α-$NaFeO_2$ Structure: ABC2_hR4_166_a_b_c-009

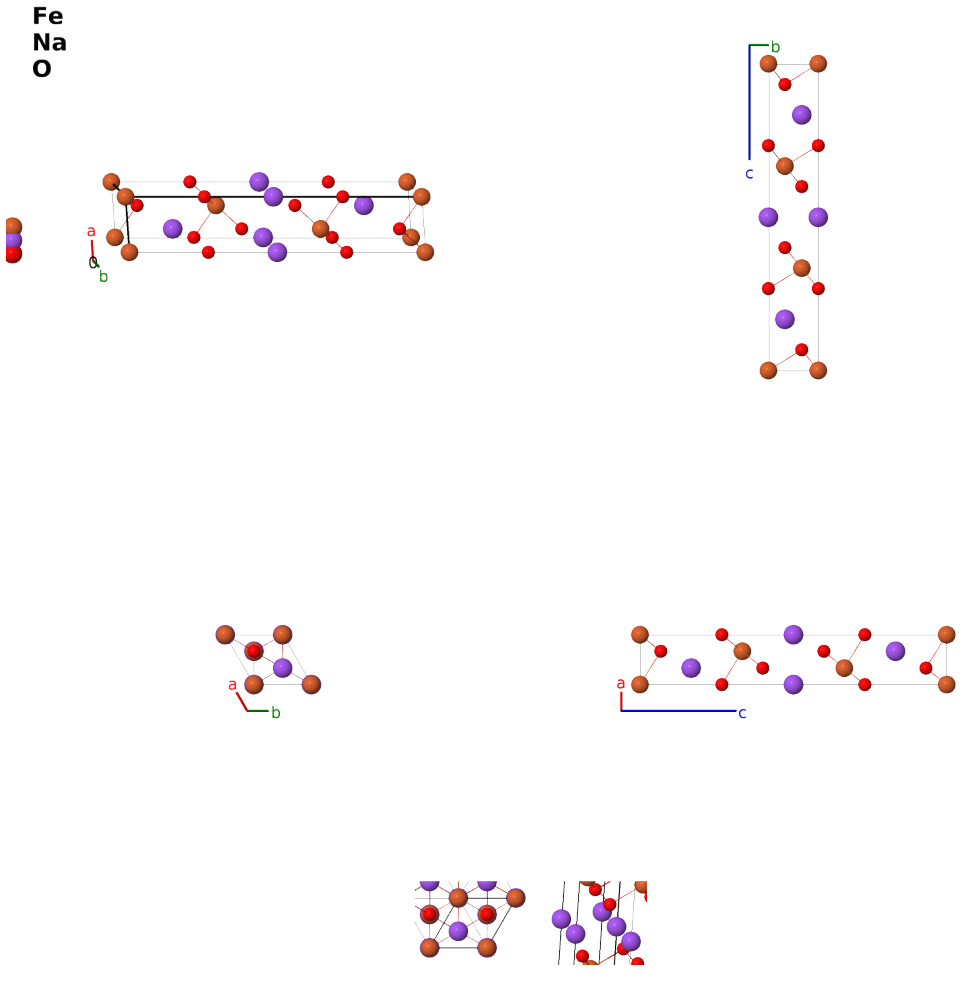
Cite this page as:

- 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/5FG5

https://aflow.org/prototype-encyclopedia/ABC2_hR4_166_a_b_c-009



Prototype	$FeNaO_2$
AFLOW prototype label	ABC2_hR4_166_a_b_c-009
ICSD	187705
CCDC	1696781
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=`$a, c/a, x_3$

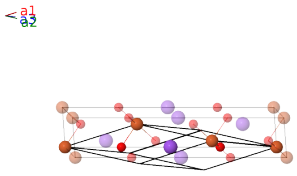
Other compounds with this structure

$AgAlO_2$, $AgAsSe_2$, $AgBiSe_2$, $AgBiTe_2$, $AgGaO_2$, $AgInS_2$, $AgInSe_2$, $AgSbTe_2$, $AlLiSe_2$, $AsICa_2$, $BeSiN_2$, $BiRbS_2$, $BiTlSe_2$, $BrNZn_2$, $CeRbO_2$, $CeRbS_2$, $CeRbSe_2$, $CeRbTe_2$, $ClCLa_2$, $ClNSr_2$, $ClNZn_2$, $CoLiO_2$, $CsCeS_2$, $CsCeSe_2$, $CsDyS_2$, $CsErS_2$, $CsEuS_2$, $CsGdS_2$, $CsHoS_2$, $CsLaS_2$, $CsLaSe_2$, $CsLuS_2$, $CsNdO_2$, $CsNdS_2$, $CsNdSe_2$, $CsNdTe_2$, $CsPrS_2$, $CsPrSe_2$, $CsSmS_2$, $CsSmSe_2$, $CsTbS_2$, $CsTmS_2$, $CsYO_2$, $CsYbS_2$, $CsYbSe_2$, $CuGaO_2$, $DNSr_2$, $DyTlS_2$, $ErNaSe_2$, $ErTlS_2$, $EuNaSe_2$, Gd_2ClC, $GdNaS_2$, $GdNaSe_2$, $GdTlS_2$, $GdTlSe_2$, $GdTlTe_2$, $GeZnN_2$, $HoNaS_2$, $HoNaSe_2$, $HoTe_2Tl$, $HoTlS_2$, $HoTlSe_2$, $InKO_2$, $InNaS_2$, InNaSSe, $InTlS_2$, $KBiS_2$, $KBiSe_2$, $KCeS_2$, $KCeSe_2$, $KCrO_2$, $KCrS_2$, $KDyS_2$, $KErO_2$, $KErS_2$, $KErTe_2$, $KEuS_2$, $KGdS_2$, $KGdSe_2$, $KGdTe_2$, $KHoS_2$, $KHoSe_2$, $KLaO_2$, $KLaS_2$, $KLaSe_2$, $KLaTe_2$, $KLuS_2$, $KLuSe_2$, $KLuTe_2$, $KNdS_2$, $KNdSe_2$, $KNdTe_2$, $KPrO_2$, $KPrS_2$, $KPrSe_2$, $KPrTe_2$, $KScO_2$, $KScS_2$, $KScTe_2$, $KSmS_2$, $KSmTe_2$, $KSnS_2$, $KTbS_2$, $KTiS_2$, $KTlO_2$, $KTmS_2$, $KTmSe_2$, $KTmTe_2$, KYO_2, KYS_2, $KYTe_2$, $KYbS_2$, $KYbSe_2$, $KZrS_2$, $LaNaSe_2$, $LiAlO_2$, $LiCoO_2$, $LiCrO_2$, $LiDyS_2$, $LiDySe_2$, $LiErS_2$, $LiErSe_2$, $LiFeO_2$, $LiGaO_2$, $LiGaS_2$, $LiGaSe_2$, $LiGdSe_2$, $LiHoS_2$, $LiHoSe_2$, $LiHoTe_2$, $LiInSe_2$, $LiLuSe_2$, $LiLuTe_2$, $LiMoO_2$, $LiNi_2$, $LiNiO_2$, $LiScS_2$, $LiScSe_2$, $LiSnS_2$, $LiTbSe_2$, $LiTiS_2$, $LiTmSe_2$, $LiTmTe_2$, $LiVO_2$, $LiYS_2$, $LiYSe_2$, $LiYbS_2$, $LuTlS_2$, $LuTlSe_2$, $LuTlTe_2$, $MgGeN_2$, $MgSiN_2$, $MnGeN_2$, $MnSiN_2$, $NBrBa_2$, $NBrCa_2$, $NBrSr_2$, $NBrZn_2$, $NClBa_2$, $NClCa_2$, $NClMg_2$, $NClSr_2$, $NClZn_2$, $NFBa_2$, $NISr_2$, $NaAlO_2$, $NaCeSe_2$, $NaCoO_2$, $NaCrO_2$, $NaCrS_2$, $NaCrSe_2$, $NaDyS_2$, $NaDySe_2$, $NaErO_2$, $NaErS_2$, $NaErSe_2$, $NaEuS_2$, $NaFeO_2$, $NaGaO_2$, $NaGdS_2$, $NaGdSe_2$, $NaHoO_2$, $NaHoS_2$, $NaHoSe_2$, $NaInO_2$, $NaInS_2$, $NaInSe_2$, $NaLuS_2$, $NaLuTe_2$, $NaMoO_2$, $NaNbN_2$, $NaNdS_2$, $NaNdSe_2$, $NaPrSe_2$, $NaRhO_2$, $NaRuO_2$, $NaScO_2$, $NaScS_2$, $NaScSe_2$, $NaScTe_2$, $NaSmS_2$, $NaSmSe_2$, $NaSnS_2$, $NaTaN_2$, $NaTbS_2$, $NaTbSe_2$, $NaTiO_2$, $NaTiS_2$, $NaTlO_2$, $NaTmS_2$, $NaTmTe_2$, $NaVO_2$, $NaVS_2$, $NaVSe_2$, $NaYO_2$, $NaYS_2$, $NaYSe_2$, $NaYbO_2$, $NaYbS_2$, $NaYbSe_2$, $NaYbSe_2$, $NdRbTe_2$, $NdTlS_2$, $NdTlSe_2$, $NdTlTe_2$, $PBrEu_2$, $PClBa_2$, $PICa_2$, $PIEu_2$, $PrTlSe_2$, $PrTlTe_2$, $RbCeS_2$, $RbCeSe_2$, $RbCeTe_2$, $RbDyO_2$, $RbDyS_2$, $RbErO_2$, $RbErS_2$, $RbErSe_2$, $RbEuO_2$, $RbEuS_2$, $RbGdO_2$, $RbGdS_2$, $RbGdSe_2$, $RbHoO_2$, $RbHoS_2$, $RbHoSe_2$, $RbHoTe_2$, $RbLaO_2$, $RbLaS_2$, $RbLaSe_2$, $RbLuO_2$, $RbLuS_2$, $RbLuSe_2$, $RbLuTe_2$, $RbNdO_2$, $RbNdS_2$, $RbNdSe_2$, $RbPrS_2$, $RbPrSe_2$, $RbScO_2$, $RbScS_2$, $RbSmO_2$, $RbSmS_2$, $RbSmSe_2$, $RbSnS_2$, $RbTbS_2$, $RbTbSe_2$, $RbTlO_2$, $RbTmO_2$, $RbTmS_2$, $RbYO_2$, $RbYS_2$, $RbYTe_2$, $RbYbO_2$, $RbYbS_2$, $RhLiO_2$, $SbTlTe_2$, $SmTlS_2$, $SmTlSe_2$, $SmTlTe_2$, $SrCeN_2$, $SrHfN_2$, $SrZrN_2$, $TbTlS_2$, $TbTlSe_2$, $TbTlTe_2$, $TlBiS_2$, $TlBiSe_2$, $TlBiTe_2$, $TlDyS_2$, $TlDySe_2$, $TlDyTe_2$, $TlErS_2$, $TlErSe_2$, $TlErTe_2$, $TlEuS_2$, $TlGdSe_2$, $TlHoSe_2$, $TlInS_2$, $TlNdSe_2$, $TlSbTe_2$, $TlScSe_2$, $TlScTe_2$, $TlTbSe_2$, $TlTmS_2$, $TlTmSe_2$, $TlTmTe_2$, $TlYS_2$, $TlYSe_2$, $TlYTe_2$, $TlYbS_2$, $TlYbSe_2$, $ZnGeN_2$, $ZnSiN_2$

- $NaFeO_3$ is found in three different forms (El-Shobaky, 1988; Singh 2018).
  - α-$NaFeO_2$ (this structure) is the low temperature structure
  - β-$NaFeO_2$ is the intermediate temperature structure, which exists at room temperature, and
  - γ-$NaFeO_2$, the high temperature form, is in the γ-$LiAlO_2$ structure.
- 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, $CuFeO_2$, caswellsilverite ($F5_1$), $LiNiO_2$ and $Li_2Mn_3O_7$. The difference in c/a, the internal parameter z_3, and site occupation 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

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



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.

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.