

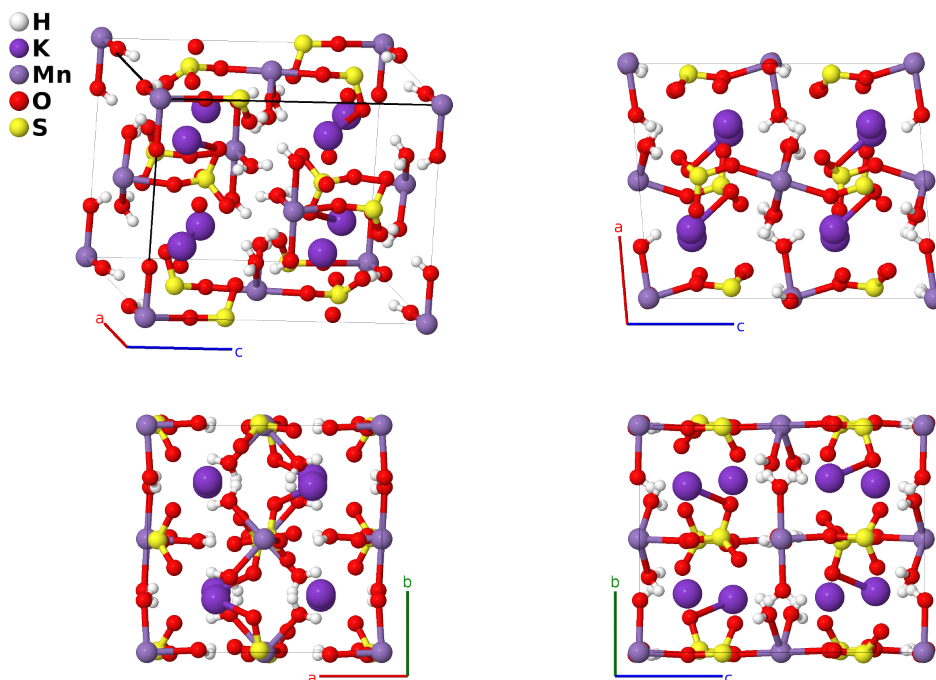
Manganese-leonite 110K [K₂Mn(SO₄)₂·4H₂O] Structure: A8B2CD12E2_mP100_14_8e_2e_ab_12e_2e-001

This structure originally had the label A8B2CD12E2_mP100_14_8e_2e_ad_12e_2e. Calls to that address will be redirected here.

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<https://aflow.org/p/V1SG>

https://aflow.org/p/A8B2CD12E2_mP100_14_8e_2e_ab_12e_2e-001



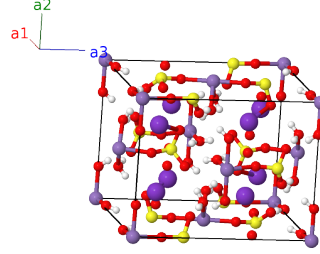
| | |
|-------------------------|---|
| Prototype | H ₈ K ₂ MnO ₁₂ S ₂ |
| AFLOW prototype label | A8B2CD12E2_mP100_14_8e_2e_ab_12e_2e-001 |
| Mineral name | manganese-leonite |
| ICSD | 92702 |
| Pearson symbol | mP100 |
| Space group number | 14 |
| Space group symbol | <i>P</i> 2 ₁ / <i>c</i> |
| AFLOW prototype command | <pre>aflow --proto=A8B2CD12E2_mP100_14_8e_2e_ab_12e_2e-001 --params=a,b/a,c/a,β,x₃,y₃,z₃,x₄,y₄,z₄,x₅,y₅,z₅,x₆,y₆,z₆,x₇,y₇,z₇,x₈,y₈,z₈,x₉, y₉,z₉,x₁₀,y₁₀,z₁₀,x₁₁,y₁₁,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,x₂₁,y₂₁,z₂₁,x₂₂,y₂₂,z₂₂,x₂₃,y₂₃,z₂₃,x₂₄, y₂₄,z₂₄,x₂₅,y₂₅,z₂₅,x₂₆,y₂₆,z₂₆</pre> |

Other compounds with this structure
K₂Mg(SO₄)₂·4H₂O (leonite)

- Manganese-leonite is found in three forms:
 - This low-temperature structure, stable below 168K.
 - An 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 SO₄ radicals. The data was taken from a sample held at 100K.
- (Hertweck, 2001) give crystallographic information of this phase in the $P2_1/a$ setting of space group #14. We used FINDSYM to transform this to the $P2_1/c$ setting, which resulted in a switching of the a - and c -axes.

Simple Monoclinic primitive vectors

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



Basis vectors

| | Lattice coordinates | = | Cartesian coordinates | Wyckoff position | Atom type |
|-------------------|---|---|---|------------------|-----------|
| \mathbf{B}_1 | 0 | = | 0 | (2a) | Mn I |
| \mathbf{B}_2 | $\frac{1}{2} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$ | = | $\frac{1}{2} c \cos \beta \hat{\mathbf{x}} + \frac{1}{2} b \hat{\mathbf{y}} + \frac{1}{2} c \sin \beta \hat{\mathbf{z}}$ | (2a) | Mn I |
| \mathbf{B}_3 | $\frac{1}{2} \mathbf{a}_1$ | = | $\frac{1}{2} a \hat{\mathbf{x}}$ | (2b) | Mn II |
| \mathbf{B}_4 | $\frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$ | = | $\frac{1}{2} (a + c \cos \beta) \hat{\mathbf{x}} + \frac{1}{2} b \hat{\mathbf{y}} + \frac{1}{2} c \sin \beta \hat{\mathbf{z}}$ | (2b) | Mn II |
| \mathbf{B}_5 | $x_3 \mathbf{a}_1 + y_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$ | = | $(ax_3 + cz_3 \cos \beta) \hat{\mathbf{x}} + by_3 \hat{\mathbf{y}} + cz_3 \sin \beta \hat{\mathbf{z}}$ | (4e) | H I |
| \mathbf{B}_6 | $-x_3 \mathbf{a}_1 + (y_3 + \frac{1}{2}) \mathbf{a}_2 - (z_3 - \frac{1}{2}) \mathbf{a}_3$ | = | $-(ax_3 + c(z_3 - \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} + b(y_3 + \frac{1}{2}) \hat{\mathbf{y}} - c(z_3 - \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$ | (4e) | H I |
| \mathbf{B}_7 | $-x_3 \mathbf{a}_1 - y_3 \mathbf{a}_2 - z_3 \mathbf{a}_3$ | = | $-(ax_3 + cz_3 \cos \beta) \hat{\mathbf{x}} - by_3 \hat{\mathbf{y}} - cz_3 \sin \beta \hat{\mathbf{z}}$ | (4e) | H I |
| \mathbf{B}_8 | $x_3 \mathbf{a}_1 - (y_3 - \frac{1}{2}) \mathbf{a}_2 + (z_3 + \frac{1}{2}) \mathbf{a}_3$ | = | $(ax_3 + c(z_3 + \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} - b(y_3 - \frac{1}{2}) \hat{\mathbf{y}} + c(z_3 + \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$ | (4e) | H I |
| \mathbf{B}_9 | $x_4 \mathbf{a}_1 + y_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$ | = | $(ax_4 + cz_4 \cos \beta) \hat{\mathbf{x}} + by_4 \hat{\mathbf{y}} + cz_4 \sin \beta \hat{\mathbf{z}}$ | (4e) | H II |
| \mathbf{B}_{10} | $-x_4 \mathbf{a}_1 + (y_4 + \frac{1}{2}) \mathbf{a}_2 - (z_4 - \frac{1}{2}) \mathbf{a}_3$ | = | $-(ax_4 + c(z_4 - \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} + b(y_4 + \frac{1}{2}) \hat{\mathbf{y}} - c(z_4 - \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$ | (4e) | H II |
| \mathbf{B}_{11} | $-x_4 \mathbf{a}_1 - y_4 \mathbf{a}_2 - z_4 \mathbf{a}_3$ | = | $-(ax_4 + cz_4 \cos \beta) \hat{\mathbf{x}} - by_4 \hat{\mathbf{y}} - cz_4 \sin \beta \hat{\mathbf{z}}$ | (4e) | H II |
| \mathbf{B}_{12} | $x_4 \mathbf{a}_1 - (y_4 - \frac{1}{2}) \mathbf{a}_2 + (z_4 + \frac{1}{2}) \mathbf{a}_3$ | = | $(ax_4 + c(z_4 + \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} - b(y_4 - \frac{1}{2}) \hat{\mathbf{y}} + c(z_4 + \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$ | (4e) | H II |
| \mathbf{B}_{13} | $x_5 \mathbf{a}_1 + y_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$ | = | $(ax_5 + cz_5 \cos \beta) \hat{\mathbf{x}} + by_5 \hat{\mathbf{y}} + cz_5 \sin \beta \hat{\mathbf{z}}$ | (4e) | H III |
| \mathbf{B}_{14} | $-x_5 \mathbf{a}_1 + (y_5 + \frac{1}{2}) \mathbf{a}_2 - (z_5 - \frac{1}{2}) \mathbf{a}_3$ | = | $-(ax_5 + c(z_5 - \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} + b(y_5 + \frac{1}{2}) \hat{\mathbf{y}} - c(z_5 - \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$ | (4e) | H III |
| \mathbf{B}_{15} | $-x_5 \mathbf{a}_1 - y_5 \mathbf{a}_2 - z_5 \mathbf{a}_3$ | = | $-(ax_5 + cz_5 \cos \beta) \hat{\mathbf{x}} - by_5 \hat{\mathbf{y}} - cz_5 \sin \beta \hat{\mathbf{z}}$ | (4e) | H III |
| \mathbf{B}_{16} | $x_5 \mathbf{a}_1 - (y_5 - \frac{1}{2}) \mathbf{a}_2 + (z_5 + \frac{1}{2}) \mathbf{a}_3$ | = | $(ax_5 + c(z_5 + \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} - b(y_5 - \frac{1}{2}) \hat{\mathbf{y}} + c(z_5 + \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$ | (4e) | H III |
| \mathbf{B}_{17} | $x_6 \mathbf{a}_1 + y_6 \mathbf{a}_2 + z_6 \mathbf{a}_3$ | = | $(ax_6 + cz_6 \cos \beta) \hat{\mathbf{x}} + by_6 \hat{\mathbf{y}} + cz_6 \sin \beta \hat{\mathbf{z}}$ | (4e) | H IV |

$$\mathbf{B}_{98} = \begin{matrix} -x_{26} \mathbf{a}_1 + (y_{26} + \frac{1}{2}) \mathbf{a}_2 - \\ (z_{26} - \frac{1}{2}) \mathbf{a}_3 \end{matrix} = \begin{matrix} - (ax_{26} + c(z_{26} - \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} + \\ b(y_{26} + \frac{1}{2}) \hat{\mathbf{y}} - c(z_{26} - \frac{1}{2}) \sin \beta \hat{\mathbf{z}} \end{matrix} \quad (4e) \quad \text{S II}$$

$$\mathbf{B}_{99} = -x_{26} \mathbf{a}_1 - y_{26} \mathbf{a}_2 - z_{26} \mathbf{a}_3 = \begin{matrix} - (ax_{26} + cz_{26} \cos \beta) \hat{\mathbf{x}} - by_{26} \hat{\mathbf{y}} - \\ cz_{26} \sin \beta \hat{\mathbf{z}} \end{matrix} \quad (4e) \quad \text{S II}$$

$$\mathbf{B}_{100} = \begin{matrix} x_{26} \mathbf{a}_1 - (y_{26} - \frac{1}{2}) \mathbf{a}_2 + \\ (z_{26} + \frac{1}{2}) \mathbf{a}_3 \end{matrix} = \begin{matrix} (ax_{26} + c(z_{26} + \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} - \\ b(y_{26} - \frac{1}{2}) \hat{\mathbf{y}} + c(z_{26} + \frac{1}{2}) \sin \beta \hat{\mathbf{z}} \end{matrix} \quad (4e) \quad \text{S II}$$

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.