This is likely the phase (Kanno, 1996) refers to as β-$LiFeO_2$.
  - γ-$LiFeO_2$ is created by low-temperature synthesis below 500°C and can be considered as an ordered version of α-$LiFeO_2$, 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 α-$LiFeO_2$ above 600°C.

- In β-$LiFeO_2$ 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_x and β-$LiFeO_2$ 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

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



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, $LiFeO_2$, 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. 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.

[4] Y. S. Lee, S. Sato, Y. K. Sun, K. Kobayakawa, and Y.Sato, *A new type of orthorhombic $LiFeO_2$ 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 $AFeO_2$ (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 β' and γ phases of $LiFeO_2$*, J. Solid State Chem. **182**, 2549–2554 (2009), doi:10.1016/j.jssc.2009.06.029.

First cited in

H. Eckert, S. Divilov, M. J. Mehl, D. Hicks, A. C. Zettel, M. Esters, X. Campilongo, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 4*, Comput. Mater. Sci. **240**, 112988 (2024), doi: 10.1016/j.commatsci.2024.112988.