Poster Presentations

[MS18-P14] Similarities and Pecularities between the Crystal Structures of the Hydrates of Sodium Sulphates and Selenates

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A study of the systems $Na_2SO_4.10H_2O$ – $Na_2SeO_4.10H_2O$ – H_2O and Na2SO4.7H2O – $Na_2SeO_4.7H_2O$ – H_2O at 15° C shows the formation of interrupted series of mixed crystals in both systems. The calculated values for Gibbs free energy of phase transitions (kJ·mol–1), for transformation of one type mixed crystals into the other type mixed crystals, in the case of decahydrates are significantly smaller than those for heptahydrates [3]. This means, that the differences in the structures between the crystal structures of heptahydrates are essential in contrast to those between the decahydrates. The crystal structures of $Na_2SO_4.10H_2O$ [4-7] and $Na_2SO_4.7H_2O$ [8] are known. For the crystal structures of $Na_2SeO_4.10H_2O$ and $Na_2SeO_4.7H_2O$ there are no data at all. The existing data for the crystal structure of $Na_2SO_4.10H_2O$ are taken at/ above 180 K and some disorder in the crystal structure was observed. For this reason it was of interest to study this crystal structure at low temperatures as well.

The crystal structure of $Na_2SO_4.7H_2O$, studied by Oswald et al [8] at 150 K ,shows a slight distortion in the structure. For that reason we have studied the crystal structures of the all 4 hydrates $Na_2SO_4.10H_2O$, $Na_2SO_4.7H_2O$, $Na_2SeO_4.10H_2O$ and $Na_2SO_4.7H_2O$.

A surprising result of our studies is, that the metastable hydrate of sodium selenate was found to be $Na_2SeO_4.7{,}5H_2O$, instead of $Na_2SeO_4.7\,H_2O$ as described former [2].

An interesting result of our study is, that two salts with different chemical compositions and different crystal structures ($Na_2SO_4.{}_7H_2O$, tetragonal, space group $P4_12_12$ and $Na_2SeO_4.7{,}5H_2O$, monoclinic, space group *C2/c*) can act mutually as crystal nucleus, so that either of these two salts can initiate crystallization of the other from their supersaturated solutions. As a result, from the comparison between these two salts, fragments of their crystal structure with a certain similarity were determined. Thus, it could be supposed, that similarity even only between certain structural elements of both salts could acts as a nucleation agent.

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