

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

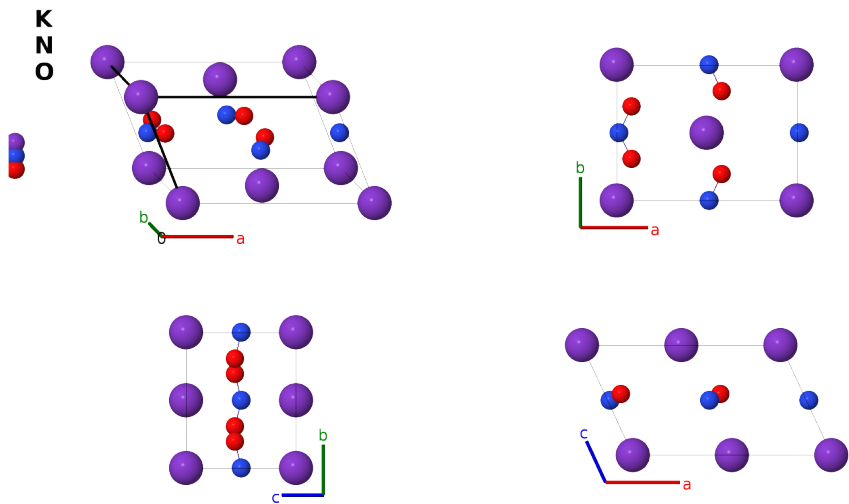
This structure previously used the label(s) ABC2_mC8_8_a_a_b. Calls to these addresses will be redirected here.

Cite this page as:

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<https://aflow.org/prototype-encyclopedia/X9AR>

https://aflow.org/prototype-encyclopedia/ABC2_mC8_8_a_a_b-001



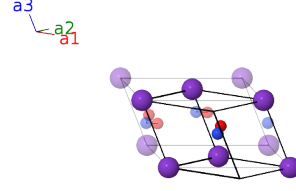
Prototype	KNO_2
AFLOW prototype label	ABC2_mC8_8_a_a_b-001
<i>Strukturbericht</i> designation	$F5_{11}$
ICSD	26764
CCDC	1602148
Pearson symbol	mC8
Space group number	8
Space group symbol	Cm
AFLOW prototype command	<code>aflow --proto=ABC2_mC8_8_a_a_b-001</code> <code>--params=a,b/a,c/a,β,x_1,z_1,x_2,z_2,x_3,y_3,z_3</code>

- “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

$$\begin{aligned}\mathbf{a}_1 &= \frac{1}{2}a \hat{\mathbf{x}} - \frac{1}{2}b \hat{\mathbf{y}} \\ \mathbf{a}_2 &= \frac{1}{2}a \hat{\mathbf{x}} + \frac{1}{2}b \hat{\mathbf{y}} \\ \mathbf{a}_3 &= c \cos \beta \hat{\mathbf{x}} + c \sin \beta \hat{\mathbf{z}}\end{aligned}$$



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 Nitrites, Nitrates, and Carbonates* (National Bureau of Standards, 1975). National Standard Reference Data Series, NSRDS-NBS 53.

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