representation of $(Et_4N)[NbOCl_3(ttfa)]$ (tetraethylammonium counter-ion omitted).

Keywords: hydrolysis, bidentate, kinetics, crystallization

MS29-P12 Temperature structural studies of spin crossover 1D coordination polymer $[Fe(4\text{-amino-}1,2,4\text{-triazole})_3]SO_4$

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Spin crossover (SCO) usually occurs in octahedral $3d^4$-d^7 transition metal complexes. SCO can be induced by change of temperature, application of pressure or by light irradiation and is accompanied by change of magnetic, optical and dielectric properties. What is important, transition from high spin (HS, $t_{2g}^4e_g^2$, S=2) to low spin (LS, $t_{2g}^6e_g^0$, S=0) form in iron(II) complexes is accompanied by shortening of Fe-ligand distance at about 0.2 Å. Although SCO phenomenon is of molecular nature, a perturbation produced by shrinkage of complex molecule (as a result of Fe-ligand bond shortening) spreads on the whole crystal lattice through intermolecular interactions. Therefore it was postulated that an incorporation of direct linkage between metal ions should enhanced transmission of perturbation. Thus it should lead to the more cooperative spin transitions. Indeed, in the coordination polymers in which iron(II) ions are bridged by small and rigid ligands, SCO very often proceeds in narrow temperature range. In particular iron(II) complexes based on 1H,2,4-triazole or 4-amino-1,2,4-triazole (NH_2trz) exhibit very abrupt spin transitions accompanied by hysteresis loops [1]. Unfortunately, synthesis of these type of complexes does not lead to the formation of crystalline samples suitable for single crystal X-Ray diffraction studies. Initially, postulated structure of one dimensional (1D) polymeric chains in which metal ions are bridged by three 1,2,4-triazole rings was supported by elucidation of crystal structure of copper(II) complexes [2].

The subject of performed studies are spin crossover 1D coordination polymers $[Fe_{1-x}Zn_x(4\text{-amino-}1,2,4\text{-triazole})_3]SO_4$ (for x=0.0, 0,09, 0.20, 0.40, 0.60, 1.00) that represent an examples of NH_2trz based SCO systems containing divalent anion [3]. The complex exhibits complete one step, abrupt spin crossover slightly above room temperature and is accompanied by the hysteresis loop. Based on the synchrotron powder diffraction measurements we have determined the crystal structure of the studied compounds.

Literature

[1] M. M. Dirtu, C. Neuhausen, A.D. Naik, A. Rotaru, L. Spinu, Y. Garcia, Inorg. Chem., **2010**, 49, 5723-5736.

[2] K. Drabent, Z. Ciunik, Chem. Commun., **2001**, 14, 1254-1255.

[3] K. Drabent, R. Bronisz, M. F. Rudolf, Italian Physical Society Conference Proceedings, **1996**, 50, 15-18.

Keywords: Spin crossover, synchrotron powder diffraction study, Fe(II) compounds