

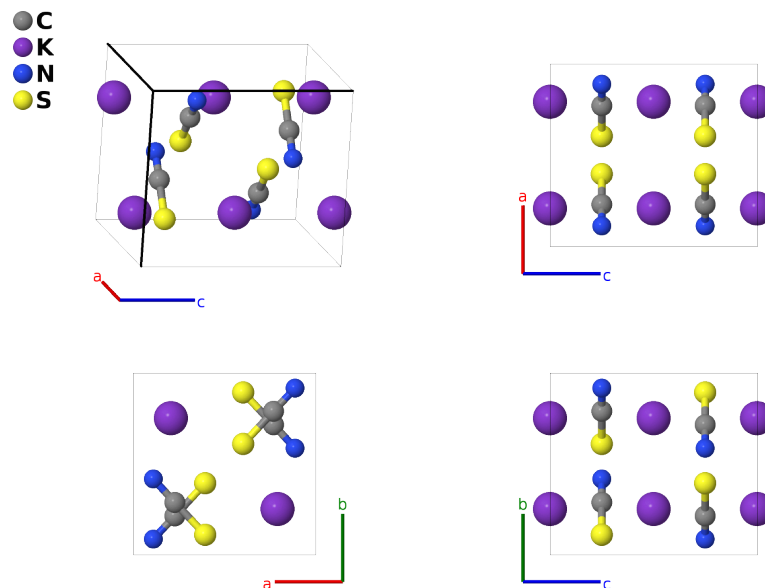
KNCS ($F5_9$) Structure: ABCD_oP16_57_d_c_d_d-001

This structure originally had the label ABCD_oP16_57_d_c_d_d. Calls to that address will be redirected here.

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<https://aflow.org/p/K4A8>

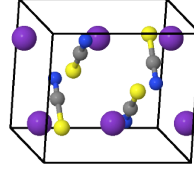
https://aflow.org/p/ABCD_oP16_57_d_c_d_d-001



Prototype	CKNS
AFLOW prototype label	ABCD_oP16_57_d_c_d_d-001
<i>Strukturbericht</i> designation	$F5_9$
ICSD	67582
Pearson symbol	oP16
Space group number	57
Space group symbol	$Pbcm$
AFLOW prototype command	<code>aflow --proto=ABCD_oP16_57_d_c_d_d-001 --params=a, b/a, c/a, x₁, x₂, y₂, x₃, y₃, x₄, y₄</code>

Simple Orthorhombic primitive vectors

a2
a1 a3



$$\begin{aligned}\mathbf{a}_1 &= a \hat{\mathbf{x}} \\ \mathbf{a}_2 &= b \hat{\mathbf{y}} \\ \mathbf{a}_3 &= c \hat{\mathbf{z}}\end{aligned}$$

Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
\mathbf{B}_1	$= x_1 \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2$	$=$	$ax_1 \hat{\mathbf{x}} + \frac{1}{4}b \hat{\mathbf{y}}$	(4c)	K I
\mathbf{B}_2	$= -x_1 \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$-ax_1 \hat{\mathbf{x}} + \frac{3}{4}b \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}}$	(4c)	K I
\mathbf{B}_3	$= -x_1 \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2$	$=$	$-ax_1 \hat{\mathbf{x}} + \frac{3}{4}b \hat{\mathbf{y}}$	(4c)	K I
\mathbf{B}_4	$= x_1 \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$ax_1 \hat{\mathbf{x}} + \frac{1}{4}b \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}}$	(4c)	K I
\mathbf{B}_5	$= x_2 \mathbf{a}_1 + y_2 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$ax_2 \hat{\mathbf{x}} + by_2 \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	(4d)	C I
\mathbf{B}_6	$= -x_2 \mathbf{a}_1 - y_2 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$-ax_2 \hat{\mathbf{x}} - by_2 \hat{\mathbf{y}} + \frac{3}{4}c \hat{\mathbf{z}}$	(4d)	C I
\mathbf{B}_7	$= -x_2 \mathbf{a}_1 + (y_2 + \frac{1}{2}) \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$-ax_2 \hat{\mathbf{x}} + b(y_2 + \frac{1}{2}) \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	(4d)	C I
\mathbf{B}_8	$= x_2 \mathbf{a}_1 - (y_2 - \frac{1}{2}) \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$ax_2 \hat{\mathbf{x}} - b(y_2 - \frac{1}{2}) \hat{\mathbf{y}} + \frac{3}{4}c \hat{\mathbf{z}}$	(4d)	C I
\mathbf{B}_9	$= x_3 \mathbf{a}_1 + y_3 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$ax_3 \hat{\mathbf{x}} + by_3 \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	(4d)	N I
\mathbf{B}_{10}	$= -x_3 \mathbf{a}_1 - y_3 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$-ax_3 \hat{\mathbf{x}} - by_3 \hat{\mathbf{y}} + \frac{3}{4}c \hat{\mathbf{z}}$	(4d)	N I
\mathbf{B}_{11}	$= -x_3 \mathbf{a}_1 + (y_3 + \frac{1}{2}) \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$-ax_3 \hat{\mathbf{x}} + b(y_3 + \frac{1}{2}) \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	(4d)	N I
\mathbf{B}_{12}	$= x_3 \mathbf{a}_1 - (y_3 - \frac{1}{2}) \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$ax_3 \hat{\mathbf{x}} - b(y_3 - \frac{1}{2}) \hat{\mathbf{y}} + \frac{3}{4}c \hat{\mathbf{z}}$	(4d)	N I
\mathbf{B}_{13}	$= x_4 \mathbf{a}_1 + y_4 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$ax_4 \hat{\mathbf{x}} + by_4 \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	(4d)	S I
\mathbf{B}_{14}	$= -x_4 \mathbf{a}_1 - y_4 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$-ax_4 \hat{\mathbf{x}} - by_4 \hat{\mathbf{y}} + \frac{3}{4}c \hat{\mathbf{z}}$	(4d)	S I
\mathbf{B}_{15}	$= -x_4 \mathbf{a}_1 + (y_4 + \frac{1}{2}) \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$-ax_4 \hat{\mathbf{x}} + b(y_4 + \frac{1}{2}) \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	(4d)	S I
\mathbf{B}_{16}	$= x_4 \mathbf{a}_1 - (y_4 - \frac{1}{2}) \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$ax_4 \hat{\mathbf{x}} - b(y_4 - \frac{1}{2}) \hat{\mathbf{y}} + \frac{3}{4}c \hat{\mathbf{z}}$	(4d)	S I

References

- [1] D. J. Cookson, M. M. Elcombe, and T. R. Finlayson, *Phonon dispersion relations for potassium thiocyanate at and above room temperature*, J. Phys.: Condens. Matter **4**, 7851–7864 (1992), doi:10.1088/0953-8984/4/39/001.

Found in

- [1] E. Nakamura, *SpringerMaterials – Inorganic Substances other than Oxides·M21 KSCN [(A)]* (2005). Y. Shiozaki, E. Nakamura, T. Mitsui (ed.).