

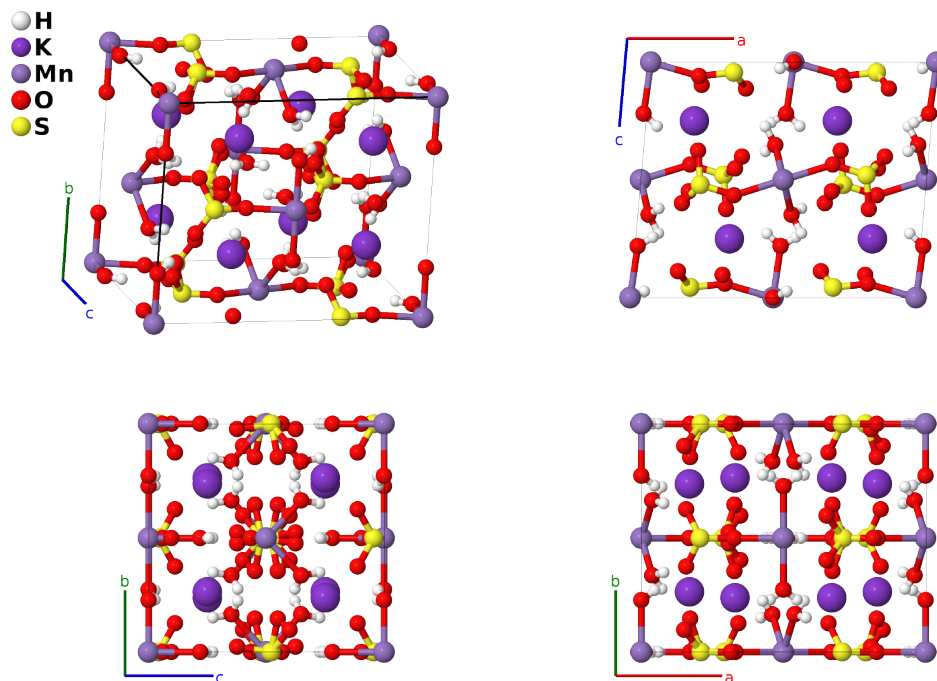
Manganese-leonite $[K_2Mn(SO_4)_2 \cdot 4H_2O, H4_{23}]$ Structure: A8B2CD15E2_mC112_12_2i3j_j_ac_g4i5j_2i-001

This structure originally had the label A8B2CD15E2_mC112_12_2i3j_j_ad_g4i5j_2i. Calls to that address will be redirected here.

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<https://aflow.org/p/KYS8>

https://aflow.org/p/A8B2CD15E2_mC112_12_2i3j_j_ac_g4i5j_2i-001



Prototype	$H_8K_2MnO_{12}S_2$
AFLOW prototype label	A8B2CD15E2_mC112_12_2i3j_j_ac_g4i5j_2i-001
<i>Strukturbericht</i> designation	$H4_{23}$
Mineral name	manganese-leonite
ICSD	92700
Pearson symbol	mC112
Space group number	12
Space group symbol	$C2/m$
AFLOW prototype command	<pre>aflow --proto=A8B2CD15E2_mC112_12_2i3j_j_ac_g4i5j_2i-001 --params=a,b/a,c/a,beta,y3,x4,z4,x5,z5,x6,z6,x7,z7,x8,z8,x9,z9,x10,z10,x11,z11, x12,y12,z12,x13,y13,z13,x14,y14,z14,x15,y15,z15,x16,y16,z16,x17,y17,z17,x18,y18,z18,x19, y19,z19,x20,y20,z20</pre>

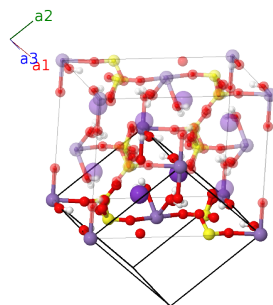
Other compounds with this structure

(NH₂)₂Co(SO₄)₂·4H₂O, (NH₂)₂Cu(SO₄)₂·4H₂O, (NH₂)₂Fe(SO₄)₂·4H₂O, (NH₂)₂Mg(SO₄)₂·4H₂O, (NH₂)₂Mn(SO₄)₂·4H₂O, Cd₂Co(SO₄)₂·4H₂O, Cd₂Cu(SO₄)₂·4H₂O, Cd₂Fe(SO₄)₂·4H₂O, Cd₂Mg(SO₄)₂·4H₂O, Cd₂Mn(SO₄)₂·4H₂O, Cs₂Co(SO₄)₂·4H₂O, Cs₂Cu(SO₄)₂·4H₂O, Cs₂Fe(SO₄)₂·4H₂O, Cs₂Mg(SO₄)₂·4H₂O, Cs₂Mn(SO₄)₂·4H₂O, K₂Co(SO₄)₂·4H₂O, K₂Cu(SO₄)₂·4H₂O, K₂Fe(SO₄)₂·4H₂O (mererite), K₂Mg(SO₄)₂·4H₂O (leonite), Rb₂Co(SO₄)₂·4H₂O, Rb₂Cu(SO₄)₂·4H₂O, Rb₂Fe(SO₄)₂·4H₂O, Rb₂Mg(SO₄)₂·4H₂O, Rb₂Mn(SO₄)₂·4H₂O, Tl₂Co(SO₄)₂·4H₂O, Tl₂Cu(SO₄)₂·4H₂O, Tl₂Fe(SO₄)₂·4H₂O, Tl₂Mg(SO₄)₂·4H₂O, Tl₂Mn(SO₄)₂·4H₂O

- Manganese-leonite is found in three forms:
 - A low-temperature structure, stable below 168K.
 - An intermediate-temperature structure, stable in between 168 and 205K.
 - This room temperature structure, *Strukturbericht H4₂₃*, stable above 205K.
- Properly the prototype of leonite is K₂Mg(SO₄)₂·4H₂O, but (Herrmann, 1943) gives manganese-leonite *Strukturbericht* symbol *H4₂₃*, so we will use Mn-leonite as the prototype.
- Unlike the lower temperature structures, this leonite structure is characterized by the disorder of the second sulfate group, centered on atom S-II (Hertweck, 2001). The oxygen sites around S-II, labeled O-VII, O-VIII, and O-IX in our notation, are only occupied 50% of the time. (Anspach, 1939), who did the original determination of this structure, was not able to see the disorder and so gives an ordered structure for both sulfates.
- We use the structure determined by (Hertweck, 2001) at room temperature, 293K.

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	(2a)	Mn I
\mathbf{B}_2	$\frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2}c \cos \beta \hat{\mathbf{x}} + \frac{1}{2}c \sin \beta \hat{\mathbf{z}}$	(2c)	Mn II
\mathbf{B}_3	$-y_3 \mathbf{a}_1 + y_3 \mathbf{a}_2$	$=$	$by_3 \hat{\mathbf{y}}$	(4g)	O I
\mathbf{B}_4	$y_3 \mathbf{a}_1 - y_3 \mathbf{a}_2$	$=$	$-by_3 \hat{\mathbf{y}}$	(4g)	O I
\mathbf{B}_5	$x_4 \mathbf{a}_1 + x_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$(ax_4 + cz_4 \cos \beta) \hat{\mathbf{x}} + cz_4 \sin \beta \hat{\mathbf{z}}$	(4i)	H I
\mathbf{B}_6	$-x_4 \mathbf{a}_1 - x_4 \mathbf{a}_2 - z_4 \mathbf{a}_3$	$=$	$-(ax_4 + cz_4 \cos \beta) \hat{\mathbf{x}} - cz_4 \sin \beta \hat{\mathbf{z}}$	(4i)	H I
\mathbf{B}_7	$x_5 \mathbf{a}_1 + x_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$(ax_5 + cz_5 \cos \beta) \hat{\mathbf{x}} + cz_5 \sin \beta \hat{\mathbf{z}}$	(4i)	H II
\mathbf{B}_8	$-x_5 \mathbf{a}_1 - x_5 \mathbf{a}_2 - z_5 \mathbf{a}_3$	$=$	$-(ax_5 + cz_5 \cos \beta) \hat{\mathbf{x}} - cz_5 \sin \beta \hat{\mathbf{z}}$	(4i)	H II
\mathbf{B}_9	$x_6 \mathbf{a}_1 + x_6 \mathbf{a}_2 + z_6 \mathbf{a}_3$	$=$	$(ax_6 + cz_6 \cos \beta) \hat{\mathbf{x}} + cz_6 \sin \beta \hat{\mathbf{z}}$	(4i)	O II
\mathbf{B}_{10}	$-x_6 \mathbf{a}_1 - x_6 \mathbf{a}_2 - z_6 \mathbf{a}_3$	$=$	$-(ax_6 + cz_6 \cos \beta) \hat{\mathbf{x}} - cz_6 \sin \beta \hat{\mathbf{z}}$	(4i)	O II
\mathbf{B}_{11}	$x_7 \mathbf{a}_1 + x_7 \mathbf{a}_2 + z_7 \mathbf{a}_3$	$=$	$(ax_7 + cz_7 \cos \beta) \hat{\mathbf{x}} + cz_7 \sin \beta \hat{\mathbf{z}}$	(4i)	O III
\mathbf{B}_{12}	$-x_7 \mathbf{a}_1 - x_7 \mathbf{a}_2 - z_7 \mathbf{a}_3$	$=$	$-(ax_7 + cz_7 \cos \beta) \hat{\mathbf{x}} - cz_7 \sin \beta \hat{\mathbf{z}}$	(4i)	O III

$$\begin{aligned}
\mathbf{B}_{40} &= \begin{pmatrix} (x_{16} + y_{16}) \mathbf{a}_1 + \\ (x_{16} - y_{16}) \mathbf{a}_2 + z_{16} \mathbf{a}_3 \end{pmatrix} = (ax_{16} + cz_{16} \cos \beta) \hat{\mathbf{x}} - by_{16} \hat{\mathbf{y}} + cz_{16} \sin \beta \hat{\mathbf{z}} & (8j) & \text{O VI} \\
\mathbf{B}_{41} &= \begin{pmatrix} (x_{17} - y_{17}) \mathbf{a}_1 + \\ (x_{17} + y_{17}) \mathbf{a}_2 + z_{17} \mathbf{a}_3 \end{pmatrix} = (ax_{17} + cz_{17} \cos \beta) \hat{\mathbf{x}} + by_{17} \hat{\mathbf{y}} + cz_{17} \sin \beta \hat{\mathbf{z}} & (8j) & \text{O VII} \\
\mathbf{B}_{42} &= \begin{pmatrix} -(x_{17} + y_{17}) \mathbf{a}_1 - \\ (x_{17} - y_{17}) \mathbf{a}_2 - z_{17} \mathbf{a}_3 \end{pmatrix} = -(ax_{17} + cz_{17} \cos \beta) \hat{\mathbf{x}} + by_{17} \hat{\mathbf{y}} - cz_{17} \sin \beta \hat{\mathbf{z}} & (8j) & \text{O VII} \\
\mathbf{B}_{43} &= \begin{pmatrix} -(x_{17} - y_{17}) \mathbf{a}_1 - \\ (x_{17} + y_{17}) \mathbf{a}_2 - z_{17} \mathbf{a}_3 \end{pmatrix} = -(ax_{17} + cz_{17} \cos \beta) \hat{\mathbf{x}} - by_{17} \hat{\mathbf{y}} - cz_{17} \sin \beta \hat{\mathbf{z}} & (8j) & \text{O VII} \\
\mathbf{B}_{44} &= \begin{pmatrix} (x_{17} + y_{17}) \mathbf{a}_1 + \\ (x_{17} - y_{17}) \mathbf{a}_2 + z_{17} \mathbf{a}_3 \end{pmatrix} = (ax_{17} + cz_{17} \cos \beta) \hat{\mathbf{x}} - by_{17} \hat{\mathbf{y}} + cz_{17} \sin \beta \hat{\mathbf{z}} & (8j) & \text{O VII} \\
\mathbf{B}_{45} &= \begin{pmatrix} (x_{18} - y_{18}) \mathbf{a}_1 + \\ (x_{18} + y_{18}) \mathbf{a}_2 + z_{18} \mathbf{a}_3 \end{pmatrix} = (ax_{18} + cz_{18} \cos \beta) \hat{\mathbf{x}} + by_{18} \hat{\mathbf{y}} + cz_{18} \sin \beta \hat{\mathbf{z}} & (8j) & \text{O VIII} \\
\mathbf{B}_{46} &= \begin{pmatrix} -(x_{18} + y_{18}) \mathbf{a}_1 - \\ (x_{18} - y_{18}) \mathbf{a}_2 - z_{18} \mathbf{a}_3 \end{pmatrix} = -(ax_{18} + cz_{18} \cos \beta) \hat{\mathbf{x}} + by_{18} \hat{\mathbf{y}} - cz_{18} \sin \beta \hat{\mathbf{z}} & (8j) & \text{O VIII} \\
\mathbf{B}_{47} &= \begin{pmatrix} -(x_{18} - y_{18}) \mathbf{a}_1 - \\ (x_{18} + y_{18}) \mathbf{a}_2 - z_{18} \mathbf{a}_3 \end{pmatrix} = -(ax_{18} + cz_{18} \cos \beta) \hat{\mathbf{x}} - by_{18} \hat{\mathbf{y}} - cz_{18} \sin \beta \hat{\mathbf{z}} & (8j) & \text{O VIII} \\
\mathbf{B}_{48} &= \begin{pmatrix} (x_{18} + y_{18}) \mathbf{a}_1 + \\ (x_{18} - y_{18}) \mathbf{a}_2 + z_{18} \mathbf{a}_3 \end{pmatrix} = (ax_{18} + cz_{18} \cos \beta) \hat{\mathbf{x}} - by_{18} \hat{\mathbf{y}} + cz_{18} \sin \beta \hat{\mathbf{z}} & (8j) & \text{O VIII} \\
\mathbf{B}_{49} &= \begin{pmatrix} (x_{19} - y_{19}) \mathbf{a}_1 + \\ (x_{19} + y_{19}) \mathbf{a}_2 + z_{19} \mathbf{a}_3 \end{pmatrix} = (ax_{19} + cz_{19} \cos \beta) \hat{\mathbf{x}} + by_{19} \hat{\mathbf{y}} + cz_{19} \sin \beta \hat{\mathbf{z}} & (8j) & \text{O IX} \\
\mathbf{B}_{50} &= \begin{pmatrix} -(x_{19} + y_{19}) \mathbf{a}_1 - \\ (x_{19} - y_{19}) \mathbf{a}_2 - z_{19} \mathbf{a}_3 \end{pmatrix} = -(ax_{19} + cz_{19} \cos \beta) \hat{\mathbf{x}} + by_{19} \hat{\mathbf{y}} - cz_{19} \sin \beta \hat{\mathbf{z}} & (8j) & \text{O IX} \\
\mathbf{B}_{51} &= \begin{pmatrix} -(x_{19} - y_{19}) \mathbf{a}_1 - \\ (x_{19} + y_{19}) \mathbf{a}_2 - z_{19} \mathbf{a}_3 \end{pmatrix} = -(ax_{19} + cz_{19} \cos \beta) \hat{\mathbf{x}} - by_{19} \hat{\mathbf{y}} - cz_{19} \sin \beta \hat{\mathbf{z}} & (8j) & \text{O IX} \\
\mathbf{B}_{52} &= \begin{pmatrix} (x_{19} + y_{19}) \mathbf{a}_1 + \\ (x_{19} - y_{19}) \mathbf{a}_2 + z_{19} \mathbf{a}_3 \end{pmatrix} = (ax_{19} + cz_{19} \cos \beta) \hat{\mathbf{x}} - by_{19} \hat{\mathbf{y}} + cz_{19} \sin \beta \hat{\mathbf{z}} & (8j) & \text{O IX} \\
\mathbf{B}_{53} &= \begin{pmatrix} (x_{20} - y_{20}) \mathbf{a}_1 + \\ (x_{20} + y_{20}) \mathbf{a}_2 + z_{20} \mathbf{a}_3 \end{pmatrix} = (ax_{20} + cz_{20} \cos \beta) \hat{\mathbf{x}} + by_{20} \hat{\mathbf{y}} + cz_{20} \sin \beta \hat{\mathbf{z}} & (8j) & \text{O X} \\
\mathbf{B}_{54} &= \begin{pmatrix} -(x_{20} + y_{20}) \mathbf{a}_1 - \\ (x_{20} - y_{20}) \mathbf{a}_2 - z_{20} \mathbf{a}_3 \end{pmatrix} = -(ax_{20} + cz_{20} \cos \beta) \hat{\mathbf{x}} + by_{20} \hat{\mathbf{y}} - cz_{20} \sin \beta \hat{\mathbf{z}} & (8j) & \text{O X} \\
\mathbf{B}_{55} &= \begin{pmatrix} -(x_{20} - y_{20}) \mathbf{a}_1 - \\ (x_{20} + y_{20}) \mathbf{a}_2 - z_{20} \mathbf{a}_3 \end{pmatrix} = -(ax_{20} + cz_{20} \cos \beta) \hat{\mathbf{x}} - by_{20} \hat{\mathbf{y}} - cz_{20} \sin \beta \hat{\mathbf{z}} & (8j) & \text{O X} \\
\mathbf{B}_{56} &= \begin{pmatrix} (x_{20} + y_{20}) \mathbf{a}_1 + \\ (x_{20} - y_{20}) \mathbf{a}_2 + z_{20} \mathbf{a}_3 \end{pmatrix} = (ax_{20} + cz_{20} \cos \beta) \hat{\mathbf{x}} - by_{20} \hat{\mathbf{y}} + cz_{20} \sin \beta \hat{\mathbf{z}} & (8j) & \text{O X}
\end{aligned}$$

References

- [1] B. Hertweck, G. Giester, and E. Libowitzky, *The crystal structures of the low-temperature phases of leonite-type compounds, $K_2\text{Me}(\text{SO}_4)_2 \cdot 4\text{H}_2\text{O}$ ($\text{Me}^{2+} = \text{Mg}, \text{Mn}, \text{Fe}$)*, Am. Mineral. **86**, 1282–1292 (2001), doi:10.2138/am-2001-1016.
- [2] H. Anspach, *Die Struktur von Mn-Leonit*, Z. Kristallogr. **101**, 39–77 (1939), doi:10.1524/zkri.1939.101.1.39.
- [3] K. Herrmann, ed., *Strukturbericht Band VII 1939* (Akademische Verlagsgesellschaft M. B. H., Leipzig, 1943).