Poster

Slow Thermally-Induced Spin Crossover in the Two-Dimensional Network $[Fe(bbtr)_3](BF_4)_2$

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The electron configuration of the transition metals in the coordination compounds can be switched by changes in temperature, pressure or light irradiation with a specific wavelength (Light-Induced Excited Spin-State Trapping, i.e. LIESST effect) [1]. The new spin state, obtained in this way, has an influence on the alterations of the magnetic, optical and structural properties. Changing the absorbance bands results in the variation of the colour of the crystal. However, in structural terms, the change of the spin state causes shortening of the metal-ligand bond length by about 0.2Å [1].

Coordination compounds, where spin transition associated with the phase transition occurs, are particularly interesting. They allow us to understand the relationship between these two phenomena and to obtain information whether the phase transition induces a spin transition, whether the spin transition leads to a phase transition or whether both processes occur simultaneously.

The X-ray temperature studies carried so far for the $[Fe(bbtr)_3](ClO_4)_2$ showed that the spin transition in this coordination compound is preceded by the phase transition (from P-3 space group to P-1 space group). Interestingly, in the measured temperature range up to 80 K a similar effect was not observed for the complex $[Fe(bbtr)_3](BF_4)_2$ [2].

High-pressure, X-ray structural studies at room temperature for the $[Fe(bbtr)_3](BF_4)_2$ showed that a spin transition occurs with increasing pressure (a reduction in the length of Fe-N bonds associated with a change of the spin state was observed). Then a phase transition occurs in which the structure changes the space group from P-3 to P-1.

The crystal structures determined at pressure 1.064 GPa for perchlorate and 1.212 GPa for tetrafluoroborate indicate the occurrence of P-3 → P-1 phase transition. The average Fe-N distances are equal to 2.0 and 2.0 Å, respectively, that is, the spin crossover is practically completed. It is clearly visible that, unlike ambient pressure, the mechanism of spin crossover under high pressure conditions is very similar for both complexes. Moreover, obtained results confirm that for perchlorate mechanism of spin crossover was changed upon transition from ambient pressure, where structural phase transition preceded spin crossover, to higher pressures where spin crossover starts before phase transition.

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