Poster Presentation

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Crystal structures of 2D coordination networks in [M(bbtr)3](ClO4)2 (M=Mn, Cd)

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[Fe(bbtr)3](ClO4)2 (bbtr=1,4-di(1,2,3-triazol-1-yl)butane) represents a spin crossover (SCO) system where the first coordination sphere consists of 1,2,3-triazole rings coordinated by exodentate nitrogen atoms [1]. Iron(II) ion is linked to six other iron(II) ions by bbtr ligands. This creates two dimensional (2D) polymeric layers. SCO is abrupt, accompanied by hysteresis loop. In the cooling mode P-3 -> P-1 structural phase transition precedes SCO. The non-magnetic structural transformation is accompanied by reorganization of weak intermolecular interactions and shift of 2D layers with respect to each other. Surprisingly, an analog [Fe(bbtr)3](BF4)2, does not exhibit in cooling mode neither thermally SCO nor structural phase transition [2]. To clarify the role of structural phase transition on SCO we have performed structural modifications by exchanging the kind of anions and/or metal ions. An exchange of perchlorate on triflate anion involves deeper structural changes. A topology of the polymeric layer remains the same, but the SCO is shifted to higher temperature and structural phase transition is not observed. The studies of isostructural zinc(II) analogs confirmed the crucial role of anion in the occurrence of non-magnetic structural phase transition. The [Zn(bbtr)3](ClO4)2 exhibites P-3 -> P-1 structural phase transition which is not present in tetrafluoroborate analog [2]. We expand studies on other hexacoordinating metal(II) ions. Reactions between manganese(II) or cadmium(II) perchlorates and bbtr in acetonitrile lead to [M(bbtr)3](ClO4)2 (M=Mn, Cd) complexes. Single crystal X-ray diffraction studies revealed that both compounds create a 2D polymeric networks. The temperature dependence of lattice parameters for these complexes showed that, in contrast to [Fe(bbtr)3](ClO4)2 and [Zn(bbtr)3](ClO4)2 systems, the structural phase transition is not present. This work was funded by the Polish National Science Centre Grant No. DEC-2011/01/B/ST5/06311.

[1] *R. Bronisz, Inorg. Chem. 2005, 44, 4463–4465,* ***[2]*** *J. Kusz, R. Bronisz, M. Zubko, G. Bednarek, Chem. Eur. J. 2011, 17, 6807–6820*

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