α-$NaFeO_2$ Structure: ABC2_hR4_166_a_b_c-009

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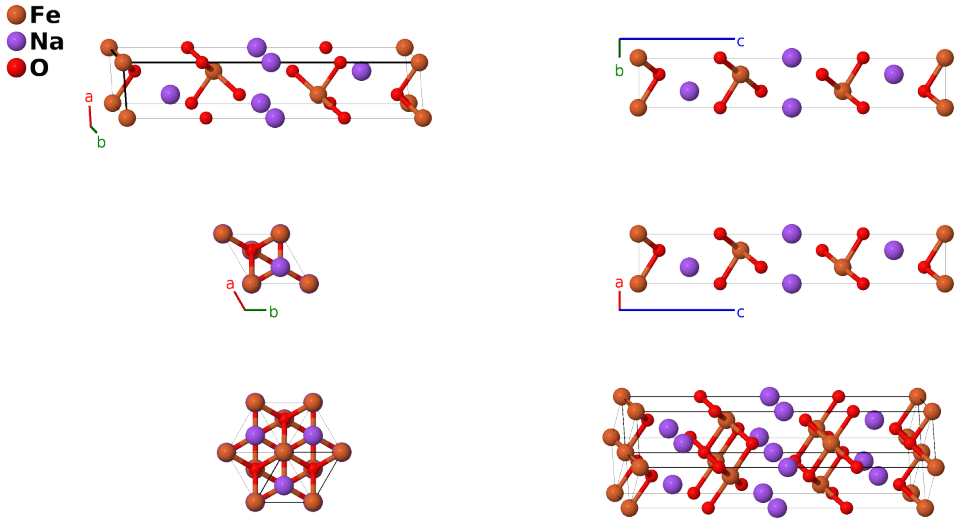
https://aflow.org/p/5FG5

https://aflow.org/p/ABC2_hR4_166_a_b_c-009



Prototype	$FeNaO_2$
AFLOW prototype label	ABC2_hR4_166_a_b_c-009
ICSD	187705
Pearson symbol	hR4
Space group number	166
Space group symbol	$R\bar{3}m$
AFLOW prototype command	`aflow --proto=ABC2_hR4_166_a_b_c-009 --params=`$a, c/a, x_3$

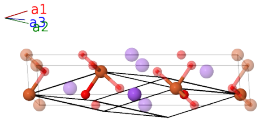
Other compounds with this structure
$CeRbO_2$, $CeRbS_2$, CeRbSSe, $CeRbSe_2$, $CeRbTe_2$, $CeRbTeSe_2$, $CsYbSe_2$, $KCeS_2$, $LiCoO_2$, $LiNi_2$, $NaCoO_2$, $NaYbO_2$, $NaYbS_2$, $NaYbSe_2$

- This is also referred to as O3-$NaFeO_2$.
- This structure is related to O2-$LiCoO_2$, O4-$LiCoO_2$, and OP4-$LiNaCo_2O_4$.
- α-$NaFeO_2$ has the same AFLOW Label, ABC2_hR4_166_a_b_c, as rhombohedral delafossite, $CuFeO_2$ and caswellsilverite ($F5_1$). The difference in the internal parameter z_3 causes a large change in the bonding of the crystals, so we present them as different structures.
- The structures are generated by the same symmetry operations with different sets of parameters (`--params`) specified in their corresponding CIF files.

- Hexagonal settings of this structure can be obtained with the option `--hex`.

Rhombohedral primitive vectors

$$\mathbf{a_1} = \frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \frac{1}{3}c\,\hat{\mathbf{z}}$$
$$\mathbf{a_2} = \frac{1}{\sqrt{3}}a\,\hat{\mathbf{y}} + \frac{1}{3}c\,\hat{\mathbf{z}}$$
$$\mathbf{a_3} = -\frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \frac{1}{3}c\,\hat{\mathbf{z}}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	0	=	0	(1a)	Fe I
$\mathbf{B_2}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}c\,\hat{\mathbf{z}}$	(1b)	Na I
$\mathbf{B_3}$	=	$x_3\,\mathbf{a}_1 + x_3\,\mathbf{a}_2 + x_3\,\mathbf{a}_3$	=	$cx_3\,\hat{\mathbf{z}}$	(2c)	O I
$\mathbf{B_4}$	=	$-x_3\,\mathbf{a}_1 - x_3\,\mathbf{a}_2 - x_3\,\mathbf{a}_3$	=	$-cx_3\,\hat{\mathbf{z}}$	(2c)	O I

References

[1] N. Yabuuchi, H. Yoshida, and S. Komaba, *Crystal Structures and Electrode Performance of Alpha-$NaFeO_2$ for Rechargeable Sodium Batteries*, Electrochemistry **80**, 716–719 (2012), doi:10.5796/electrochemistry.80.716.