SPIN-TRANSITION TEMPERATURE TUNING OF A NOVEL GROUP OF MOLECULAR Fe(II) SCO-PL COMPLEXES

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Multifunctional spin crossover (SCO) compounds combine classical SCO properties with additional features (e.g. non-linear optics, bulk magnetic ordering, …), thus opening the possibility for prospective and versatile applications.[1]

Besides the usually performed magnetic measurements concerning SCO nanomaterials a more straightforward spin state detection method, which allows a precise tracking even in small clusters, is required. The spin state dependent modulation of photoluminescence (PL) is one approach fulfilling these demands. In addition to the development of SCO-PL systems for feasible applications, investigations on the only partially understood mechanism of this phenomenon still need to be conducted.[2]

We recently developed a heteroleptic octahedral Fe(II)-complex consisting of four 1,3,5,7-tetramethyl-8-((1H-tetrazol-1-yl)methyl)-BODIPY (2TzBODIPY) ligands and two apically arranged acetonitrile (MeCN) ligands. The structure of $[Fe(2TzBODIPY)_4(MeCN)_2](ClO_4)_2$ was confirmed by single crystal XRD analysis as shown in **Figure 1**. This novel SCO-PL system exhibits a spin transition at $T_{½} = 265$ K and shows strong fluorescence in solid state at room temperature. This multifunctional compound allows a straightforward tuning of the spin transition temperature by replacing the apical ligands with various nitrile (R-CN) species. This paves the way for detailed investigations – regarding the electronic and steric influence of the apical ligands on the Fe(II) coordination center – and for its possible future applications as multifunctional materials. The magnetic behavior of the developed system with varying apical ligands (R-CN) is depicted in **Figure 2**.

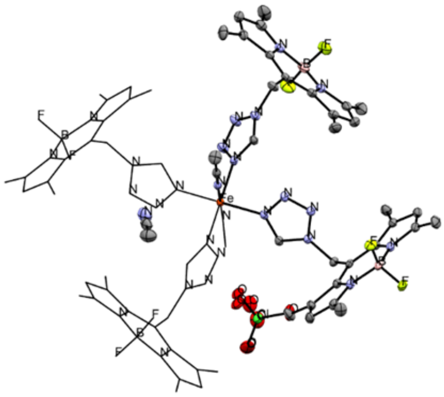

Figure 1: single crystal structure of $[Fe(2TzBODIPY)_4(MeCN)_2](ClO_4)_2$

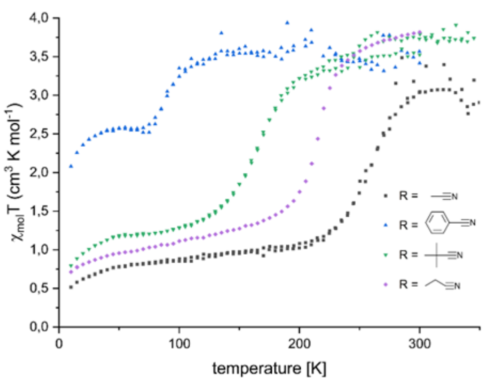

Figure 2: magnetic properties of $[Fe(2TzBODIPY)_4(RCN)_2](ClO_4)_2$

[1] Senthil Kumar, K.; Ruben, M. *Coordination Chemistry Reviews* 2017, *346*, 176-205.

[2] Shepherd, H. J.; Quintero, C. M.; Molnár, G.; Salmon, L.; Bousseksou, A. *Spin-Crossover Materials*, 2013, pp. 347-373.