

MS27-2-7 Decoupling spin-crossover and structural phase transition in iron(II) molecular complex #MS27-2-7

D. Paliwoda¹, L. Vendier¹, G. Molnár¹, A. Bousseksou¹
¹LCC, CNRS & Université de Toulouse (UPS, INP), - 31077 Toulouse (France)

Abstract

Spin-crossover (SCO) materials are sensitive to external stimuli. SCO transition arouses curiosity because the change of the spin state of metal ion involves appearance of serious structural perturbation related to changes of metal-ligand distances. The interest in Fe(II) spin crossover systems is enhanced by the fact that the spin state can be conveniently switched by changing the temperature, applying pressure, light irradiation or by the action of a chemical agent¹. Hence, these compounds are considered as materials for potential applications² for example in medicinal diagnostic³, as sensors⁴, displays⁵ and memory devices⁶.

We have recently investigated pressure induced spin-crossover (SCO) transitions in Fe(II) molecular complexes: **(1)** [Fe^{II}(H₂B(pz)₂)₂(bipy)] and **(2)** [Fe^{II}(H₂B(pz)₂)₂(phen)] pz: pyrazole; bipy: 2,2'-bipyridine; and phen: phenanthroline).

We have performed a series of high-pressure measurements of **(1)** and **(2)** using wide-opening angle diamond anvil cell (One20DAC) and four-circle Rigaku Synergy-S XtaLab diffractometer equipped with Hypix6000 hybrid pixel Si detector. At normal conditions **(1)** and **(2)** form monoclinic crystals of space group C2/c. Both complexes undergo SCO transition when cooled down to 160 K, which is manifested indirectly by abrupt shortening of Fe-N(ligand) distance of about 0.2 Å. While **(1)** remains monoclinic upon further cooling, the low temperature high spin (HS) to low spin (LS) transition in **(2)** is

1

accompanied by the structural transformation from monoclinic C2/c form to triclinic P phase.

Compression of **(2)** decouples SCO and structural transition which allows to detect monoclinic LS form, so far undetectable upon cooling^{7,8}.

Acknowledgements: Financial support from regional Nanomat PRRI Project and ERC "E-MOTION" Advanced Grant is gratefully acknowledged.

References

- [1] A. B. Gaspar, G. Molnár, A. Rotaru; H. J. Shepherd, *C.R. Chimie*, 2018, **21**, 1095.
- [2] A. Bousseksou, G. Molnár, L. Salmon, W. Nicolazzi, *Chem. Soc. Rev.* 2011, **40**, 3313.
- [3] R. N. Muller, L. V. Elst and S. J. Laurent, *J. Am. Chem. Soc.*, 2003, **125**, 8405.
- [4] C. Bartual-Murgui, A. Akou, C. Thibault, G. Molnar, C. Vieu, L. Salmon, A. Bousseksou, *J. Mater. Chem. C*, 2015, **3**, 1277.
- [5] O. Kahn, C. J. Martinez, *Science*, 1988, **279**, 44.
- [6] J.-F. Letard, P. Guionneau, L. Goux-Capes, *Top. Curr. Chem.*, 2004, **235**, 221;
- [7] J. A. Real, M. Carmen Muñoz, J. Faus, X. Solans, *Inorg. Chem.*, 1997, **36**, 3008.
- [8] A. L. Thompson, A. E. Goeta, J. A. Real, A. Galet, M. Carmen Muñoz, *Chem. Comm.*, 2004, **12**, 1390.

Unit cell angles α/γ of **(2)** and av. Fe-N distances

