Ferroelectric $NaNO_2$ ($F5_5$) Structure: ABC2_oI8_44_a_a_c-001

This structure originally had the label `ABC2_oI8_44_a_a_c`. Calls to that address will be redirected here.

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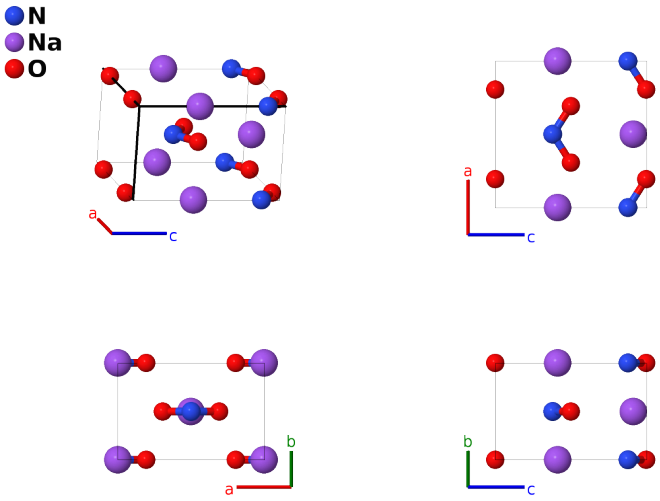
https://aflow.org/p/JZVB

https://aflow.org/p/ABC2_oI8_44_a_a_c-001



Prototype	$NaNO_2$
AFLOW prototype label	ABC2_oI8_44_a_a_c-001
***Strukturbericht* designation**	$F5_5$
Mineral name	sodium nitrite
ICSD	15400
Pearson symbol	oI8
Space group number	44
Space group symbol	$Imm2$
AFLOW prototype command	`aflow --proto=ABC2_oI8_44_a_a_c-001 --params=`$a, b/a, c/a, z_1, z_2, x_3, z_3$

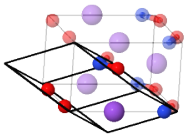
Other compounds with this structure
$AgNO_3$ ($F5_{12}$)

- This is the low-temperature phase of $NaNO_2$, ferroelectric below 158°C.
- (Kay, 1961) gives the structure in the $Im2m$ setting of space group #44. We have used FINDSYM to put it in the standard $Imm2$ setting.

- This structure is very similar to silver nitrite, $AgNO_2$, $F5_{12}$. We present both structures as they are listed separately in the *Strukturbericht* volumes.
- The original publications give Wyckoff positions giving $NaNO_2$ the AFLOW prototype label ABC2_oI8_44_a_a_c and $AgNO_2$ the label ABC2_oI8_44_a_a_d. When we apply our AFLOW prototype label rules, however, the label for both structures becomes ABC2_oI8_44_a_a_c. The two structures are generated by the same symmetry operations with different sets of parameters (`--params`) specified in their corresponding CIF files.
- The origin of the z coordinate in $Imm2$, or the y coordinate in $Im2m$, is arbitrary. Here z_3 is set to zero.

Body-centered Orthorhombic primitive vectors

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



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$z_1\,\mathbf{a}_1 + z_1\,\mathbf{a}_2$	=	$cz_1\,\hat{\mathbf{z}}$	(2a)	N I
$\mathbf{B_2}$	=	$z_2\,\mathbf{a}_1 + z_2\,\mathbf{a}_2$	=	$cz_2\,\hat{\mathbf{z}}$	(2a)	Na I
$\mathbf{B_3}$	=	$z_3\,\mathbf{a}_1 + (x_3 + z_3)\,\mathbf{a}_2 + x_3\,\mathbf{a}_3$	=	$ax_3\,\hat{\mathbf{x}} + cz_3\,\hat{\mathbf{z}}$	(4c)	O I
$\mathbf{B_4}$	=	$z_3\,\mathbf{a}_1 - (x_3 - z_3)\,\mathbf{a}_2 - x_3\,\mathbf{a}_3$	=	$-ax_3\,\hat{\mathbf{x}} + cz_3\,\hat{\mathbf{z}}$	(4c)	O I

References

[1] M. I. Kay and B. C. Frazier, *A neutron diffraction refinement of the low temperature phase of $NaNO_2$*, Acta Cryst. **14**, 56–57 (1961), doi:10.1107/S0365110X61000103.