Orthorhombic $LiFeO_2$ (o-$LiFeO_2$) Structure: ABC2_oP8_59_a_a_2b-004

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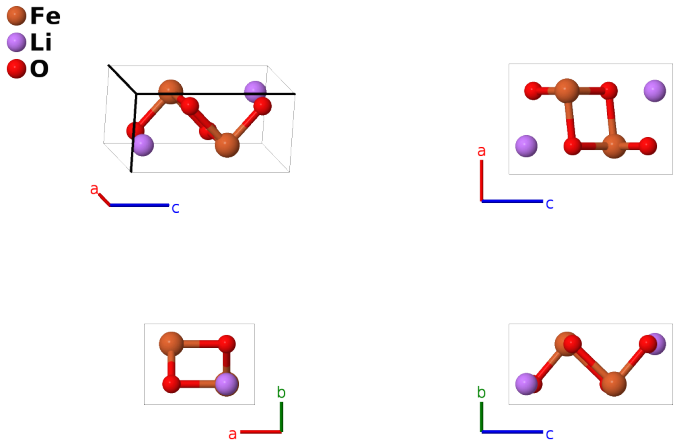
https://aflow.org/p/WEQC

https://aflow.org/p/ABC2_oP8_59_a_a_2b-004



Prototype	$FeLiO_2$
AFLOW prototype label	ABC2_oP8_59_a_a_2b-004
ICSD	none
Pearson symbol	oP8
Space group number	59
Space group symbol	$Pmmn$
AFLOW prototype command	`aflow --proto=ABC2_oP8_59_a_a_2b-004 --params=`$a, b/a, c/a, z_1, z_2, z_3, z_4$

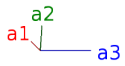
Other compounds with this structure
$LiMnO_2$, $NaMnO_2$

- $FeLiO_2$ 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.
  - 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-$LiFeO_2$.

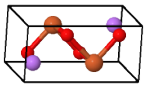
  - γ-$LiFeO_2$ is created by low-temperature synthesis below 500°C and can be considered as an ordered version of α-$LiFeO_2$, with a doubled unit cell.
  - o-$LiFeO_2$ (this structure) is orthorhombic, produced by an ion exchange interaction. It is (meta)-stable below 400°C, transforming to α-$LiFeO_2$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

- We used the data for the sample of o-$LiFeO_2$ studied by (Kanno, 1996) by X-ray diffraction. It has moderate disorder. The Fe (2a) site is 91% iron and 9% lithium, while the Li (2a) site is 91% lithium and 9% iron.

Simple Orthorhombic primitive vectors



$$\mathbf{a_1} = a\,\hat{\mathbf{x}}$$
$$\mathbf{a_2} = b\,\hat{\mathbf{y}}$$
$$\mathbf{a_3} = c\,\hat{\mathbf{z}}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$\frac{1}{4}\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 + z_1\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + \frac{1}{4}b\,\hat{\mathbf{y}} + cz_1\,\hat{\mathbf{z}}$	(2a)	Fe I
$\mathbf{B_2}$	=	$\frac{3}{4}\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 - z_1\,\mathbf{a}_3$	=	$\frac{3}{4}a\,\hat{\mathbf{x}} + \frac{3}{4}b\,\hat{\mathbf{y}} - cz_1\,\hat{\mathbf{z}}$	(2a)	Fe I
$\mathbf{B_3}$	=	$\frac{1}{4}\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 + z_2\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + \frac{1}{4}b\,\hat{\mathbf{y}} + cz_2\,\hat{\mathbf{z}}$	(2a)	Li I
$\mathbf{B_4}$	=	$\frac{3}{4}\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 - z_2\,\mathbf{a}_3$	=	$\frac{3}{4}a\,\hat{\mathbf{x}} + \frac{3}{4}b\,\hat{\mathbf{y}} - cz_2\,\hat{\mathbf{z}}$	(2a)	Li I
$\mathbf{B_5}$	=	$\frac{1}{4}\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 + z_3\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + \frac{3}{4}b\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$	(2b)	O I
$\mathbf{B_6}$	=	$\frac{3}{4}\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 - z_3\,\mathbf{a}_3$	=	$\frac{3}{4}a\,\hat{\mathbf{x}} + \frac{1}{4}b\,\hat{\mathbf{y}} - cz_3\,\hat{\mathbf{z}}$	(2b)	O I
$\mathbf{B_7}$	=	$\frac{1}{4}\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 + z_4\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + \frac{3}{4}b\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$	(2b)	O II
$\mathbf{B_8}$	=	$\frac{3}{4}\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 - z_4\,\mathbf{a}_3$	=	$\frac{3}{4}a\,\hat{\mathbf{x}} + \frac{1}{4}b\,\hat{\mathbf{y}} - cz_4\,\hat{\mathbf{z}}$	(2b)	O II

References

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