

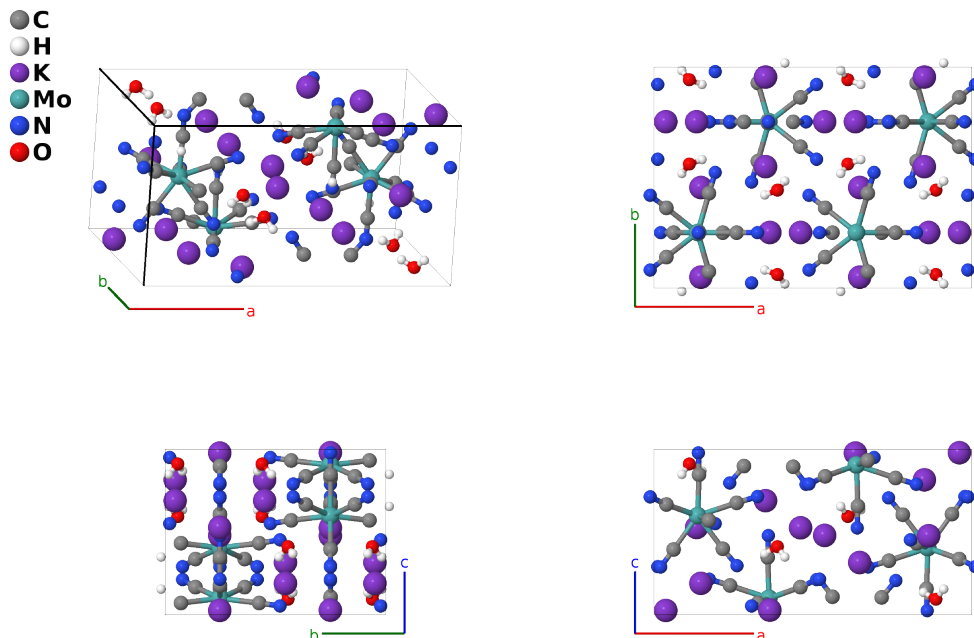
$K_4[Mo(CN)_8] \cdot 2H_2O$ ($F2_1$) Structure: A8B4C4DE8F2_oP108_62_4c2d_2d_2cd_c_4c2d_d-001

This structure originally had the label A8B4C4DE8F2_oP108_62_4c2d_2d_2cd_c_4c2d_d. Calls to that address will be redirected here.

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<https://aflow.org/p/BH4W>

https://aflow.org/p/A8B4C4DE8F2_oP108_62_4c2d_2d_2cd_c_4c2d_d-001

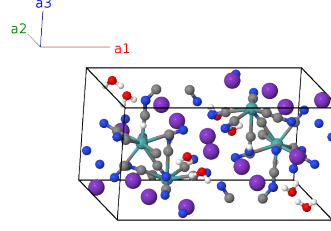


Prototype	$C_8H_4K_4MoN_8O_2$
AFLOW prototype label	A8B4C4DE8F2_oP108_62_4c2d_2d_2cd_c_4c2d_d-001
<i>Strukturbericht</i> designation	$F2_1$
ICSD	none
Pearson symbol	oP108
Space group number	62
Space group symbol	$Pnma$
AFLOW prototype command	aflow --proto=A8B4C4DE8F2_oP108_62_4c2d_2d_2cd_c_4c2d_d-001 --params=a,b/a,c/a,x ₁ ,z ₁ ,x ₂ ,z ₂ ,x ₃ ,z ₃ ,x ₄ ,z ₄ ,x ₅ ,z ₅ ,x ₆ ,z ₆ ,x ₇ ,z ₇ ,x ₈ ,z ₈ ,x ₉ ,z ₉ ,x ₁₀ ,z ₁₀ ,x ₁₁ ,z ₁₁ ,x ₁₂ ,z ₁₂ ,x ₁₃ ,z ₁₃ ,x ₁₄ ,z ₁₄ ,x ₁₅ ,z ₁₅ ,x ₁₆ ,z ₁₆ ,x ₁₇ ,z ₁₇ ,x ₁₈ ,z ₁₈ ,x ₁₉ ,z ₁₉

- (Hoard, 1939) originally determined this structure, but were unable to locate the hydrogen atoms. (Herrmann, 1943) gave this the *Strukturbericht* designation $F2_1$. (Typilo, 2010) were able to refine the structure at 173K, including the hydrogen positions. Since the space group and Wyckoff positions are otherwise unchanged we use the newer structure as our prototype.

Simple Orthorhombic primitive vectors

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



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
\mathbf{B}_1	$= x_1 \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_1 \mathbf{a}_3$	$=$	$ax_1 \hat{\mathbf{x}} + \frac{1}{4}b \hat{\mathbf{y}} + cz_1 \hat{\mathbf{z}}$	(4c)	C I
\mathbf{B}_2	$= -(x_1 - \frac{1}{2}) \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + (z_1 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-a(x_1 - \frac{1}{2}) \hat{\mathbf{x}} + \frac{3}{4}b \hat{\mathbf{y}} + c(z_1 + \frac{1}{2}) \hat{\mathbf{z}}$	(4c)	C I
\mathbf{B}_3	$= -x_1 \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_1 \mathbf{a}_3$	$=$	$-ax_1 \hat{\mathbf{x}} + \frac{3}{4}b \hat{\mathbf{y}} - cz_1 \hat{\mathbf{z}}$	(4c)	C I
\mathbf{B}_4	$= (x_1 + \frac{1}{2}) \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 - (z_1 - \frac{1}{2}) \mathbf{a}_3$	$=$	$a(x_1 + \frac{1}{2}) \hat{\mathbf{x}} + \frac{1}{4}b \hat{\mathbf{y}} - c(z_1 - \frac{1}{2}) \hat{\mathbf{z}}$	(4c)	C I
\mathbf{B}_5	$= x_2 \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_2 \mathbf{a}_3$	$=$	$ax_2 \hat{\mathbf{x}} + \frac{1}{4}b \hat{\mathbf{y}} + cz_2 \hat{\mathbf{z}}$	(4c)	C II
\mathbf{B}_6	$= -(x_2 - \frac{1}{2}) \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + (z_2 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-a(x_2 - \frac{1}{2}) \hat{\mathbf{x}} + \frac{3}{4}b \hat{\mathbf{y}} + c(z_2 + \frac{1}{2}) \hat{\mathbf{z}}$	(4c)	C II
\mathbf{B}_7	$= -x_2 \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_2 \mathbf{a}_3$	$=$	$-ax_2 \hat{\mathbf{x}} + \frac{3}{4}b \hat{\mathbf{y}} - cz_2 \hat{\mathbf{z}}$	(4c)	C II
\mathbf{B}_8	$= (x_2 + \frac{1}{2}) \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 - (z_2 - \frac{1}{2}) \mathbf{a}_3$	$=$	$a(x_2 + \frac{1}{2}) \hat{\mathbf{x}} + \frac{1}{4}b \hat{\mathbf{y}} - c(z_2 - \frac{1}{2}) \hat{\mathbf{z}}$	(4c)	C II
\mathbf{B}_9	$= x_3 \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$ax_3 \hat{\mathbf{x}} + \frac{1}{4}b \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}}$	(4c)	C III
\mathbf{B}_{10}	$= -(x_3 - \frac{1}{2}) \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + (z_3 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-a(x_3 - \frac{1}{2}) \hat{\mathbf{x}} + \frac{3}{4}b \hat{\mathbf{y}} + c(z_3 + \frac{1}{2}) \hat{\mathbf{z}}$	(4c)	C III
\mathbf{B}_{11}	$= -x_3 \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_3 \mathbf{a}_3$	$=$	$-ax_3 \hat{\mathbf{x}} + \frac{3}{4}b \hat{\mathbf{y}} - cz_3 \hat{\mathbf{z}}$	(4c)	C III
\mathbf{B}_{12}	$= (x_3 + \frac{1}{2}) \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 - (z_3 - \frac{1}{2}) \mathbf{a}_3$	$=$	$a(x_3 + \frac{1}{2}) \hat{\mathbf{x}} + \frac{1}{4}b \hat{\mathbf{y}} - c(z_3 - \frac{1}{2}) \hat{\mathbf{z}}$	(4c)	C III
\mathbf{B}_{13}	$= x_4 \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$ax_4 \hat{\mathbf{x}} + \frac{1}{4}b \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}}$	(4c)	C IV
\mathbf{B}_{14}	$= -(x_4 - \frac{1}{2}) \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + (z_4 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-a(x_4 - \frac{1}{2}) \hat{\mathbf{x}} + \frac{3}{4}b \hat{\mathbf{y}} + c(z_4 + \frac{1}{2}) \hat{\mathbf{z}}$	(4c)	C IV
\mathbf{B}_{15}	$= -x_4 \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_4 \mathbf{a}_3$	$=$	$-ax_4 \hat{\mathbf{x}} + \frac{3}{4}b \hat{\mathbf{y}} - cz_4 \hat{\mathbf{z}}$	(4c)	C IV
\mathbf{B}_{16}	$= (x_4 + \frac{1}{2}) \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 - (z_4 - \frac{1}{2}) \mathbf{a}_3$	$=$	$a(x_4 + \frac{1}{2}) \hat{\mathbf{x}} + \frac{1}{4}b \hat{\mathbf{y}} - c(z_4 - \frac{1}{2}) \hat{\mathbf{z}}$	(4c)	C IV
\mathbf{B}_{17}	$= x_5 \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$ax_5 \hat{\mathbf{x}} + \frac{1}{4}b \hat{\mathbf{y}} + cz_5 \hat{\mathbf{z}}$	(4c)	K I
\mathbf{B}_{18}	$= -(x_5 - \frac{1}{2}) \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + (z_5 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-a(x_5 - \frac{1}{2}) \hat{\mathbf{x}} + \frac{3}{4}b \hat{\mathbf{y}} + c(z_5 + \frac{1}{2}) \hat{\mathbf{z}}$	(4c)	K I
\mathbf{B}_{19}	$= -x_5 \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_5 \mathbf{a}_3$	$=$	$-ax_5 \hat{\mathbf{x}} + \frac{3}{4}b \hat{\mathbf{y}} - cz_5 \hat{\mathbf{z}}$	(4c)	K I
\mathbf{B}_{20}	$= (x_5 + \frac{1}{2}) \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 - (z_5 - \frac{1}{2}) \mathbf{a}_3$	$=$	$a(x_5 + \frac{1}{2}) \hat{\mathbf{x}} + \frac{1}{4}b \hat{\mathbf{y}} - c(z_5 - \frac{1}{2}) \hat{\mathbf{z}}$	(4c)	K I
\mathbf{B}_{21}	$= x_6 \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_6 \mathbf{a}_3$	$=$	$ax_6 \hat{\mathbf{x}} + \frac{1}{4}b \hat{\mathbf{y}} + cz_6 \hat{\mathbf{z}}$	(4c)	K II
\mathbf{B}_{22}	$= -(x_6 - \frac{1}{2}) \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + (z_6 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-a(x_6 - \frac{1}{2}) \hat{\mathbf{x}} + \frac{3}{4}b \hat{\mathbf{y}} + c(z_6 + \frac{1}{2}) \hat{\mathbf{z}}$	(4c)	K II
\mathbf{B}_{23}	$= -x_6 \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_6 \mathbf{a}_3$	$=$	$-ax_6 \hat{\mathbf{x}} + \frac{3}{4}b \hat{\mathbf{y}} - cz_6 \hat{\mathbf{z}}$	(4c)	K II
\mathbf{B}_{24}	$= (x_6 + \frac{1}{2}) \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 - (z_6 - \frac{1}{2}) \mathbf{a}_3$	$=$	$a(x_6 + \frac{1}{2}) \hat{\mathbf{x}} + \frac{1}{4}b \hat{\mathbf{y}} - c(z_6 - \frac{1}{2}) \hat{\mathbf{z}}$	(4c)	K II
\mathbf{B}_{25}	$= x_7 \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_7 \mathbf{a}_3$	$=$	$ax_7 \hat{\mathbf{x}} + \frac{1}{4}b \hat{\mathbf{y}} + cz_7 \hat{\mathbf{z}}$	(4c)	Mo I

$$\begin{aligned}
\mathbf{B}_{87} &= -x_{17} \mathbf{a}_1 + (y_{17} + \frac{1}{2}) \mathbf{a}_2 - z_{17} \mathbf{a}_3 &= & -ax_{17} \hat{\mathbf{x}} + b(y_{17} + \frac{1}{2}) \hat{\mathbf{y}} - cz_{17} \hat{\mathbf{z}} & (8d) & \text{N V} \\
\mathbf{B}_{88} &= (x_{17} + \frac{1}{2}) \mathbf{a}_1 - (y_{17} - \frac{1}{2}) \mathbf{a}_2 - &= & a(x_{17} + \frac{1}{2}) \hat{\mathbf{x}} - b(y_{17} - \frac{1}{2}) \hat{\mathbf{y}} - & (8d) & \text{N V} \\
& (z_{17} - \frac{1}{2}) \mathbf{a}_3 & & c(z_{17} - \frac{1}{2}) \hat{\mathbf{z}} & & \\
\mathbf{B}_{89} &= -x_{17} \mathbf{a}_1 - y_{17} \mathbf{a}_2 - z_{17} \mathbf{a}_3 &= & -ax_{17} \hat{\mathbf{x}} - by_{17} \hat{\mathbf{y}} - cz_{17} \hat{\mathbf{z}} & (8d) & \text{N V} \\
\mathbf{B}_{90} &= (x_{17} + \frac{1}{2}) \mathbf{a}_1 + y_{17} \mathbf{a}_2 - &= & a(x_{17} + \frac{1}{2}) \hat{\mathbf{x}} + by_{17} \hat{\mathbf{y}} - c(z_{17} - \frac{1}{2}) \hat{\mathbf{z}} & (8d) & \text{N V} \\
& (z_{17} - \frac{1}{2}) \mathbf{a}_3 & & & & \\
\mathbf{B}_{91} &= x_{17} \mathbf{a}_1 - (y_{17} - \frac{1}{2}) \mathbf{a}_2 + z_{17} \mathbf{a}_3 &= & ax_{17} \hat{\mathbf{x}} - b(y_{17} - \frac{1}{2}) \hat{\mathbf{y}} + cz_{17} \hat{\mathbf{z}} & (8d) & \text{N V} \\
\mathbf{B}_{92} &= -(x_{17} - \frac{1}{2}) \mathbf{a}_1 + (y_{17} + \frac{1}{2}) \mathbf{a}_2 + &= & -a(x_{17} - \frac{1}{2}) \hat{\mathbf{x}} + b(y_{17} + \frac{1}{2}) \hat{\mathbf{y}} + & (8d) & \text{N V} \\
& (z_{17} + \frac{1}{2}) \mathbf{a}_3 & & c(z_{17} + \frac{1}{2}) \hat{\mathbf{z}} & & \\
\mathbf{B}_{93} &= x_{18} \mathbf{a}_1 + y_{18} \mathbf{a}_2 + z_{18} \mathbf{a}_3 &= & ax_{18} \hat{\mathbf{x}} + by_{18} \hat{\mathbf{y}} + cz_{18} \hat{\mathbf{z}} & (8d) & \text{N VI} \\
\mathbf{B}_{94} &= -(x_{18} - \frac{1}{2}) \mathbf{a}_1 - y_{18} \mathbf{a}_2 + &= & -a(x_{18} - \frac{1}{2}) \hat{\mathbf{x}} - by_{18} \hat{\mathbf{y}} + c(z_{18} + \frac{1}{2}) \hat{\mathbf{z}} & (8d) & \text{N VI} \\
& (z_{18} + \frac{1}{2}) \mathbf{a}_3 & & & & \\
\mathbf{B}_{95} &= -x_{18} \mathbf{a}_1 + (y_{18} + \frac{1}{2}) \mathbf{a}_2 - z_{18} \mathbf{a}_3 &= & -ax_{18} \hat{\mathbf{x}} + b(y_{18} + \frac{1}{2}) \hat{\mathbf{y}} - cz_{18} \hat{\mathbf{z}} & (8d) & \text{N VI} \\
\mathbf{B}_{96} &= (x_{18} + \frac{1}{2}) \mathbf{a}_1 - (y_{18} - \frac{1}{2}) \mathbf{a}_2 - &= & a(x_{18} + \frac{1}{2}) \hat{\mathbf{x}} - b(y_{18} - \frac{1}{2}) \hat{\mathbf{y}} - & (8d) & \text{N VI} \\
& (z_{18} - \frac{1}{2}) \mathbf{a}_3 & & c(z_{18} - \frac{1}{2}) \hat{\mathbf{z}} & & \\
\mathbf{B}_{97} &= -x_{18} \mathbf{a}_1 - y_{18} \mathbf{a}_2 - z_{18} \mathbf{a}_3 &= & -ax_{18} \hat{\mathbf{x}} - by_{18} \hat{\mathbf{y}} - cz_{18} \hat{\mathbf{z}} & (8d) & \text{N VI} \\
\mathbf{B}_{98} &= (x_{18} + \frac{1}{2}) \mathbf{a}_1 + y_{18} \mathbf{a}_2 - &= & a(x_{18} + \frac{1}{2}) \hat{\mathbf{x}} + by_{18} \hat{\mathbf{y}} - c(z_{18} - \frac{1}{2}) \hat{\mathbf{z}} & (8d) & \text{N VI} \\
& (z_{18} - \frac{1}{2}) \mathbf{a}_3 & & & & \\
\mathbf{B}_{99} &= x_{18} \mathbf{a}_1 - (y_{18} - \frac{1}{2}) \mathbf{a}_2 + z_{18} \mathbf{a}_3 &= & ax_{18} \hat{\mathbf{x}} - b(y_{18} - \frac{1}{2}) \hat{\mathbf{y}} + cz_{18} \hat{\mathbf{z}} & (8d) & \text{N VI} \\
\mathbf{B}_{100} &= -(x_{18} - \frac{1}{2}) \mathbf{a}_1 + (y_{18} + \frac{1}{2}) \mathbf{a}_2 + &= & -a(x_{18} - \frac{1}{2}) \hat{\mathbf{x}} + b(y_{18} + \frac{1}{2}) \hat{\mathbf{y}} + & (8d) & \text{N VI} \\
& (z_{18} + \frac{1}{2}) \mathbf{a}_3 & & c(z_{18} + \frac{1}{2}) \hat{\mathbf{z}} & & \\
\mathbf{B}_{101} &= x_{19} \mathbf{a}_1 + y_{19} \mathbf{a}_2 + z_{19} \mathbf{a}_3 &= & ax_{19} \hat{\mathbf{x}} + by_{19} \hat{\mathbf{y}} + cz_{19} \hat{\mathbf{z}} & (8d) & \text{O I} \\
\mathbf{B}_{102} &= -(x_{19} - \frac{1}{2}) \mathbf{a}_1 - y_{19} \mathbf{a}_2 + &= & -a(x_{19} - \frac{1}{2}) \hat{\mathbf{x}} - by_{19} \hat{\mathbf{y}} + c(z_{19} + \frac{1}{2}) \hat{\mathbf{z}} & (8d) & \text{O I} \\
& (z_{19} + \frac{1}{2}) \mathbf{a}_3 & & & & \\
\mathbf{B}_{103} &= -x_{19} \mathbf{a}_1 + (y_{19} + \frac{1}{2}) \mathbf{a}_2 - z_{19} \mathbf{a}_3 &= & -ax_{19} \hat{\mathbf{x}} + b(y_{19} + \frac{1}{2}) \hat{\mathbf{y}} - cz_{19} \hat{\mathbf{z}} & (8d) & \text{O I} \\
\mathbf{B}_{104} &= (x_{19} + \frac{1}{2}) \mathbf{a}_1 - (y_{19} - \frac{1}{2}) \mathbf{a}_2 - &= & a(x_{19} + \frac{1}{2}) \hat{\mathbf{x}} - b(y_{19} - \frac{1}{2}) \hat{\mathbf{y}} - & (8d) & \text{O I} \\
& (z_{19} - \frac{1}{2}) \mathbf{a}_3 & & c(z_{19} - \frac{1}{2}) \hat{\mathbf{z}} & & \\
\mathbf{B}_{105} &= -x_{19} \mathbf{a}_1 - y_{19} \mathbf{a}_2 - z_{19} \mathbf{a}_3 &= & -ax_{19} \hat{\mathbf{x}} - by_{19} \hat{\mathbf{y}} - cz_{19} \hat{\mathbf{z}} & (8d) & \text{O I} \\
\mathbf{B}_{106} &= (x_{19} + \frac{1}{2}) \mathbf{a}_1 + y_{19} \mathbf{a}_2 - &= & a(x_{19} + \frac{1}{2}) \hat{\mathbf{x}} + by_{19} \hat{\mathbf{y}} - c(z_{19} - \frac{1}{2}) \hat{\mathbf{z}} & (8d) & \text{O I} \\
& (z_{19} - \frac{1}{2}) \mathbf{a}_3 & & & & \\
\mathbf{B}_{107} &= x_{19} \mathbf{a}_1 - (y_{19} - \frac{1}{2}) \mathbf{a}_2 + z_{19} \mathbf{a}_3 &= & ax_{19} \hat{\mathbf{x}} - b(y_{19} - \frac{1}{2}) \hat{\mathbf{y}} + cz_{19} \hat{\mathbf{z}} & (8d) & \text{O I} \\
\mathbf{B}_{108} &= -(x_{19} - \frac{1}{2}) \mathbf{a}_1 + (y_{19} + \frac{1}{2}) \mathbf{a}_2 + &= & -a(x_{19} - \frac{1}{2}) \hat{\mathbf{x}} + b(y_{19} + \frac{1}{2}) \hat{\mathbf{y}} + & (8d) & \text{O I} \\
& (z_{19} + \frac{1}{2}) \mathbf{a}_3 & & c(z_{19} + \frac{1}{2}) \hat{\mathbf{z}} & &
\end{aligned}$$

References

- [1] I. Typilo, O. Sereda, H. Stoeckli-Evans, R. Gladyshevskii, and D. Semenyshyn, *Refinement of the crystal structure of potassium octacyanomolybdate(IV) dihydrate*, Chem. Met. Alloys **3**, 49–52 (2010).
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- [3] K. Herrmann, ed., *Strukturbericht Band VII 1939* (Akademische Verlagsgesellschaft M. B. H., Leipzig, 1943).