Monoclinic $NaNiO_2$ Structure: ABC2_mC8_12_a_c_i-004

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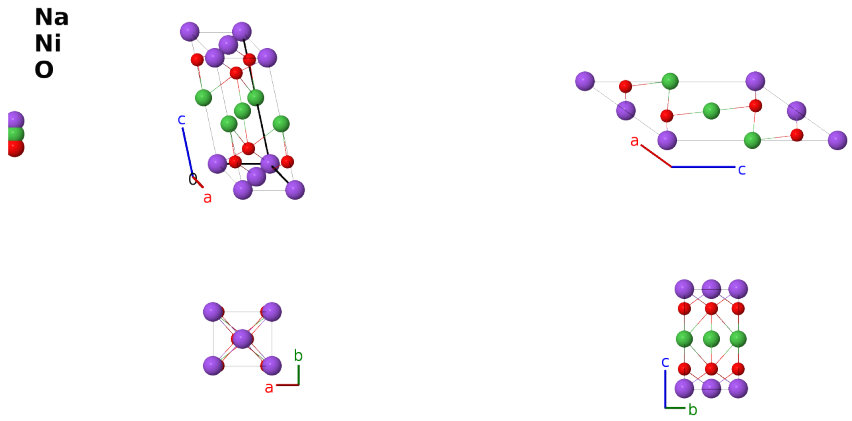
https://aflow.org/prototype-encyclopedia/9GYS

https://aflow.org/prototype-encyclopedia/ABC2_mC8_12_a_c_i-004



Prototype	$NaNiO_2$
AFLOW prototype label	ABC2_mC8_12_a_c_i-004
ICSD	415072
CCDC	1729252
Pearson symbol	mC8
Space group number	12
Space group symbol	$C2/m$
AFLOW prototype command	`aflow --proto=ABC2_mC8_12_a_c_i-004 --params=`$a, b/a, c/a, \beta, x_3, z_3$

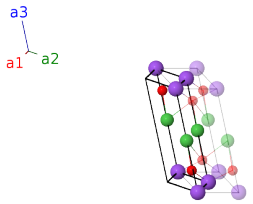
Other compounds with this structure

$AgCuO_2$, $AgMnO_2$, $CdHgO_2$, $CuMnO_2$ (crednerite), $LiCuO_2$, $LiMnO_2$, $LiMoO_2$, $NaCoO_2$, $NaCuO_2$, $NaMnO_2$, $NaTiO_2$, $NaVO_2$

- Above 220°C $NaNiO_2$ transforms into the rhombohedral $LiNiO_2$ structure (Dyer, 1954).
- In the current structure, the AFLOW protocol label algorithm switches the nickel atom from the (2d) Wyckoff position to the (2c) site. This requires a shift of the lattice vector $\vec{a}_3 \to \vec{a}_3 - \vec{a}_1$.

Base-centered Monoclinic primitive vectors

$$\mathbf{a_1} = \frac{1}{2}a\,\hat{\mathbf{x}} - \frac{1}{2}b\,\hat{\mathbf{y}}$$
$$\mathbf{a_2} = \frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}b\,\hat{\mathbf{y}}$$
$$\mathbf{a_3} = c\cos\beta\,\hat{\mathbf{x}} + c\sin\beta\,\hat{\mathbf{z}}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	0	=	0	(2a)	Na I
$\mathbf{B_2}$	=	$\frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}c\cos\beta\,\hat{\mathbf{x}} + \frac{1}{2}c\sin\beta\,\hat{\mathbf{z}}$	(2c)	Ni I
$\mathbf{B_3}$	=	$x_3\,\mathbf{a}_1 + x_3\,\mathbf{a}_2 + z_3\,\mathbf{a}_3$	=	$(ax_3 + cz_3\cos\beta)\,\hat{\mathbf{x}} + cz_3\sin\beta\,\hat{\mathbf{z}}$	(4i)	O I
$\mathbf{B_4}$	=	$-x_3\,\mathbf{a}_1 - x_3\,\mathbf{a}_2 - z_3\,\mathbf{a}_3$	=	$-(ax_3 + cz_3\cos\beta)\,\hat{\mathbf{x}} - cz_3\sin\beta\,\hat{\mathbf{z}}$	(4i)	O I

References

[1] M. Sofin and M. Jansen, *New Route of Preparation and Properties of $NaNiO_2$*, Z. Naturforsch. B **60**, 701–704 (2005), doi:10.1515/znb-2005-0615.

[2] L. D. Dyer, B. S. B. Jr., and G. P. Smith, *Alkali Metal-Nickel Oxides of the Type $MNiO_2$*, J. Am. Chem. Soc. **76**, 1499–1503 (1954), doi:10.1021/ja01635a012.

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