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Crystal Structures and Anisotropic Expansion of Coordination Compounds from the Mg(SCN)2 ·x H2O/THF System

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- Introduction

Magnesium halides and pseudo-halides are essential compounds for many applications ranging from biochemistry to construction and building materials. These phases exhibit a great variety of chemical and structural properties and hence, were extensively studied. However, in the row of magnesium pseudo-halides, i.e. cyanides, cyanates etc., the thiocyanates were often overseen and are therefore still only poorly characterized.

- Objectives

Mg(SCN)2 ·x H2O/THF coordination compounds were synthesized, characterized, their crystal structures solved ab initio from X-ray powder diffraction (XRPD) data and their thermal expansion properties investigated by temperature dependent in situ XRPD.

- Results

The recrystallization of Mg(SCN)2 ·4 H2O in THF yields the novel compounds Mg(SCN)2 ·2 (H2O, THF) and α-Mg(SCN)2 ·4 THF. By heating, α-Mg(SCN)2 ·4 THF undergoes a phase transition into β-Mg(SCN)2 ·4 THF that is associated with an increasing disorder of the THF molecules. Finally, two THF molecules are released, which leads to the formation of Mg(SCN)2 ·2 THF. The investigated compounds show a remarkable anisotropic thermal expansion and the growing disorder of THF molecules has a major impact on the expansion properties.

- Conclusions

The coordination chemistry of Mg(SCN)2 turned out to be rich and has the potential to go beyond H2O and THF as ligands. An expansion towards other metals like nickel, cobalt or iron appears to be very feasible.

Fig. 1. Octahedral coordination of Mg2+ with SCN- and THF for a) α-Mg(SCN)2 · 4 THF; b); β-Mg(SCN)2 · 4 THF, Plots showing the variation of the thermal expansion coefficient α with the principal directions X1, X2 and X3 of c) α-Mg(SCN)2 · 4 THF, d) β-Mg(SCN)2 · 4 THF

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