$F5_{11}$ (KNO_2) Structure (*Obsolete*): ABC2_mC8_8_a_a_b-001

This structure originally had the label `ABC2_mC8_8_a_a_b`. Calls to that address will be redirected here.

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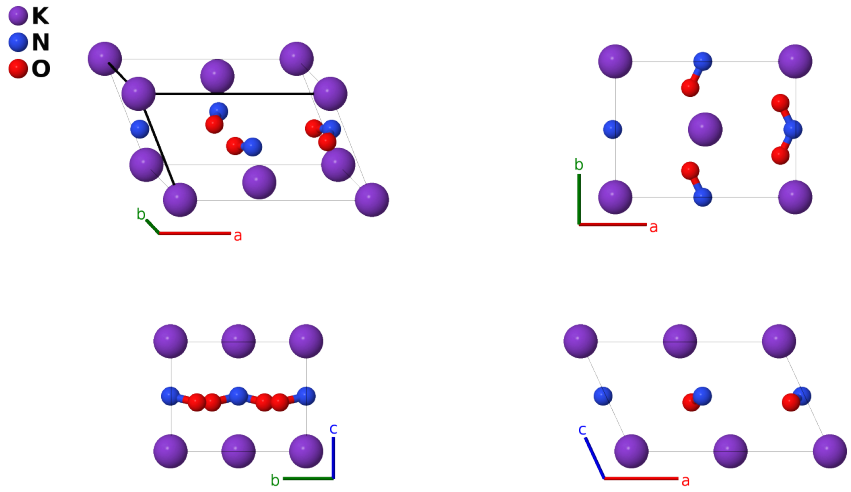
https://aflow.org/p/X9AR

https://aflow.org/p/ABC2_mC8_8_a_a_b-001

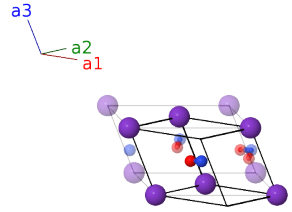


Prototype	KNO_2
AFLOW prototype label	ABC2_mC8_8_a_a_b-001
***Strukturbericht* designation**	$F5_{11}$
ICSD	26764
Pearson symbol	mC8
Space group number	8
Space group symbol	Cm
AFLOW prototype command	`aflow --proto=ABC2_mC8_8_a_a_b-001 --params=`$a, b/a, c/a, \beta, x_1, z_1, x_2, z_2, x_3, y_3, z_3$

- "The room-temperature structure of KNO_2 was first considered to have monoclinic symmetry, ..., but recent studies have established the structure to be rhombohedral ..." (Rao, 1975). The $F5_{11}$ structure is thus neither the ground state structure of KNO_2 nor the room-temperature structure, which is somewhat disordered with space group $R\bar{3}m$ #166. We present this structure as part of the historical record.
- (Ziegler, 1936) gave this structure in the Am setting of space group #8. We used FINDSYM to transform it to the standard Cm setting, which involved a considerable change in the orientation and length of the primitive lattice vectors.

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
$\mathbf{B_1}$	=	$x_1\,\mathbf{a}_1 + x_1\,\mathbf{a}_2 + z_1\,\mathbf{a}_3$	=	$(ax_1 + cz_1\cos\beta)\,\hat{\mathbf{x}} + cz_1\sin\beta\,\hat{\mathbf{z}}$	(2a)	K I
$\mathbf{B_2}$	=	$x_2\,\mathbf{a}_1 + x_2\,\mathbf{a}_2 + z_2\,\mathbf{a}_3$	=	$(ax_2 + cz_2\cos\beta)\,\hat{\mathbf{x}} + cz_2\sin\beta\,\hat{\mathbf{z}}$	(2a)	N I
$\mathbf{B_3}$	=	$(x_3 - y_3)\,\mathbf{a}_1 + (x_3 + y_3)\,\mathbf{a}_2 + z_3\,\mathbf{a}_3$	=	$(ax_3 + cz_3\cos\beta)\,\hat{\mathbf{x}} + by_3\,\hat{\mathbf{y}} + cz_3\sin\beta\,\hat{\mathbf{z}}$	(4b)	O I
$\mathbf{B_4}$	=	$(x_3 + y_3)\,\mathbf{a}_1 + (x_3 - y_3)\,\mathbf{a}_2 + z_3\,\mathbf{a}_3$	=	$(ax_3 + cz_3\cos\beta)\,\hat{\mathbf{x}} - by_3\,\hat{\mathbf{y}} + cz_3\sin\beta\,\hat{\mathbf{z}}$	(4b)	O I

References

[1] G. E. Ziegler, *The Crystal Structure of Potassium Nitrite, KNO_2*, Z. Kristallogr. A **94**, 491–499 (1936), doi:10.1524/zkri.1936.94.1.491.

[2] C. N. R. Rao, B. Prakash, and M. Natarajan, *Crystal Structure Transformations in Inorganic Nitrities, Nitrates, and Carbonates* (National Bureau of Standards, 1975). National Standard Reference Data Series, NSRDS-NBS 53.