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MS29-P7 Crystal structure of the 1D coordination polymer $[Fe(ebtz)_2(CH_3CN)_2](BF_4)_2 \cdot 2CH_3CN$

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Spin crossover (SCO) depends on alteration of electronic structure of metal ion which can be triggered by the change of temperature, an application of pressure, by light irradiation or using pulsing magnetic field as well as by chemical perturbation.[1] SCO in octahedral iron(II) complexes is associated with the shift of two electrons between t_{2g} and e_g electronic levels. This results in alteration of magnetic, optical and dielectric properties. Transition from high spin HS(S=2) to low spin LS(S=0) state is accompanied by the reduction of Fe-donor distance from 2.0 to 2.2 Å. This becomes a source of perturbation which spreading on the crystal lattice may trigger further structural transformations within a complex molecule and in the network of intermolecular interactions.

$[Fe(ebtz)_2(C_2H_3CN)_2](ClO_4)_2$(**1**) represents an example in which SCO is associated with structural changes.[2] In this complex neighbouring Fe(II) ions are linked by 1,2-di(tetrazol-2-yl)ethane (ebtz). This bridging mode leads to formation of the polymeric chain. Adjusted polymeric chains form supramolecular layers which are parallel to each other. Nitrile molecules adopt uncommon orientation in relation to coordination octahedron. The angle Fe-N-C(nitrile) in HS is lesser that 150° (145.9° at 110 K). SCO in this complex is very abrupt and accompanied by wide hysteresis loop ($T_{1/2}^{\downarrow} \approx 112$ K, $T_{1/2}^{\uparrow} \approx 141$ K). It was found that HS→LS transition is associated with reorientation of propionitrile molecule (<Fe-N-C(nitrile) = 162.9° at 80 K).

On the poster will be presented the crystal structure and magnetic properties of 1D coordination polymer $[Fe(ebtz)_2(CH_3CN)_2](BF_4)_2 \cdot 2CH_3CN$ (**2**). In this complex the polymeric chains form supramolecular layers. Axially coordinated acetonitrile molecules are also directed towards space between layers. But the angle of Fe-N-C(CH_3) fragment in HS of **2** is significantly greater (167.95°) than in **1** and after HS→LS transition increases only slightly (171.61°). SCO in **2** is more gradual and accompanied by a narrow hysteresis loop ($T_{1/2}^{\downarrow} \approx 161.0$ K, $T_{1/2}^{\uparrow} \approx 163.5$ K).

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Literature

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