

Manganese-leonite 185K [K₂Mn(SO₄)₂·4H₂O] Structure: A8B2CD12E2_mC200_15_8f_2f_ae_2e11f_2f-001

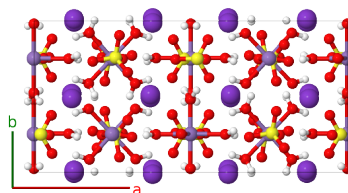
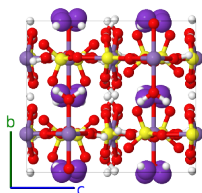
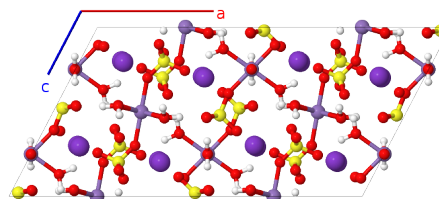
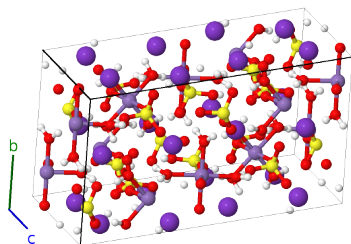
This structure originally had the label A8B2CD12E2_mC200_15_8f_2f_ce_2e11f_2f. Calls to that address will be redirected here.

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<https://aflow.org/p/5SVW>

https://aflow.org/p/A8B2CD12E2_mC200_15_8f_2f_ae_2e11f_2f-001

● H
● K
● Mn
● O
● S



Prototype	H ₈ K ₄ MnO ₁₂ S ₂
AFLOW prototype label	A8B2CD12E2_mC200_15_8f_2f_ae_2e11f_2f-001
Mineral name	manganese-leonite
ICSD	92701
Pearson symbol	mC200
Space group number	15
Space group symbol	C2/c
AFLOW prototype command	aflow --proto=A8B2CD12E2_mC200_15_8f_2f_ae_2e11f_2f-001 --params=a, b/a, c/a, β, y ₂ , y ₃ , y ₄ , x ₅ , y ₅ , z ₅ , x ₆ , y ₆ , z ₆ , x ₇ , y ₇ , z ₇ , x ₈ , y ₈ , z ₈ , x ₉ , y ₉ , z ₉ , x ₁₀ , y ₁₀ , z ₁₀ , x ₁₁ , y ₁₁ , z ₁₁ , x ₁₂ , y ₁₂ , z ₁₂ , x ₁₃ , y ₁₃ , z ₁₃ , x ₁₄ , y ₁₄ , z ₁₄ , x ₁₅ , y ₁₅ , z ₁₅ , x ₁₆ , y ₁₆ , z ₁₆ , x ₁₇ , y ₁₇ , z ₁₇ , x ₁₈ , y ₁₈ , z ₁₈ , x ₁₉ , y ₁₉ , z ₁₉ , x ₂₀ , y ₂₀ , z ₂₀ , x ₂₁ , y ₂₁ , z ₂₁ , x ₂₂ , y ₂₂ , z ₂₂ , x ₂₃ , y ₂₃ , z ₂₃ , x ₂₄ , y ₂₄ , z ₂₄ , x ₂₅ , y ₂₅ , z ₂₅ , x ₂₆ , y ₂₆ , z ₂₆ , x ₂₇ , y ₂₇ , z ₂₇

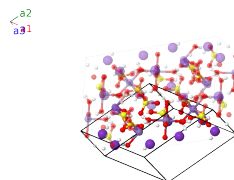
Other compounds with this structure

$\text{K}_2\text{Mg}(\text{SO}_4)_2 \cdot 4\text{H}_2\text{O}$ (leonite), $\text{K}_2\text{Fe}(\text{SO}_4)_2 \cdot 4\text{H}_2\text{O}$ (mereiterite)

- Manganese-leonite is found in three forms:
 - A low-temperature structure, stable below 168K.
 - This intermediate-temperature structure, stable in between 168 and 205K.
 - The room temperature structure, *Strukturbericht H4*₂₃, stable above 205K.
- The current structure orders all of the SO_4 radicals. The data was taken from a sample held at 185K.
- (Hertweck, 2001) give crystallographic information of the 185K phase in the $I2/a$ setting of space group #15, with the origin supposedly shifted by $(\frac{1}{4}, \frac{1}{4}, \frac{1}{2})$ from the -1 point on the a -glide plane (the symmetry operations for this setting may be found here). We were unable to use their data to construct a realistic crystal structure. Instead, we used the interpretation of their results by (Villars, 2016) to put the structure in the standard $C2/c$ setting of space group #15. Unfortunately this does not agree with the ICSD entry. We are investigating further and will update this page when we have more information.

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	0	$=$	0	(4a)	Mn I
\mathbf{B}_2	$\frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2}c \cos \beta \hat{\mathbf{x}} + \frac{1}{2}c \sin \beta \hat{\mathbf{z}}$	(4a)	Mn I
\mathbf{B}_3	$-y_2 \mathbf{a}_1 + y_2 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$\frac{1}{4}c \cos \beta \hat{\mathbf{x}} + by_2 \hat{\mathbf{y}} + \frac{1}{4}c \sin \beta \hat{\mathbf{z}}$	(4e)	Mn II
\mathbf{B}_4	$y_2 \mathbf{a}_1 - y_2 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$\frac{3}{4}c \cos \beta \hat{\mathbf{x}} - by_2 \hat{\mathbf{y}} + \frac{3}{4}c \sin \beta \hat{\mathbf{z}}$	(4e)	Mn II
\mathbf{B}_5	$-y_3 \mathbf{a}_1 + y_3 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$\frac{1}{4}c \cos \beta \hat{\mathbf{x}} + by_3 \hat{\mathbf{y}} + \frac{1}{4}c \sin \beta \hat{\mathbf{z}}$	(4e)	O I
\mathbf{B}_6	$y_3 \mathbf{a}_1 - y_3 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$\frac{3}{4}c \cos \beta \hat{\mathbf{x}} - by_3 \hat{\mathbf{y}} + \frac{3}{4}c \sin \beta \hat{\mathbf{z}}$	(4e)	O I
\mathbf{B}_7	$-y_4 \mathbf{a}_1 + y_4 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$\frac{1}{4}c \cos \beta \hat{\mathbf{x}} + by_4 \hat{\mathbf{y}} + \frac{1}{4}c \sin \beta \hat{\mathbf{z}}$	(4e)	O II
\mathbf{B}_8	$y_4 \mathbf{a}_1 - y_4 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$\frac{3}{4}c \cos \beta \hat{\mathbf{x}} - by_4 \hat{\mathbf{y}} + \frac{3}{4}c \sin \beta \hat{\mathbf{z}}$	(4e)	O II
\mathbf{B}_9	$(x_5 - y_5) \mathbf{a}_1 + (x_5 + y_5) \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$(ax_5 + cz_5 \cos \beta) \hat{\mathbf{x}} + by_5 \hat{\mathbf{y}} + cz_5 \sin \beta \hat{\mathbf{z}}$	(8f)	H I
\mathbf{B}_{10}	$-(x_5 + y_5) \mathbf{a}_1 - (x_5 - y_5) \mathbf{a}_2 - (z_5 - \frac{1}{2}) \mathbf{a}_3$	$=$	$-(ax_5 + c(z_5 - \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} + by_5 \hat{\mathbf{y}} - c(z_5 - \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$	(8f)	H I
\mathbf{B}_{11}	$-(x_5 - y_5) \mathbf{a}_1 - (x_5 + y_5) \mathbf{a}_2 - z_5 \mathbf{a}_3$	$=$	$-(ax_5 + cz_5 \cos \beta) \hat{\mathbf{x}} - by_5 \hat{\mathbf{y}} - cz_5 \sin \beta \hat{\mathbf{z}}$	(8f)	H I
\mathbf{B}_{12}	$(x_5 + y_5) \mathbf{a}_1 + (x_5 - y_5) \mathbf{a}_2 + (z_5 + \frac{1}{2}) \mathbf{a}_3$	$=$	$(ax_5 + c(z_5 + \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} - by_5 \hat{\mathbf{y}} + c(z_5 + \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$	(8f)	H I
\mathbf{B}_{13}	$(x_6 - y_6) \mathbf{a}_1 + (x_6 + y_6) \mathbf{a}_2 + z_6 \mathbf{a}_3$	$=$	$(ax_6 + cz_6 \cos \beta) \hat{\mathbf{x}} + by_6 \hat{\mathbf{y}} + cz_6 \sin \beta \hat{\mathbf{z}}$	(8f)	H II
\mathbf{B}_{14}	$-(x_6 + y_6) \mathbf{a}_1 - (x_6 - y_6) \mathbf{a}_2 - (z_6 - \frac{1}{2}) \mathbf{a}_3$	$=$	$-(ax_6 + c(z_6 - \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} + by_6 \hat{\mathbf{y}} - c(z_6 - \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$	(8f)	H II

$$\begin{aligned}
\mathbf{B}_{15} &= -(x_6 - y_6) \mathbf{a}_1 - (x_6 + y_6) \mathbf{a}_2 - z_6 \mathbf{a}_3 = -(ax_6 + cz_6 \cos \beta) \hat{\mathbf{x}} - by_6 \hat{\mathbf{y}} - cz_6 \sin \beta \hat{\mathbf{z}} & (8f) & \text{H II} \\
\mathbf{B}_{16} &= (x_6 + y_6) \mathbf{a}_1 + (x_6 - y_6) \mathbf{a}_2 + (z_6 + \frac{1}{2}) \mathbf{a}_3 = (ax_6 + c(z_6 + \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} - by_6 \hat{\mathbf{y}} + c(z_6 + \frac{1}{2}) \sin \beta \hat{\mathbf{z}} & (8f) & \text{H II} \\
\mathbf{B}_{17} &= (x_7 - y_7) \mathbf{a}_1 + (x_7 + y_7) \mathbf{a}_2 + z_7 \mathbf{a}_3 = (ax_7 + cz_7 \cos \beta) \hat{\mathbf{x}} + by_7 \hat{\mathbf{y}} + cz_7 \sin \beta \hat{\mathbf{z}} & (8f) & \text{H III} \\
\mathbf{B}_{18} &= -(x_7 + y_7) \mathbf{a}_1 - (x_7 - y_7) \mathbf{a}_2 - (z_7 - \frac{1}{2}) \mathbf{a}_3 = -(ax_7 + c(z_7 - \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} + by_7 \hat{\mathbf{y}} - c(z_7 - \frac{1}{2}) \sin \beta \hat{\mathbf{z}} & (8f) & \text{H III} \\
\mathbf{B}_{19} &= -(x_7 - y_7) \mathbf{a}_1 - (x_7 + y_7) \mathbf{a}_2 - z_7 \mathbf{a}_3 = -(ax_7 + cz_7 \cos \beta) \hat{\mathbf{x}} - by_7 \hat{\mathbf{y}} - cz_7 \sin \beta \hat{\mathbf{z}} & (8f) & \text{H III} \\
\mathbf{B}_{20} &= (x_7 + y_7) \mathbf{a}_1 + (x_7 - y_7) \mathbf{a}_2 + (z_7 + \frac{1}{2}) \mathbf{a}_3 = (ax_7 + c(z_7 + \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} - by_7 \hat{\mathbf{y}} + c(z_7 + \frac{1}{2}) \sin \beta \hat{\mathbf{z}} & (8f) & \text{H III} \\
\mathbf{B}_{21} &= (x_8 - y_8) \mathbf{a}_1 + (x_8 + y_8) \mathbf{a}_2 + z_8 \mathbf{a}_3 = (ax_8 + cz_8 \cos \beta) \hat{\mathbf{x}} + by_8 \hat{\mathbf{y}} + cz_8 \sin \beta \hat{\mathbf{z}} & (8f) & \text{H IV} \\
\mathbf{B}_{22} &= -(x_8 + y_8) \mathbf{a}_1 - (x_8 - y_8) \mathbf{a}_2 - (z_8 - \frac{1}{2}) \mathbf{a}_3 = -(ax_8 + c(z_8 - \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} + by_8 \hat{\mathbf{y}} - c(z_8 - \frac{1}{2}) \sin \beta \hat{\mathbf{z}} & (8f) & \text{H IV} \\
\mathbf{B}_{23} &= -(x_8 - y_8) \mathbf{a}_1 - (x_8 + y_8) \mathbf{a}_2 - z_8 \mathbf{a}_3 = -(ax_8 + cz_8 \cos \beta) \hat{\mathbf{x}} - by_8 \hat{\mathbf{y}} - cz_8 \sin \beta \hat{\mathbf{z}} & (8f) & \text{H IV} \\
\mathbf{B}_{24} &= (x_8 + y_8) \mathbf{a}_1 + (x_8 - y_8) \mathbf{a}_2 + (z_8 + \frac{1}{2}) \mathbf{a}_3 = (ax_8 + c(z_8 + \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} - by_8 \hat{\mathbf{y}} + c(z_8 + \frac{1}{2}) \sin \beta \hat{\mathbf{z}} & (8f) & \text{H IV} \\
\mathbf{B}_{25} &= (x_9 - y_9) \mathbf{a}_1 + (x_9 + y_9) \mathbf{a}_2 + z_9 \mathbf{a}_3 = (ax_9 + cz_9 \cos \beta) \hat{\mathbf{x}} + by_9 \hat{\mathbf{y}} + cz_9 \sin \beta \hat{\mathbf{z}} & (8f) & \text{H V} \\
\mathbf{B}_{26} &= -(x_9 + y_9) \mathbf{a}_1 - (x_9 - y_9) \mathbf{a}_2 - (z_9 - \frac{1}{2}) \mathbf{a}_3 = -(ax_9 + c(z_9 - \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} + by_9 \hat{\mathbf{y}} - c(z_9 - \frac{1}{2}) \sin \beta \hat{\mathbf{z}} & (8f) & \text{H V} \\
\mathbf{B}_{27} &= -(x_9 - y_9) \mathbf{a}_1 - (x_9 + y_9) \mathbf{a}_2 - z_9 \mathbf{a}_3 = -(ax_9 + cz_9 \cos \beta) \hat{\mathbf{x}} - by_9 \hat{\mathbf{y}} - cz_9 \sin \beta \hat{\mathbf{z}} & (8f) & \text{H V} \\
\mathbf{B}_{28} &= (x_9 + y_9) \mathbf{a}_1 + (x_9 - y_9) \mathbf{a}_2 + (z_9 + \frac{1}{2}) \mathbf{a}_3 = (ax_9 + c(z_9 + \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} - by_9 \hat{\mathbf{y}} + c(z_9 + \frac{1}{2}) \sin \beta \hat{\mathbf{z}} & (8f) & \text{H V} \\
\mathbf{B}_{29} &= (x_{10} - y_{10}) \mathbf{a}_1 + (x_{10} + y_{10}) \mathbf{a}_2 + z_{10} \mathbf{a}_3 = (ax_{10} + cz_{10} \cos \beta) \hat{\mathbf{x}} + by_{10} \hat{\mathbf{y}} + cz_{10} \sin \beta \hat{\mathbf{z}} & (8f) & \text{H VI} \\
\mathbf{B}_{30} &= -(x_{10} + y_{10}) \mathbf{a}_1 - (x_{10} - y_{10}) \mathbf{a}_2 - (z_{10} - \frac{1}{2}) \mathbf{a}_3 = -(ax_{10} + c(z_{10} - \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} + by_{10} \hat{\mathbf{y}} - c(z_{10} - \frac{1}{2}) \sin \beta \hat{\mathbf{z}} & (8f) & \text{H VI} \\
\mathbf{B}_{31} &= -(x_{10} - y_{10}) \mathbf{a}_1 - (x_{10} + y_{10}) \mathbf{a}_2 - z_{10} \mathbf{a}_3 = -(ax_{10} + cz_{10} \cos \beta) \hat{\mathbf{x}} - by_{10} \hat{\mathbf{y}} - cz_{10} \sin \beta \hat{\mathbf{z}} & (8f) & \text{H VI} \\
\mathbf{B}_{32} &= (x_{10} + y_{10}) \mathbf{a}_1 + (x_{10} - y_{10}) \mathbf{a}_2 + (z_{10} + \frac{1}{2}) \mathbf{a}_3 = (ax_{10} + c(z_{10} + \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} - by_{10} \hat{\mathbf{y}} + c(z_{10} + \frac{1}{2}) \sin \beta \hat{\mathbf{z}} & (8f) & \text{H VI} \\
\mathbf{B}_{33} &= (x_{11} - y_{11}) \mathbf{a}_1 + (x_{11} + y_{11}) \mathbf{a}_2 + z_{11} \mathbf{a}_3 = (ax_{11} + cz_{11} \cos \beta) \hat{\mathbf{x}} + by_{11} \hat{\mathbf{y}} + cz_{11} \sin \beta \hat{\mathbf{z}} & (8f) & \text{H VII} \\
\mathbf{B}_{34} &= -(x_{11} + y_{11}) \mathbf{a}_1 - (x_{11} - y_{11}) \mathbf{a}_2 - (z_{11} - \frac{1}{2}) \mathbf{a}_3 = -(ax_{11} + c(z_{11} - \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} + by_{11} \hat{\mathbf{y}} - c(z_{11} - \frac{1}{2}) \sin \beta \hat{\mathbf{z}} & (8f) & \text{H VII} \\
\mathbf{B}_{35} &= -(x_{11} - y_{11}) \mathbf{a}_1 - (x_{11} + y_{11}) \mathbf{a}_2 - z_{11} \mathbf{a}_3 = -(ax_{11} + cz_{11} \cos \beta) \hat{\mathbf{x}} - by_{11} \hat{\mathbf{y}} - cz_{11} \sin \beta \hat{\mathbf{z}} & (8f) & \text{H VII} \\
\mathbf{B}_{36} &= (x_{11} + y_{11}) \mathbf{a}_1 + (x_{11} - y_{11}) \mathbf{a}_2 + (z_{11} + \frac{1}{2}) \mathbf{a}_3 = (ax_{11} + c(z_{11} + \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} - by_{11} \hat{\mathbf{y}} + c(z_{11} + \frac{1}{2}) \sin \beta \hat{\mathbf{z}} & (8f) & \text{H VII} \\
\mathbf{B}_{37} &= (x_{12} - y_{12}) \mathbf{a}_1 + (x_{12} + y_{12}) \mathbf{a}_2 + z_{12} \mathbf{a}_3 = (ax_{12} + cz_{12} \cos \beta) \hat{\mathbf{x}} + by_{12} \hat{\mathbf{y}} + cz_{12} \sin \beta \hat{\mathbf{z}} & (8f) & \text{H VIII}
\end{aligned}$$

$$\begin{aligned}
\mathbf{B}_{84} &= \begin{pmatrix} (x_{23} + y_{23}) \mathbf{a}_1 + \\ (x_{23} - y_{23}) \mathbf{a}_2 + (z_{23} + \frac{1}{2}) \mathbf{a}_3 \end{pmatrix} = \begin{pmatrix} (ax_{23} + c(z_{23} + \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} - by_{23} \hat{\mathbf{y}} + \\ c(z_{23} + \frac{1}{2}) \sin \beta \hat{\mathbf{z}} \end{pmatrix} & (8f) & \text{O XI} \\
\mathbf{B}_{85} &= \begin{pmatrix} (x_{24} - y_{24}) \mathbf{a}_1 + \\ (x_{24} + y_{24}) \mathbf{a}_2 + z_{24} \mathbf{a}_3 \end{pmatrix} = \begin{pmatrix} (ax_{24} + cz_{24} \cos \beta) \hat{\mathbf{x}} + by_{24} \hat{\mathbf{y}} + cz_{24} \sin \beta \hat{\mathbf{z}} \end{pmatrix} & (8f) & \text{O XII} \\
\mathbf{B}_{86} &= \begin{pmatrix} -(x_{24} + y_{24}) \mathbf{a}_1 - \\ (x_{24} - y_{24}) \mathbf{a}_2 - (z_{24} - \frac{1}{2}) \mathbf{a}_3 \end{pmatrix} = \begin{pmatrix} -(ax_{24} + c(z_{24} - \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} + by_{24} \hat{\mathbf{y}} - \\ c(z_{24} - \frac{1}{2}) \sin \beta \hat{\mathbf{z}} \end{pmatrix} & (8f) & \text{O XII} \\
\mathbf{B}_{87} &= \begin{pmatrix} -(x_{24} - y_{24}) \mathbf{a}_1 - \\ (x_{24} + y_{24}) \mathbf{a}_2 - z_{24} \mathbf{a}_3 \end{pmatrix} = \begin{pmatrix} -(ax_{24} + cz_{24} \cos \beta) \hat{\mathbf{x}} - by_{24} \hat{\mathbf{y}} - \\ cz_{24} \sin \beta \hat{\mathbf{z}} \end{pmatrix} & (8f) & \text{O XII} \\
\mathbf{B}_{88} &= \begin{pmatrix} (x_{24} + y_{24}) \mathbf{a}_1 + \\ (x_{24} - y_{24}) \mathbf{a}_2 + (z_{24} + \frac{1}{2}) \mathbf{a}_3 \end{pmatrix} = \begin{pmatrix} (ax_{24} + c(z_{24} + \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} - by_{24} \hat{\mathbf{y}} + \\ c(z_{24} + \frac{1}{2}) \sin \beta \hat{\mathbf{z}} \end{pmatrix} & (8f) & \text{O XII} \\
\mathbf{B}_{89} &= \begin{pmatrix} (x_{25} - y_{25}) \mathbf{a}_1 + \\ (x_{25} + y_{25}) \mathbf{a}_2 + z_{25} \mathbf{a}_3 \end{pmatrix} = \begin{pmatrix} (ax_{25} + cz_{25} \cos \beta) \hat{\mathbf{x}} + by_{25} \hat{\mathbf{y}} + cz_{25} \sin \beta \hat{\mathbf{z}} \end{pmatrix} & (8f) & \text{O XIII} \\
\mathbf{B}_{90} &= \begin{pmatrix} -(x_{25} + y_{25}) \mathbf{a}_1 - \\ (x_{25} - y_{25}) \mathbf{a}_2 - (z_{25} - \frac{1}{2}) \mathbf{a}_3 \end{pmatrix} = \begin{pmatrix} -(ax_{25} + c(z_{25} - \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} + by_{25} \hat{\mathbf{y}} - \\ c(z_{25} - \frac{1}{2}) \sin \beta \hat{\mathbf{z}} \end{pmatrix} & (8f) & \text{O XIII} \\
\mathbf{B}_{91} &= \begin{pmatrix} -(x_{25} - y_{25}) \mathbf{a}_1 - \\ (x_{25} + y_{25}) \mathbf{a}_2 - z_{25} \mathbf{a}_3 \end{pmatrix} = \begin{pmatrix} -(ax_{25} + cz_{25} \cos \beta) \hat{\mathbf{x}} - by_{25} \hat{\mathbf{y}} - \\ cz_{25} \sin \beta \hat{\mathbf{z}} \end{pmatrix} & (8f) & \text{O XIII} \\
\mathbf{B}_{92} &= \begin{pmatrix} (x_{25} + y_{25}) \mathbf{a}_1 + \\ (x_{25} - y_{25}) \mathbf{a}_2 + (z_{25} + \frac{1}{2}) \mathbf{a}_3 \end{pmatrix} = \begin{pmatrix} (ax_{25} + c(z_{25} + \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} - by_{25} \hat{\mathbf{y}} + \\ c(z_{25} + \frac{1}{2}) \sin \beta \hat{\mathbf{z}} \end{pmatrix} & (8f) & \text{O XIII} \\
\mathbf{B}_{93} &= \begin{pmatrix} (x_{26} - y_{26}) \mathbf{a}_1 + \\ (x_{26} + y_{26}) \mathbf{a}_2 + z_{26} \mathbf{a}_3 \end{pmatrix} = \begin{pmatrix} (ax_{26} + cz_{26} \cos \beta) \hat{\mathbf{x}} + by_{26} \hat{\mathbf{y}} + cz_{26} \sin \beta \hat{\mathbf{z}} \end{pmatrix} & (8f) & \text{S I} \\
\mathbf{B}_{94} &= \begin{pmatrix} -(x_{26} + y_{26}) \mathbf{a}_1 - \\ (x_{26} - y_{26}) \mathbf{a}_2 - (z_{26} - \frac{1}{2}) \mathbf{a}_3 \end{pmatrix} = \begin{pmatrix} -(ax_{26} + c(z_{26} - \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} + by_{26} \hat{\mathbf{y}} - \\ c(z_{26} - \frac{1}{2}) \sin \beta \hat{\mathbf{z}} \end{pmatrix} & (8f) & \text{S I} \\
\mathbf{B}_{95} &= \begin{pmatrix} -(x_{26} - y_{26}) \mathbf{a}_1 - \\ (x_{26} + y_{26}) \mathbf{a}_2 - z_{26} \mathbf{a}_3 \end{pmatrix} = \begin{pmatrix} -(ax_{26} + cz_{26} \cos \beta) \hat{\mathbf{x}} - by_{26} \hat{\mathbf{y}} - \\ cz_{26} \sin \beta \hat{\mathbf{z}} \end{pmatrix} & (8f) & \text{S I} \\
\mathbf{B}_{96} &= \begin{pmatrix} (x_{26} + y_{26}) \mathbf{a}_1 + \\ (x_{26} - y_{26}) \mathbf{a}_2 + (z_{26} + \frac{1}{2}) \mathbf{a}_3 \end{pmatrix} = \begin{pmatrix} (ax_{26} + c(z_{26} + \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} - by_{26} \hat{\mathbf{y}} + \\ c(z_{26} + \frac{1}{2}) \sin \beta \hat{\mathbf{z}} \end{pmatrix} & (8f) & \text{S I} \\
\mathbf{B}_{97} &= \begin{pmatrix} (x_{27} - y_{27}) \mathbf{a}_1 + \\ (x_{27} + y_{27}) \mathbf{a}_2 + z_{27} \mathbf{a}_3 \end{pmatrix} = \begin{pmatrix} (ax_{27} + cz_{27} \cos \beta) \hat{\mathbf{x}} + by_{27} \hat{\mathbf{y}} + cz_{27} \sin \beta \hat{\mathbf{z}} \end{pmatrix} & (8f) & \text{S II} \\
\mathbf{B}_{98} &= \begin{pmatrix} -(x_{27} + y_{27}) \mathbf{a}_1 - \\ (x_{27} - y_{27}) \mathbf{a}_2 - (z_{27} - \frac{1}{2}) \mathbf{a}_3 \end{pmatrix} = \begin{pmatrix} -(ax_{27} + c(z_{27} - \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} + by_{27} \hat{\mathbf{y}} - \\ c(z_{27} - \frac{1}{2}) \sin \beta \hat{\mathbf{z}} \end{pmatrix} & (8f) & \text{S II} \\
\mathbf{B}_{99} &= \begin{pmatrix} -(x_{27} - y_{27}) \mathbf{a}_1 - \\ (x_{27} + y_{27}) \mathbf{a}_2 - z_{27} \mathbf{a}_3 \end{pmatrix} = \begin{pmatrix} -(ax_{27} + cz_{27} \cos \beta) \hat{\mathbf{x}} - by_{27} \hat{\mathbf{y}} - \\ cz_{27} \sin \beta \hat{\mathbf{z}} \end{pmatrix} & (8f) & \text{S II} \\
\mathbf{B}_{100} &= \begin{pmatrix} (x_{27} + y_{27}) \mathbf{a}_1 + \\ (x_{27} - y_{27}) \mathbf{a}_2 + (z_{27} + \frac{1}{2}) \mathbf{a}_3 \end{pmatrix} = \begin{pmatrix} (ax_{27} + c(z_{27} + \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} - by_{27} \hat{\mathbf{y}} + \\ c(z_{27} + \frac{1}{2}) \sin \beta \hat{\mathbf{z}} \end{pmatrix} & (8f) & \text{S II}
\end{aligned}$$

References

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- [2] *$K_2\text{Mn}(\text{SO}_4)_2 \cdot 4\text{H}_2\text{O}$ ($K_2\text{Mn}[\text{SO}_4]_2[\text{H}_2\text{O}]_4$ mon1, $T = 185$ K) Crystal Structure: Datasheet from “PAULING FILE Multinaries Edition – 2012” in SpringerMaterials (https://materials.springer.com/isp/crystallographic/docs/sd_1811721). Copyright 2016 Springer-Verlag Berlin Heidelberg & Material Phases Data System (MPDS), Switzerland & National Institute for Materials Science (NIMS), Japan.*