

Kristallstruktur von $\text{MgSO}_3 \cdot \text{H}_2\text{O}$

Crystal Structure of $\text{MgSO}_3 \cdot \text{H}_2\text{O}$

Willi Buchmeier, Bernward Engelen*, Holger Müller

Universität-GH Siegen, Anorganische Chemie II, D-57068 Siegen

Z. Naturforsch. **53 b**, 131–134 (1998); eingegangen am 10. November 1997

X-Ray, Sulfites, Hydrates, Magnesium, Pseudosymmetry

The crystal structure of $\text{MgSO}_3 \cdot \text{H}_2\text{O}$, space group $P2_1/n$, $Z = 4$, $D_x = 2.415 \text{ g} \cdot \text{cm}^{-3}$, $a = 4.699(1)$, $b = 12.751(3)$, $c = 5.618(1) \text{ \AA}$, $\beta = 90.49(3)^\circ$, was determined by single crystal X-ray diffraction. $\text{MgSO}_3 \cdot \text{H}_2\text{O}$ crystallizes in the $\text{MnSO}_3 \cdot \text{H}_2\text{O}$ type. The structure consists of buckled *trans* layers $\infty^2 [\text{MgSO}_3 \cdot \text{H}_2\text{O}]$, which are built up from strongly distorted $\text{MgO}_5(\text{H}_2\text{O})$ octahedra sharing four equatorial vertices, and of trigonal pyramidal SO_3^{2-} ions. It is closely related to the structures of orthorhombic $\text{MnSeO}_3 \cdot \text{D}_2\text{O}$ and monoclinic $\text{ZnSeO}_3 \cdot \text{H}_2\text{O}$. The Mg-O distances range from 2.051(3) to 2.175(4) Å. The S-O distances (1.543(3), 1.547(3) and 1.493(3) Å) and the O-S-O angles (98.4(2) and $2 \times 106.0(2)^\circ$) correspond to those in $\text{MnSO}_3 \cdot \text{H}_2\text{O}$. The distortion of the $\text{MO}_5(\text{H}_2\text{O})$ octahedra ($M = \text{Mg}, \text{Mn}$) and of the SO_3^{2-} ions is smaller in $\text{MgSO}_3 \cdot \text{H}_2\text{O}$, but with greater deviations from *m* symmetry. The distances between the H-connected $\infty^2 [\text{MSO}_3 \cdot \text{H}_2\text{O}]$ layers are greater in $\text{MgSO}_3 \cdot \text{H}_2\text{O}$, indicating weaker inter-layer hydrogen bonds. The lateral arrangement of the $\infty^2 [\text{MSO}_3 \cdot \text{H}_2\text{O}]$ layers is nearly the same in both sulfite monohydrates.

* Sonderdruckanforderungen an Prof. Dr. B. Engelen, e-mail: engelen@chemie.uni-siegen.de