

α -LiFe₅O₈ Structure:

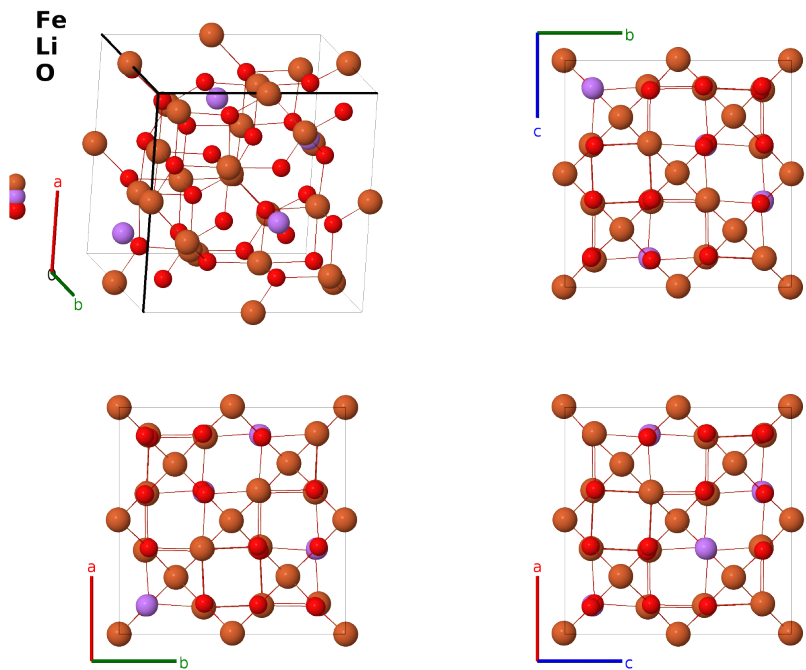
A5BC8_cP56_212_cd_a_ce-001

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- D. Hicks, M. J. Mehl, M. Esters, C. Osos, 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/694R>

https://aflow.org/prototype-encyclopedia/A5BC8_cP56_212_cd_a_ce-001



Prototype	Fe ₅ LiO ₈
AFLOW prototype label	A5BC8_cP56_212_cd_a_ce-001
ICSD	162806
CCDC	1679109
Pearson symbol	cP56
Space group number	212
Space group symbol	$P4_332$
AFLOW prototype command	<code>aflow --proto=A5BC8_cP56_212_cd_a_ce-001</code> <code>--params=a, x₂, x₃, y₄, x₅, y₅, z₅</code>

Other compounds with this structure

LiAl₅O₈, LiGa₅O₈, TeCo₅O₈

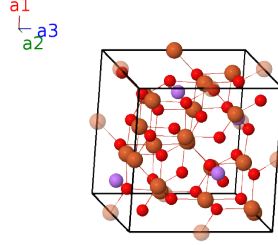
- This is the spinel-like low temperature structure of LiFe_5O_8 . Above 720-750°C the lithium and iron sites are randomly distributed on the cobalt sites of the $D7_2$ cubic spinel structure (Iliev, 2011).
- $\text{Li}_2\text{NiGe}_3\text{O}_5$ is an ordered quaternary form of this structure.
- Space group $P4_332$ #212 is a Sohncke Class II chiral space group, so this structure may also be found in the enantiomorphic space group $P4_132$ #213.

Simple Cubic primitive vectors

$$\mathbf{a}_1 = a \hat{\mathbf{x}}$$

$$\mathbf{a}_2 = a \hat{\mathbf{y}}$$

$$\mathbf{a}_3 = a \hat{\mathbf{z}}$$



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$= \frac{1}{8} \mathbf{a}_1 + \frac{1}{8} \mathbf{a}_2 + \frac{1}{8} \mathbf{a}_3$	$=$	$\frac{1}{8} a \hat{\mathbf{x}} + \frac{1}{8} a \hat{\mathbf{y}} + \frac{1}{8} a \hat{\mathbf{z}}$	(4a)	Li I
$\mathbf{B}_2$	$= \frac{3}{8} \mathbf{a}_1 + \frac{7}{8} \mathbf{a}_2 + \frac{5}{8} \mathbf{a}_3$	$=$	$\frac{3}{8} a \hat{\mathbf{x}} + \frac{7}{8} a \hat{\mathbf{y}} + \frac{5}{8} a \hat{\mathbf{z}}$	(4a)	Li I
$\mathbf{B}_3$	$= \frac{7}{8} \mathbf{a}_1 + \frac{5}{8} \mathbf{a}_2 + \frac{3}{8} \mathbf{a}_3$	$=$	$\frac{7}{8} a \hat{\mathbf{x}} + \frac{5}{8} a \hat{\mathbf{y}} + \frac{3}{8} a \hat{\mathbf{z}}$	(4a)	Li I
$\mathbf{B}_4$	$= \frac{5}{8} \mathbf{a}_1 + \frac{3}{8} \mathbf{a}_2 + \frac{7}{8} \mathbf{a}_3$	$=$	$\frac{5}{8} a \hat{\mathbf{x}} + \frac{3}{8} a \hat{\mathbf{y}} + \frac{7}{8} a \hat{\mathbf{z}}$	(4a)	Li I
$\mathbf{B}_5$	$= x_2 \mathbf{a}_1 + x_2 \mathbf{a}_2 + x_2 \mathbf{a}_3$	$=$	$ax_2 \hat{\mathbf{x}} + ax_2 \hat{\mathbf{y}} + ax_2 \hat{\mathbf{z}}$	(8c)	Fe I
$\mathbf{B}_6$	$= -\left(x_2 - \frac{1}{2}\right) \mathbf{a}_1 - x_2 \mathbf{a}_2 + \left(x_2 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-a\left(x_2 - \frac{1}{2}\right) \hat{\mathbf{x}} - ax_2 \hat{\mathbf{y}} + a\left(x_2 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(8c)	Fe I
$\mathbf{B}_7$	$= -x_2 \mathbf{a}_1 + \left(x_2 + \frac{1}{2}\right) \mathbf{a}_2 - \left(x_2 - \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-ax_2 \hat{\mathbf{x}} + a\left(x_2 + \frac{1}{2}\right) \hat{\mathbf{y}} - a\left(x_2 - \frac{1}{2}\right) \hat{\mathbf{z}}$	(8c)	Fe I
$\mathbf{B}_8$	$= \left(x_2 + \frac{1}{2}\right) \mathbf{a}_1 - \left(x_2 - \frac{1}{2}\right) \mathbf{a}_2 - x_2 \mathbf{a}_3$	$=$	$a\left(x_2 + \frac{1}{2}\right) \hat{\mathbf{x}} - a\left(x_2 - \frac{1}{2}\right) \hat{\mathbf{y}} - ax_2 \hat{\mathbf{z}}$	(8c)	Fe I
$\mathbf{B}_9$	$= \left(x_2 + \frac{1}{4}\right) \mathbf{a}_1 + \left(x_2 + \frac{3}{4}\right) \mathbf{a}_2 - \left(x_2 - \frac{3}{4}\right) \mathbf{a}_3$	$=$	$a\left(x_2 + \frac{1}{4}\right) \hat{\mathbf{x}} + a\left(x_2 + \frac{3}{4}\right) \hat{\mathbf{y}} - a\left(x_2 - \frac{3}{4}\right) \hat{\mathbf{z}}$	(8c)	Fe I
$\mathbf{B}_{10}$	$= -\left(x_2 - \frac{1}{4}\right) \mathbf{a}_1 - \left(x_2 - \frac{1}{4}\right) \mathbf{a}_2 - \left(x_2 - \frac{1}{4}\right) \mathbf{a}_3$	$=$	$-a\left(x_2 - \frac{1}{4}\right) \hat{\mathbf{x}} - a\left(x_2 - \frac{1}{4}\right) \hat{\mathbf{y}} - a\left(x_2 - \frac{1}{4}\right) \hat{\mathbf{z}}$	(8c)	Fe I
$\mathbf{B}_{11}$	$= \left(x_2 + \frac{3}{4}\right) \mathbf{a}_1 - \left(x_2 - \frac{3}{4}\right) \mathbf{a}_2 + \left(x_2 + \frac{1}{4}\right) \mathbf{a}_3$	$=$	$a\left(x_2 + \frac{3}{4}\right) \hat{\mathbf{x}} - a\left(x_2 - \frac{3}{4}\right) \hat{\mathbf{y}} + a\left(x_2 + \frac{1}{4}\right) \hat{\mathbf{z}}$	(8c)	Fe I
$\mathbf{B}_{12}$	$= -\left(x_2 - \frac{3}{4}\right) \mathbf{a}_1 + \left(x_2 + \frac{1}{4}\right) \mathbf{a}_2 + \left(x_2 + \frac{3}{4}\right) \mathbf{a}_3$	$=$	$-a\left(x_2 - \frac{3}{4}\right) \hat{\mathbf{x}} + a\left(x_2 + \frac{1}{4}\right) \hat{\mathbf{y}} + a\left(x_2 + \frac{3}{4}\right) \hat{\mathbf{z}}$	(8c)	Fe I
$\mathbf{B}_{13}$	$= x_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 + x_3 \mathbf{a}_3$	$=$	$ax_3 \hat{\mathbf{x}} + ax_3 \hat{\mathbf{y}} + ax_3 \hat{\mathbf{z}}$	(8c)	O I
$\mathbf{B}_{14}$	$= -\left(x_3 - \frac{1}{2}\right) \mathbf{a}_1 - x_3 \mathbf{a}_2 + \left(x_3 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-a\left(x_3 - \frac{1}{2}\right) \hat{\mathbf{x}} - ax_3 \hat{\mathbf{y}} + a\left(x_3 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(8c)	O I
$\mathbf{B}_{15}$	$= -x_3 \mathbf{a}_1 + \left(x_3 + \frac{1}{2}\right) \mathbf{a}_2 - \left(x_3 - \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-ax_3 \hat{\mathbf{x}} + a\left(x_3 + \frac{1}{2}\right) \hat{\mathbf{y}} - a\left(x_3 - \frac{1}{2}\right) \hat{\mathbf{z}}$	(8c)	O I
$\mathbf{B}_{16}$	$= \left(x_3 + \frac{1}{2}\right) \mathbf{a}_1 - \left(x_3 - \frac{1}{2}\right) \mathbf{a}_2 - x_3 \mathbf{a}_3$	$=$	$a\left(x_3 + \frac{1}{2}\right) \hat{\mathbf{x}} - a\left(x_3 - \frac{1}{2}\right) \hat{\mathbf{y}} - ax_3 \hat{\mathbf{z}}$	(8c)	O I

$$\begin{aligned}
\mathbf{B}_{17} &= \begin{pmatrix} (x_3 + \frac{1}{4}) \mathbf{a}_1 + (x_3 + \frac{3}{4}) \mathbf{a}_2 - \\ (x_3 - \frac{3}{4}) \mathbf{a}_3 \end{pmatrix} = a \begin{pmatrix} (x_3 + \frac{1}{4}) \hat{\mathbf{x}} + a (x_3 + \frac{3}{4}) \hat{\mathbf{y}} - a (x_3 - \frac{3}{4}) \hat{\mathbf{z}} \end{pmatrix} & (8c) & \text{O I} \\
\mathbf{B}_{18} &= \begin{pmatrix} -(x_3 - \frac{1}{4}) \mathbf{a}_1 - (x_3 - \frac{1}{4}) \mathbf{a}_2 - \\ (x_3 - \frac{1}{4}) \mathbf{a}_3 \end{pmatrix} = \begin{pmatrix} -a (x_3 - \frac{1}{4}) \hat{\mathbf{x}} - a (x_3 - \frac{1}{4}) \hat{\mathbf{y}} - \\ a (x_3 - \frac{1}{4}) \hat{\mathbf{z}} \end{pmatrix} & (8c) & \text{O I} \\
\mathbf{B}_{19} &= \begin{pmatrix} (x_3 + \frac{3}{4}) \mathbf{a}_1 - (x_3 - \frac{3}{4}) \mathbf{a}_2 + \\ (x_3 + \frac{1}{4}) \mathbf{a}_3 \end{pmatrix} = a \begin{pmatrix} (x_3 + \frac{3}{4}) \hat{\mathbf{x}} - a (x_3 - \frac{3}{4}) \hat{\mathbf{y}} + a (x_3 + \frac{1}{4}) \hat{\mathbf{z}} \end{pmatrix} & (8c) & \text{O I} \\
\mathbf{B}_{20} &= \begin{pmatrix} -(x_3 - \frac{3}{4}) \mathbf{a}_1 + (x_3 + \frac{1}{4}) \mathbf{a}_2 + \\ (x_3 + \frac{3}{4}) \mathbf{a}_3 \end{pmatrix} = \begin{pmatrix} -a (x_3 - \frac{3}{4}) \hat{\mathbf{x}} + a (x_3 + \frac{1}{4}) \hat{\mathbf{y}} + \\ a (x_3 + \frac{3}{4}) \hat{\mathbf{z}} \end{pmatrix} & (8c) & \text{O I} \\
\mathbf{B}_{21} &= \frac{1}{8} \mathbf{a}_1 + y_4 \mathbf{a}_2 - (y_4 - \frac{1}{4}) \mathbf{a}_3 = \frac{1}{8} a \hat{\mathbf{x}} + ay_4 \hat{\mathbf{y}} - a (y_4 - \frac{1}{4}) \hat{\mathbf{z}} & (12d) & \text{Fe II} \\
\mathbf{B}_{22} &= \frac{3}{8} \mathbf{a}_1 - y_4 \mathbf{a}_2 - (y_4 - \frac{3}{4}) \mathbf{a}_3 = \frac{3}{8} a \hat{\mathbf{x}} - ay_4 \hat{\mathbf{y}} - a (y_4 - \frac{3}{4}) \hat{\mathbf{z}} & (12d) & \text{Fe II} \\
\mathbf{B}_{23} &= \frac{7}{8} \mathbf{a}_1 + (y_4 + \frac{1}{2}) \mathbf{a}_2 + (y_4 + \frac{1}{4}) \mathbf{a}_3 = \frac{7}{8} a \hat{\mathbf{x}} + a (y_4 + \frac{1}{2}) \hat{\mathbf{y}} + a (y_4 + \frac{1}{4}) \hat{\mathbf{z}} & (12d) & \text{Fe II} \\
\mathbf{B}_{24} &= \frac{5}{8} \mathbf{a}_1 - (y_4 - \frac{1}{2}) \mathbf{a}_2 + (y_4 + \frac{3}{4}) \mathbf{a}_3 = \frac{5}{8} a \hat{\mathbf{x}} - a (y_4 - \frac{1}{2}) \hat{\mathbf{y}} + a (y_4 + \frac{3}{4}) \hat{\mathbf{z}} & (12d) & \text{Fe II} \\
\mathbf{B}_{25} &= -(y_4 - \frac{1}{4}) \mathbf{a}_1 + \frac{1}{8} \mathbf{a}_2 + y_4 \mathbf{a}_3 = -a (y_4 - \frac{1}{4}) \hat{\mathbf{x}} + \frac{1}{8} a \hat{\mathbf{y}} + ay_4 \hat{\mathbf{z}} & (12d) & \text{Fe II} \\
\mathbf{B}_{26} &= -(y_4 - \frac{3}{4}) \mathbf{a}_1 + \frac{3}{8} \mathbf{a}_2 - y_4 \mathbf{a}_3 = -a (y_4 - \frac{3}{4}) \hat{\mathbf{x}} + \frac{3}{8} a \hat{\mathbf{y}} - ay_4 \hat{\mathbf{z}} & (12d) & \text{Fe II} \\
\mathbf{B}_{27} &= (y_4 + \frac{1}{4}) \mathbf{a}_1 + \frac{7}{8} \mathbf{a}_2 + (y_4 + \frac{1}{2}) \mathbf{a}_3 = a (y_4 + \frac{1}{4}) \hat{\mathbf{x}} + \frac{7}{8} a \hat{\mathbf{y}} + a (y_4 + \frac{1}{2}) \hat{\mathbf{z}} & (12d) & \text{Fe II} \\
\mathbf{B}_{28} &= (y_4 + \frac{3}{4}) \mathbf{a}_1 + \frac{5}{8} \mathbf{a}_2 - (y_4 - \frac{1}{2}) \mathbf{a}_3 = a (y_4 + \frac{3}{4}) \hat{\mathbf{x}} + \frac{5}{8} a \hat{\mathbf{y}} - a (y_4 - \frac{1}{2}) \hat{\mathbf{z}} & (12d) & \text{Fe II} \\
\mathbf{B}_{29} &= y_4 \mathbf{a}_1 - (y_4 - \frac{1}{4}) \mathbf{a}_2 + \frac{1}{8} \mathbf{a}_3 = ay_4 \hat{\mathbf{x}} - a (y_4 - \frac{1}{4}) \hat{\mathbf{y}} + \frac{1}{8} a \hat{\mathbf{z}} & (12d) & \text{Fe II} \\
\mathbf{B}_{30} &= -y_4 \mathbf{a}_1 - (y_4 - \frac{3}{4}) \mathbf{a}_2 + \frac{3}{8} \mathbf{a}_3 = -ay_4 \hat{\mathbf{x}} - a (y_4 - \frac{3}{4}) \hat{\mathbf{y}} + \frac{3}{8} a \hat{\mathbf{z}} & (12d) & \text{Fe II} \\
\mathbf{B}_{31} &= (y_4 + \frac{1}{2}) \mathbf{a}_1 + (y_4 + \frac{1}{4}) \mathbf{a}_2 + \frac{7}{8} \mathbf{a}_3 = a (y_4 + \frac{1}{2}) \hat{\mathbf{x}} + a (y_4 + \frac{1}{4}) \hat{\mathbf{y}} + \frac{7}{8} a \hat{\mathbf{z}} & (12d) & \text{Fe II} \\
\mathbf{B}_{32} &= -(y_4 - \frac{1}{2}) \mathbf{a}_1 + (y_4 + \frac{3}{4}) \mathbf{a}_2 + \frac{5}{8} \mathbf{a}_3 = -a (y_4 - \frac{1}{2}) \hat{\mathbf{x}} + a (y_4 + \frac{3}{4}) \hat{\mathbf{y}} + \frac{5}{8} a \hat{\mathbf{z}} & (12d) & \text{Fe II} \\
\mathbf{B}_{33} &= x_5 \mathbf{a}_1 + y_5 \mathbf{a}_2 + z_5 \mathbf{a}_3 = ax_5 \hat{\mathbf{x}} + ay_5 \hat{\mathbf{y}} + az_5 \hat{\mathbf{z}} & (24e) & \text{O II} \\
\mathbf{B}_{34} &= \begin{pmatrix} -(x_5 - \frac{1}{2}) \mathbf{a}_1 - y_5 \mathbf{a}_2 + \\ (z_5 + \frac{1}{2}) \mathbf{a}_3 \end{pmatrix} = -a \begin{pmatrix} (x_5 - \frac{1}{2}) \hat{\mathbf{x}} - ay_5 \hat{\mathbf{y}} + a (z_5 + \frac{1}{2}) \hat{\mathbf{z}} \end{pmatrix} & (24e) & \text{O II} \\
\mathbf{B}_{35} &= \begin{pmatrix} -x_5 \mathbf{a}_1 + (y_5 + \frac{1}{2}) \mathbf{a}_2 - \\ (z_5 - \frac{1}{2}) \mathbf{a}_3 \end{pmatrix} = -ax_5 \hat{\mathbf{x}} + a (y_5 + \frac{1}{2}) \hat{\mathbf{y}} - a (z_5 - \frac{1}{2}) \hat{\mathbf{z}} & (24e) & \text{O II} \\
\mathbf{B}_{36} &= (x_5 + \frac{1}{2}) \mathbf{a}_1 - (y_5 - \frac{1}{2}) \mathbf{a}_2 - z_5 \mathbf{a}_3 = a \begin{pmatrix} (x_5 + \frac{1}{2}) \hat{\mathbf{x}} - a (y_5 - \frac{1}{2}) \hat{\mathbf{y}} - az_5 \hat{\mathbf{z}} \end{pmatrix} & (24e) & \text{O II} \\
\mathbf{B}_{37} &= z_5 \mathbf{a}_1 + x_5 \mathbf{a}_2 + y_5 \mathbf{a}_3 = az_5 \hat{\mathbf{x}} + ax_5 \hat{\mathbf{y}} + ay_5 \hat{\mathbf{z}} & (24e) & \text{O II} \\
\mathbf{B}_{38} &= (z_5 + \frac{1}{2}) \mathbf{a}_1 - (x_5 - \frac{1}{2}) \mathbf{a}_2 - y_5 \mathbf{a}_3 = a \begin{pmatrix} (z_5 + \frac{1}{2}) \hat{\mathbf{x}} - a (x_5 - \frac{1}{2}) \hat{\mathbf{y}} - ay_5 \hat{\mathbf{z}} \end{pmatrix} & (24e) & \text{O II} \\
\mathbf{B}_{39} &= \begin{pmatrix} -(z_5 - \frac{1}{2}) \mathbf{a}_1 - x_5 \mathbf{a}_2 + \\ (y_5 + \frac{1}{2}) \mathbf{a}_3 \end{pmatrix} = -a \begin{pmatrix} (z_5 - \frac{1}{2}) \hat{\mathbf{x}} - ax_5 \hat{\mathbf{y}} + a (y_5 + \frac{1}{2}) \hat{\mathbf{z}} \end{pmatrix} & (24e) & \text{O II} \\
\mathbf{B}_{40} &= \begin{pmatrix} -z_5 \mathbf{a}_1 + (x_5 + \frac{1}{2}) \mathbf{a}_2 - \\ (y_5 - \frac{1}{2}) \mathbf{a}_3 \end{pmatrix} = -az_5 \hat{\mathbf{x}} + a (x_5 + \frac{1}{2}) \hat{\mathbf{y}} - a (y_5 - \frac{1}{2}) \hat{\mathbf{z}} & (24e) & \text{O II} \\
\mathbf{B}_{41} &= y_5 \mathbf{a}_1 + z_5 \mathbf{a}_2 + x_5 \mathbf{a}_3 = ay_5 \hat{\mathbf{x}} + az_5 \hat{\mathbf{y}} + ax_5 \hat{\mathbf{z}} & (24e) & \text{O II} \\
\mathbf{B}_{42} &= \begin{pmatrix} -y_5 \mathbf{a}_1 + (z_5 + \frac{1}{2}) \mathbf{a}_2 - \\ (x_5 - \frac{1}{2}) \mathbf{a}_3 \end{pmatrix} = -ay_5 \hat{\mathbf{x}} + a (z_5 + \frac{1}{2}) \hat{\mathbf{y}} - a (x_5 - \frac{1}{2}) \hat{\mathbf{z}} & (24e) & \text{O II} \\
\mathbf{B}_{43} &= (y_5 + \frac{1}{2}) \mathbf{a}_1 - (z_5 - \frac{1}{2}) \mathbf{a}_2 - x_5 \mathbf{a}_3 = a \begin{pmatrix} (y_5 + \frac{1}{2}) \hat{\mathbf{x}} - a (z_5 - \frac{1}{2}) \hat{\mathbf{y}} - ax_5 \hat{\mathbf{z}} \end{pmatrix} & (24e) & \text{O II} \\
\mathbf{B}_{44} &= \begin{pmatrix} -(y_5 - \frac{1}{2}) \mathbf{a}_1 - z_5 \mathbf{a}_2 + \\ (x_5 + \frac{1}{2}) \mathbf{a}_3 \end{pmatrix} = -a \begin{pmatrix} (y_5 - \frac{1}{2}) \hat{\mathbf{x}} - az_5 \hat{\mathbf{y}} + a (x_5 + \frac{1}{2}) \hat{\mathbf{z}} \end{pmatrix} & (24e) & \text{O II} \\
\mathbf{B}_{45} &= \begin{pmatrix} (y_5 + \frac{1}{4}) \mathbf{a}_1 + (x_5 + \frac{3}{4}) \mathbf{a}_2 - \\ (z_5 - \frac{3}{4}) \mathbf{a}_3 \end{pmatrix} = a \begin{pmatrix} (y_5 + \frac{1}{4}) \hat{\mathbf{x}} + a (x_5 + \frac{3}{4}) \hat{\mathbf{y}} - a (z_5 - \frac{3}{4}) \hat{\mathbf{z}} \end{pmatrix} & (24e) & \text{O II} \\
\mathbf{B}_{46} &= \begin{pmatrix} -(y_5 - \frac{1}{4}) \mathbf{a}_1 - (x_5 - \frac{1}{4}) \mathbf{a}_2 - \\ (z_5 - \frac{1}{4}) \mathbf{a}_3 \end{pmatrix} = -a \begin{pmatrix} (y_5 - \frac{1}{4}) \hat{\mathbf{x}} - a (x_5 - \frac{1}{4}) \hat{\mathbf{y}} - a (z_5 - \frac{1}{4}) \hat{\mathbf{z}} \end{pmatrix} & (24e) & \text{O II}
\end{aligned}$$

$$\begin{aligned}
\mathbf{B}_{47} &= \begin{pmatrix} y_5 + \frac{3}{4} \\ z_5 + \frac{1}{4} \end{pmatrix} \mathbf{a}_1 - \begin{pmatrix} x_5 - \frac{3}{4} \\ y_5 - \frac{1}{4} \end{pmatrix} \mathbf{a}_2 + \begin{pmatrix} x_5 + \frac{1}{4} \\ z_5 + \frac{3}{4} \end{pmatrix} \mathbf{a}_3 &= a \begin{pmatrix} y_5 + \frac{3}{4} \\ z_5 + \frac{1}{4} \end{pmatrix} \hat{\mathbf{x}} - a \begin{pmatrix} x_5 - \frac{3}{4} \\ y_5 - \frac{1}{4} \end{pmatrix} \hat{\mathbf{y}} + a \begin{pmatrix} x_5 + \frac{1}{4} \\ z_5 + \frac{3}{4} \end{pmatrix} \hat{\mathbf{z}} &(24e) & \text{O II} \\
\mathbf{B}_{48} &= -\begin{pmatrix} y_5 - \frac{3}{4} \\ z_5 + \frac{3}{4} \end{pmatrix} \mathbf{a}_1 + \begin{pmatrix} x_5 + \frac{1}{4} \\ y_5 - \frac{1}{4} \end{pmatrix} \mathbf{a}_2 + \begin{pmatrix} x_5 + \frac{1}{4} \\ z_5 + \frac{3}{4} \end{pmatrix} \mathbf{a}_3 &= -a \begin{pmatrix} y_5 - \frac{3}{4} \\ z_5 + \frac{3}{4} \end{pmatrix} \hat{\mathbf{x}} + a \begin{pmatrix} x_5 + \frac{1}{4} \\ y_5 - \frac{1}{4} \end{pmatrix} \hat{\mathbf{y}} + a \begin{pmatrix} x_5 + \frac{1}{4} \\ z_5 + \frac{3}{4} \end{pmatrix} \hat{\mathbf{z}} &(24e) & \text{O II} \\
\mathbf{B}_{49} &= \begin{pmatrix} x_5 + \frac{1}{4} \\ y_5 - \frac{3}{4} \end{pmatrix} \mathbf{a}_1 + \begin{pmatrix} z_5 + \frac{3}{4} \\ x_5 - \frac{3}{4} \end{pmatrix} \mathbf{a}_2 - \begin{pmatrix} x_5 + \frac{1}{4} \\ z_5 + \frac{3}{4} \end{pmatrix} \mathbf{a}_3 &= a \begin{pmatrix} x_5 + \frac{1}{4} \\ y_5 - \frac{3}{4} \end{pmatrix} \hat{\mathbf{x}} + a \begin{pmatrix} z_5 + \frac{3}{4} \\ x_5 - \frac{3}{4} \end{pmatrix} \hat{\mathbf{y}} - a \begin{pmatrix} x_5 + \frac{1}{4} \\ z_5 + \frac{3}{4} \end{pmatrix} \hat{\mathbf{z}} &(24e) & \text{O II} \\
\mathbf{B}_{50} &= -\begin{pmatrix} x_5 - \frac{3}{4} \\ y_5 + \frac{3}{4} \end{pmatrix} \mathbf{a}_1 + \begin{pmatrix} z_5 + \frac{1}{4} \\ x_5 + \frac{1}{4} \end{pmatrix} \mathbf{a}_2 + \begin{pmatrix} x_5 + \frac{1}{4} \\ z_5 + \frac{3}{4} \end{pmatrix} \mathbf{a}_3 &= -a \begin{pmatrix} x_5 - \frac{3}{4} \\ y_5 + \frac{3}{4} \end{pmatrix} \hat{\mathbf{x}} + a \begin{pmatrix} z_5 + \frac{1}{4} \\ x_5 + \frac{1}{4} \end{pmatrix} \hat{\mathbf{y}} + a \begin{pmatrix} x_5 + \frac{1}{4} \\ z_5 + \frac{3}{4} \end{pmatrix} \hat{\mathbf{z}} &(24e) & \text{O II} \\
\mathbf{B}_{51} &= -\begin{pmatrix} x_5 - \frac{1}{4} \\ y_5 - \frac{1}{4} \end{pmatrix} \mathbf{a}_1 - \begin{pmatrix} z_5 - \frac{1}{4} \\ x_5 - \frac{1}{4} \end{pmatrix} \mathbf{a}_2 - \begin{pmatrix} x_5 - \frac{1}{4} \\ z_5 - \frac{1}{4} \end{pmatrix} \mathbf{a}_3 &= -a \begin{pmatrix} x_5 - \frac{1}{4} \\ y_5 - \frac{1}{4} \end{pmatrix} \hat{\mathbf{x}} - a \begin{pmatrix} z_5 - \frac{1}{4} \\ x_5 - \frac{1}{4} \end{pmatrix} \hat{\mathbf{y}} - a \begin{pmatrix} x_5 - \frac{1}{4} \\ z_5 - \frac{1}{4} \end{pmatrix} \hat{\mathbf{z}} &(24e) & \text{O II} \\
\mathbf{B}_{52} &= \begin{pmatrix} x_5 + \frac{3}{4} \\ y_5 + \frac{1}{4} \end{pmatrix} \mathbf{a}_1 - \begin{pmatrix} z_5 - \frac{3}{4} \\ x_5 - \frac{3}{4} \end{pmatrix} \mathbf{a}_2 + \begin{pmatrix} x_5 + \frac{3}{4} \\ y_5 + \frac{1}{4} \end{pmatrix} \mathbf{a}_3 &= a \begin{pmatrix} x_5 + \frac{3}{4} \\ y_5 + \frac{1}{4} \end{pmatrix} \hat{\mathbf{x}} - a \begin{pmatrix} z_5 - \frac{3}{4} \\ x_5 - \frac{3}{4} \end{pmatrix} \hat{\mathbf{y}} + a \begin{pmatrix} x_5 + \frac{3}{4} \\ y_5 + \frac{1}{4} \end{pmatrix} \hat{\mathbf{z}} &(24e) & \text{O II} \\
\mathbf{B}_{53} &= \begin{pmatrix} z_5 + \frac{1}{4} \\ x_5 - \frac{3}{4} \end{pmatrix} \mathbf{a}_1 + \begin{pmatrix} y_5 + \frac{3}{4} \\ z_5 + \frac{1}{4} \end{pmatrix} \mathbf{a}_2 - \begin{pmatrix} z_5 + \frac{1}{4} \\ x_5 - \frac{3}{4} \end{pmatrix} \mathbf{a}_3 &= a \begin{pmatrix} z_5 + \frac{1}{4} \\ x_5 - \frac{3}{4} \end{pmatrix} \hat{\mathbf{x}} + a \begin{pmatrix} y_5 + \frac{3}{4} \\ z_5 + \frac{1}{4} \end{pmatrix} \hat{\mathbf{y}} - a \begin{pmatrix} z_5 + \frac{1}{4} \\ x_5 - \frac{3}{4} \end{pmatrix} \hat{\mathbf{z}} &(24e) & \text{O II} \\
\mathbf{B}_{54} &= \begin{pmatrix} z_5 + \frac{3}{4} \\ x_5 + \frac{1}{4} \end{pmatrix} \mathbf{a}_1 - \begin{pmatrix} y_5 - \frac{3}{4} \\ x_5 + \frac{1}{4} \end{pmatrix} \mathbf{a}_2 + \begin{pmatrix} z_5 + \frac{3}{4} \\ x_5 + \frac{1}{4} \end{pmatrix} \mathbf{a}_3 &= a \begin{pmatrix} z_5 + \frac{3}{4} \\ x_5 + \frac{1}{4} \end{pmatrix} \hat{\mathbf{x}} - a \begin{pmatrix} y_5 - \frac{3}{4} \\ x_5 + \frac{1}{4} \end{pmatrix} \hat{\mathbf{y}} + a \begin{pmatrix} z_5 + \frac{3}{4} \\ x_5 + \frac{1}{4} \end{pmatrix} \hat{\mathbf{z}} &(24e) & \text{O II} \\
\mathbf{B}_{55} &= -\begin{pmatrix} z_5 - \frac{3}{4} \\ x_5 + \frac{3}{4} \end{pmatrix} \mathbf{a}_1 + \begin{pmatrix} y_5 + \frac{1}{4} \\ z_5 - \frac{3}{4} \end{pmatrix} \mathbf{a}_2 + \begin{pmatrix} z_5 - \frac{3}{4} \\ x_5 + \frac{3}{4} \end{pmatrix} \mathbf{a}_3 &= -a \begin{pmatrix} z_5 - \frac{3}{4} \\ x_5 + \frac{3}{4} \end{pmatrix} \hat{\mathbf{x}} + a \begin{pmatrix} y_5 + \frac{1}{4} \\ z_5 - \frac{3}{4} \end{pmatrix} \hat{\mathbf{y}} + a \begin{pmatrix} z_5 - \frac{3}{4} \\ x_5 + \frac{3}{4} \end{pmatrix} \hat{\mathbf{z}} &(24e) & \text{O II} \\
\mathbf{B}_{56} &= -\begin{pmatrix} z_5 - \frac{1}{4} \\ x_5 - \frac{1}{4} \end{pmatrix} \mathbf{a}_1 - \begin{pmatrix} y_5 - \frac{1}{4} \\ x_5 - \frac{1}{4} \end{pmatrix} \mathbf{a}_2 - \begin{pmatrix} z_5 - \frac{1}{4} \\ x_5 - \frac{1}{4} \end{pmatrix} \mathbf{a}_3 &= -a \begin{pmatrix} z_5 - \frac{1}{4} \\ x_5 - \frac{1}{4} \end{pmatrix} \hat{\mathbf{x}} - a \begin{pmatrix} y_5 - \frac{1}{4} \\ x_5 - \frac{1}{4} \end{pmatrix} \hat{\mathbf{y}} - a \begin{pmatrix} z_5 - \frac{1}{4} \\ x_5 - \frac{1}{4} \end{pmatrix} \hat{\mathbf{z}} &(24e) & \text{O II}
\end{aligned}$$

References

- [1] N. V. P. . A. B. K. A. I. Smolentsev, A. B. Meshalkin, *Refinement of LiFe_5O_8 crystal structure*, J. of Struct. Chem. **49**, 953–956 (2008), doi:10.1007/s10947-008-0163-8.
- [2] M. N. Iliev, V. G. Ivanov, N. D. Todorov, V. Marinova, M. V. Abrashev, R. P. Y.-Q. Wang, and A. P. Litvinchuk, *Lattice dynamics of the α and β phases of LiFe_5O_8* , Phys. Rev. B **83**, 174111 (2011), doi:10.1103/PhysRevB.83.174111.

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