γ-$LiFeO_2$ Structure: ABC2_tI16_141_a_b_e-003

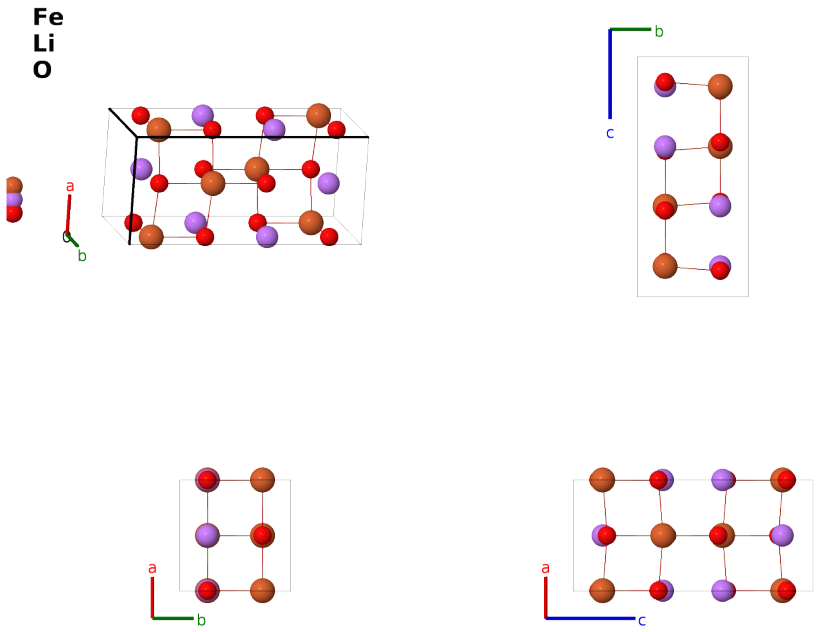
Cite this page as:

- 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/XJE5

https://aflow.org/prototype-encyclopedia/ABC2_tI16_141_a_b_e-003



Prototype	$FeLiO_2$
AFLOW prototype label	ABC2_tI16_141_a_b_e-003
ICSD	174085
CCDC	1688977
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=`$a, c/a, z_3$

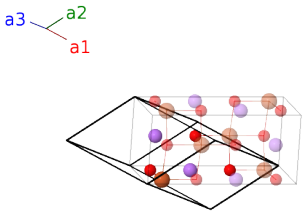
Other compounds with this structure

$ErLiO_2$, δ-$LiAlO_2$, $LiErO_2$, $LiFeO_2$, $LiInO_2$, $LiScO_2$, $LiTiO_2$, $LiTlO_2$, $LiYbO_2$, $NFMg_2$, $NaGdO_2$, $NaNdO_2$, $NaPrO_2$, $NaTbO_2$, $YbAgS_2$

- $FeLiO_2$ 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:
  - 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-$LiFeO_2$ 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-$LiFeO_2$ (this structure) 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.
- For γ-$FeLiO_2$ we use the data taken by (Barré, 2009) at 25°.

Body-centered Tetragonal primitive vectors

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



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

[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.

[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] 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.

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.