

β -NaFeO₂ Structure:

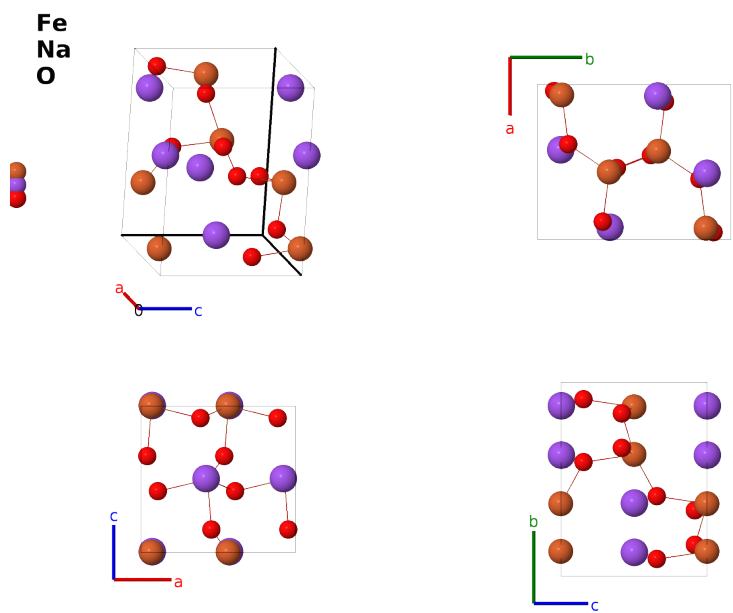
ABC2_oP16_33_a_a_2a-001

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<https://aflow.org/prototype-encyclopedia/3YWY>

https://aflow.org/prototype-encyclopedia/ABC2_oP16_33_a_a_2a-001



Prototype	NaFeO ₂
AFLOW prototype label	ABC2_oP16_33_a_a_2a-001
ICSD	186309
CCDC	169574
Pearson symbol	oP16
Space group number	33
Space group symbol	$Pna2_1$
AFLOW prototype command	<code>aflow --proto=ABC2_oP16_33_a_a_2a-001</code> <code>--params=a, b/a, c/a, x₁, y₁, z₁, x₂, y₂, z₂, x₃, y₃, z₃, x₄, y₄, z₄</code>

Other compounds with this structure

AgAlO₂, AgGaO₂, AgInS₂, AgInSe₂, BeCN₂, BeGeN₂, BeSiN₂, BrNZn₂, ClNZn₂, CuGaO₂, LiAlO₂, LiAlSe₂, LiGaO₂, LiGaS₂, LiGaSe₂, LiInSe₂, MgCN₂, MgGeN₂, MgSiN₂, MgSnN₂, MnGeN₂, MnSiN₂, NBrZn₂, NClZn₂, NaAlO₂, NaGaO₂, ZnGeN₂, ZnSiN₂

- NaFeO₃ is found in three different forms (El-Shobaky, 1988; Singh 2018).
 - α -NaFeO₂ is the low temperature structure
 - β -NaFeO₂ (this structure) is the intermediate temperature structure, which exists at room temperature, and
 - γ -NaFeO₂, the high temperature form, is in the γ -LiAlO₂ structure.
- The temperature range seems to be uncertain, β -NaFeO₂ is said to be the room temperature structure (Viret, 2012) but α -NaFeO₂ is observed at 1000°C (El-Shobaky, 1988).
- Although the title from (Viret, 2012) says “new,” this structure was first reported in 1950 by (Berataut, 1954) (ICSD 27117, CCDC 1602445).
- Space group $Pna2_1$ #33 is polar and so allows an arbitrary choice of the zero of the z -axis. Here we set $z_1 = 0$ for the Fe I atoms.
- β -NaFeO₂ and LiGaO₂ have the same AFLOW prototype label, ABC2_oP16_33_a_a_2a. They are generated by the same symmetry operations with different sets of parameters (`--params`) specified in their corresponding CIF files.

Simple Orthorhombic primitive vectors



Basis vectors

	Lattice coordinates		Cartesian coordinates		Wyckoff position	Atom type
$\mathbf{B}_1$	$= x_1 \mathbf{a}_1 + y_1 \mathbf{a}_2 + z_1 \mathbf{a}_3$	$=$	$ax_1 \hat{\mathbf{x}} + by_1 \hat{\mathbf{y}} + cz_1 \hat{\mathbf{z}}$		(4a)	Fe I
$\mathbf{B}_2$	$= -x_1 \mathbf{a}_1 - y_1 \mathbf{a}_2 + (z_1 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-ax_1 \hat{\mathbf{x}} - by_1 \hat{\mathbf{y}} + c(z_1 + \frac{1}{2}) \hat{\mathbf{z}}$		(4a)	Fe I
$\mathbf{B}_3$	$= (x_1 + \frac{1}{2}) \mathbf{a}_1 - (y_1 - \frac{1}{2}) \mathbf{a}_2 + z_1 \mathbf{a}_3$	$=$	$a(x_1 + \frac{1}{2}) \hat{\mathbf{x}} - b(y_1 - \frac{1}{2}) \hat{\mathbf{y}} + cz_1 \hat{\mathbf{z}}$		(4a)	Fe I
$\mathbf{B}_4$	$= -(x_1 - \frac{1}{2}) \mathbf{a}_1 + (y_1 + \frac{1}{2}) \mathbf{a}_2 + (z_1 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-a(x_1 - \frac{1}{2}) \hat{\mathbf{x}} + b(y_1 + \frac{1}{2}) \hat{\mathbf{y}} + c(z_1 + \frac{1}{2}) \hat{\mathbf{z}}$		(4a)	Fe I
$\mathbf{B}_5$	$= x_2 \mathbf{a}_1 + y_2 \mathbf{a}_2 + z_2 \mathbf{a}_3$	$=$	$ax_2 \hat{\mathbf{x}} + by_2 \hat{\mathbf{y}} + cz_2 \hat{\mathbf{z}}$		(4a)	Na I
$\mathbf{B}_6$	$= -x_2 \mathbf{a}_1 - y_2 \mathbf{a}_2 + (z_2 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-ax_2 \hat{\mathbf{x}} - by_2 \hat{\mathbf{y}} + c(z_2 + \frac{1}{2}) \hat{\mathbf{z}}$		(4a)	Na I
$\mathbf{B}_7$	$= (x_2 + \frac{1}{2}) \mathbf{a}_1 - (y_2 - \frac{1}{2}) \mathbf{a}_2 + z_2 \mathbf{a}_3$	$=$	$a(x_2 + \frac{1}{2}) \hat{\mathbf{x}} - b(y_2 - \frac{1}{2}) \hat{\mathbf{y}} + cz_2 \hat{\mathbf{z}}$		(4a)	Na I
$\mathbf{B}_8$	$= -(x_2 - \frac{1}{2}) \mathbf{a}_1 + (y_2 + \frac{1}{2}) \mathbf{a}_2 + (z_2 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-a(x_2 - \frac{1}{2}) \hat{\mathbf{x}} + b(y_2 + \frac{1}{2}) \hat{\mathbf{y}} + c(z_2 + \frac{1}{2}) \hat{\mathbf{z}}$		(4a)	Na I
$\mathbf{B}_9$	$= x_3 \mathbf{a}_1 + y_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$ax_3 \hat{\mathbf{x}} + by_3 \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}}$		(4a)	O I
$\mathbf{B}_{10}$	$= -x_3 \mathbf{a}_1 - y_3 \mathbf{a}_2 + (z_3 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-ax_3 \hat{\mathbf{x}} - by_3 \hat{\mathbf{y}} + c(z_3 + \frac{1}{2}) \hat{\mathbf{z}}$		(4a)	O I
$\mathbf{B}_{11}$	$= (x_3 + \frac{1}{2}) \mathbf{a}_1 - (y_3 - \frac{1}{2}) \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$a(x_3 + \frac{1}{2}) \hat{\mathbf{x}} - b(y_3 - \frac{1}{2}) \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}}$		(4a)	O I
$\mathbf{B}_{12}$	$= -(x_3 - \frac{1}{2}) \mathbf{a}_1 + (y_3 + \frac{1}{2}) \mathbf{a}_2 + (z_3 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-a(x_3 - \frac{1}{2}) \hat{\mathbf{x}} + b(y_3 + \frac{1}{2}) \hat{\mathbf{y}} + c(z_3 + \frac{1}{2}) \hat{\mathbf{z}}$		(4a)	O I
$\mathbf{B}_{13}$	$= x_4 \mathbf{a}_1 + y_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$ax_4 \hat{\mathbf{x}} + by_4 \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}}$		(4a)	O II
$\mathbf{B}_{14}$	$= -x_4 \mathbf{a}_1 - y_4 \mathbf{a}_2 + (z_4 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-ax_4 \hat{\mathbf{x}} - by_4 \hat{\mathbf{y}} + c(z_4 + \frac{1}{2}) \hat{\mathbf{z}}$		(4a)	O II

$$\mathbf{B}_{15} = \left(x_4 + \frac{1}{2}\right) \mathbf{a}_1 - \left(y_4 - \frac{1}{2}\right) \mathbf{a}_2 + z_4 \mathbf{a}_3 = a \left(x_4 + \frac{1}{2}\right) \hat{\mathbf{x}} - b \left(y_4 - \frac{1}{2}\right) \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}} \quad (4a) \quad \text{O II}$$

$$\mathbf{B}_{16} = -\left(x_4 - \frac{1}{2}\right) \mathbf{a}_1 + \left(y_4 + \frac{1}{2}\right) \mathbf{a}_2 + \left(z_4 + \frac{1}{2}\right) \mathbf{a}_3 = -a \left(x_4 - \frac{1}{2}\right) \hat{\mathbf{x}} + b \left(y_4 + \frac{1}{2}\right) \hat{\mathbf{y}} + c \left(z_4 + \frac{1}{2}\right) \hat{\mathbf{z}} \quad (4a) \quad \text{O II}$$

References

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