04.6-10 HYDROGEN BONDING AND MELTING CHARACTERISTICS OF WATER-RICH SALT hydrates: NEUTRON DIFFRACTION DATA ON SILICATES Na₂[SiO₂(OH)₄]₂·nH₂O, n = 4,5,7,8.

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Sodium silicate hydrates Na₂[SiO₂(OH)₄]₂·nH₂O, n = 4,5,7,8 have the unique monomeric tetrahedral [SiO₂(OH)₄]²⁻ anion in common. Different amounts of n water molecules enter the structure through different arrangements of dominating octahedral aquo-complexes Na⁺[O₂H₂O]₄²⁻ sharing corners or edges. From complete neutron diffraction data we reveal our approach to special features in hydrogen bonding, which are in common with all 4 individual hydrate phases. Tetrahedral coordination dominates the hydrate water molecules in all 4 structures besides some distinct fivefold coordinated oxygens. From bond length/bond strength correlations we find a corresponding harmonicity in bond strengths reaching the (water) oxygen coordination centers from all types of ligands (-H₂O,...H₂O,Na⁺).

The complete structural data, especially concerning hydrogen positions, also allows for reference standards on (H₂O)₂⁵Si-NMR-analytical data which is available for the crystalline phases as well as for the super-cooled melts.

This study is part of a general approach to deepen understanding of H₂O-X(O,OH)₄ interactions in 3-dimensional icelike networks, which show up from crystalline but also disordered glasslike solids, gels or non-Newtonian liquids. We are especially interested in the structural background data of congruently melting water rich salt hydrates. The given silicate hydrates belong to the very rare hydrates which melt congruently, definitely and which form super-cooled melts of non-Newtonian character.

04.6-11 HYDROXYSODALITE HYDRATES Na₈[Al₅Si₄O₁₄(OH)]₂·nH₂O : TEMPERATURE-INDUCED DYNAMICS AND ORDERING OF OH/H₂O - CONSTITUENTS DURING DECOMPOSITION AND EXCHANGE REACTIONS. By S. Luger and J. Felsche, Fakultät für Chemie, Universität Konstanz, Postfach 5560, 7750 Konstanz, FRG.

Samples of different H₂O-content from large scale synthetic programs have been investigated by means of X-ray/neutron diffraction and thermoanalytical studies. There is strong evidence of OH-centering in hydroxysodalite hydrates Na₈[Al₅Si₄O₁₄(OH)]₂·nH₂O. The OH-groups center the Na₄-tetrahedra within the cubic-octahedral framework structure corresponding to CI in common sodalites.

Oxygens of the hydroxyl-groups are located on position 2a and protons on position 8e of space group P₄₃m. Oxygens of the hydroxyl-groups are located on position 2a and protons on position 8e of space group P₄₃m. Oxygens of the hydroxyl-groups are located on position 2a and protons on position 8e of space group P₄₃m. Oxygens of the hydroxyl-groups are located on position 2a and protons on position 8e of space group P₄₃m. Oxygens of the hydroxyl-groups are located on position 2a and protons on position 8e of space group P₄₃m. Oxygens of the hydroxyl-groups are located on position 2a and protons on position 8e of space group P₄₃m. Oxygens of the hydroxyl-groups are located on position 2a and protons on position 8e of space group P₄₃m. Oxygens of the hydroxyl-groups are located on position 2a and protons on position 8e of space group P₄₃m. Oxygens of the hydroxyl-groups are located on position 2a and protons on position 8e of space group P₄₃m. Oxygens of the hydroxyl-groups are located on position 2a and protons on position 8e of space group P₄₃m.

There is another type of hydroxysodalite hydrate Na₈[Al₅Si₄O₁₄(OH)]₂·nH₂O, n>8 from elevated pressure (>400 bar) and temperature (200-500°C) conditions. This type reveals complex organization of OH/H₂O-groups on position 24i of space group P₄₃m as favored in the model given by HASSEN & GRUNDY (1983) or GALITSKII et al. (1974).

We observe an exothermic reaction at about 150 K from freezing the OH/H₂O thermal motion probably on running this type in DSC-experiments down to 100 K. At temp. ~325 K another structural phase transition occurs upon heating at open system conditions. Fundamental reorganization of OH/H₂O constituents starts as soon as hydrate water concentration is lowered to n<2 H₂O. (Al/Si) order/disorder phenomena probably affect this phase transition.

From exchange experiments a less basic type of sodalite Na₈[Al₅Si₄O₁₄(OH)]₂·nH₂O is obtained.