

The synthesis & structural elucidation of 3,5-bis(2-pyridyl)-1,2,4-triazolate bridged dinuclear iron(II) spin crossover compounds

C. J. Schneider, K. S. Murray, S. R. Batten, S. M. Neville, D. R. Turner, B. Moubaraki, J. D. Cashion

School of Chemistry, Monash University, Clayton, VIC, Australia

Spin crossover materials show much potential for possible application in microelectronics and information processing. Their ability to switch between either of two states via an external perturbation of temperature/optical excitation can lead to new and exciting materials with very interesting magnetic properties.

Our studies of two very closely related families of iron(II) dinuclear spin crossover compounds has led to the synthesis of new spin crossover compounds with very well defined spin transitions^[1].

The complexes are of the type $[\text{Fe}(\text{NCX})(\text{py})]_2 \cdot m (\text{L})_2$ ($\text{X} = \text{S}, \text{Se}, \text{BH}_3$) ($\text{L} = \text{bpytz}^-$ or bpypz^-). The two iron(II) centres are equatorially, coplanar bridged by either the 3,5-bis(2-pyridyl)-1,2,4-triazolate (bpytz^-) (Fig.1) or 3,5-bis(2-pyridyl)pyrazolate (bpypz^-) ligand with unidentate pyridine and NCX^- ligands coordinated apically. In each dinuclear family the NCX^- ligand is varied, with profound effects on the magnetic behaviour being observed. Of the bpytz^- family, the structure of $[\text{Fe}(\text{NCS})(\text{py})]_2 \cdot m (\text{bpytz})_2$ is known however, only $[\text{Fe}(\text{NCBH}_3)(\text{py})]_2 \cdot m (\text{bpytz})_2$ shows a well resolved two step spin transition with interesting Mössbauer data.

As well, for the first time, we present the fully resolved structure of the previously reported spin crossover complex $[\text{Fe}(\text{NCS})(\text{py})]_2 \cdot m (\text{bpypz})_2$ ^[2], the crystals of which, surprisingly, do not show any spin crossover.

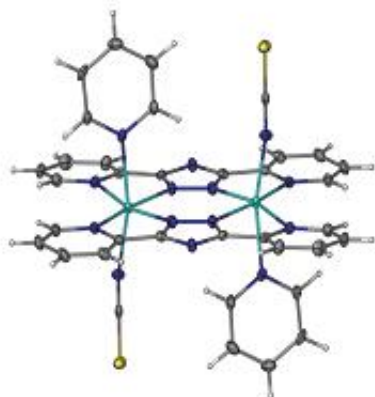


Figure 1: The structure of $[\text{Fe}(\text{NCS})(\text{py})]_2 \cdot m(\text{bpytz})_2$

(1) 1. C.J Schneider, J.D. Cashion, B.M. Moubaraki, S.M. Neville, S.R. Batten, D.R. Turner K.S. Murray. *Polyhedron*, 2006, in press

(2)

(3) 2. K. Nakano, N. Suemura, S. Kawata, A. Fuyuhiko, T. Yagi, S. Nasu, S. Morimoto, S. Kaizaki, *Dalton Trans.* 2004, 982-988