

Guest seminar lecture room MB155 - Tuesday 21 April at 3 pm.

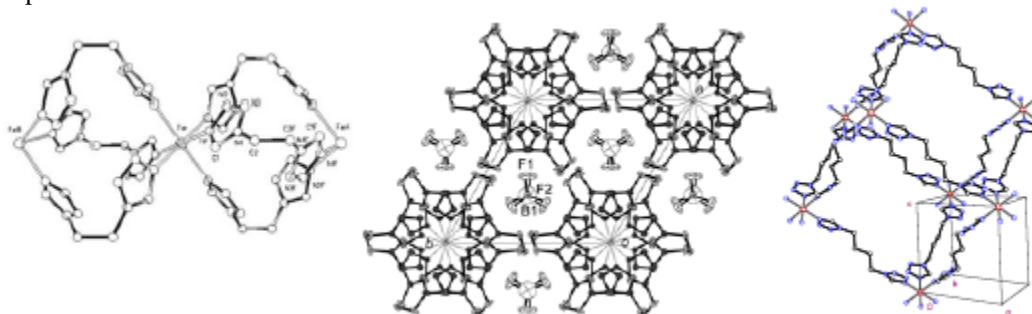
## ELUCIDATION OF THE INFLUENCE OF STERIC AND ELECTRONIC FACTORS ON THE SPIN TRANSITION BEHAVIOUR OF FE(II) SPIN-CROSSOVER COMPOUNDS

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### ABSTRACT

Despite of the existence of rare predictive models, *e.g.* for 1D chain type triazole-based Fe(II) coordination polymers [1], it is still impossible to predict the spin transition behaviour of almost any new spin-crossover (SCO) compound. But within a series of homologue ligands a systematic variation may elucidate the impact of steric and/or electronic factors upon the spin transition properties such as the spin transition temperature  $T_{1/2}$  and the abruptness of the transition. A comparative study on mononuclear as well as polynuclear complexes based on the extremely versatile building block system of N1-substituted tetrazole ligands sheds light on these factors governing the spin transition properties. Examples of the impact of the spacer chain length within the class of  $\alpha,\omega$ -ditetrazolyl-alkanes shows dramatic changes from a rather flexible 1D chain-type [2] to a more rigid 1D chain-type [3] and a very rigid 3D threefold interpenetrated [4] coordination polymer and its consequences for the spin crossover behaviour.



Molecular Structures of [2] (left), [3] (center) and [4] (right)

### REFERENCES

- [1] Dirtu M.M., Rotaru A., Gillard D., Linares J., Codjovi E., Tinant B. and Garcia Y., "Prediction of the Spin Transition Temperature in Fe(II) One-Dimensional Coordination Polymers: an Anion Based Database", *Inorg. Chem.*, 48, (2009), pp 7838-7852.
- [2] Schweifer J., Weinberger P., Mereiter K., Boca M., Reichl C., Wiesinger G., Hilscher G., van Koningsbruggen P.J., Kooijman H., Grunert M. and Linert W., "Catena [ $\mu$ -Tris(1,2-bis(tetrazol-1-yl)ethane-*N*4,*N*4')iron(II)] Bis(tetrafluoroborate): Synthesis, Structural, Vibrational and Magnetic Characterisation of a Chain-type Coordination Polymer Spin-Crossover Compound", *Inorg. Chim. Acta*, 339, (2002), pp 297- 306.
- [3] Müller D., Knoll C., Stöger B., Artner W., Reissner M. and Weinberger P., "A modified synthetic pathway for the synthesis of so far inaccessible N1-functionalized tetrazole ligands - synthesis and characterisation of the 1D chain-type Spin Crossover compound [Fe(3ditz)<sub>3</sub>](BF<sub>4</sub>)<sub>2</sub>", *Eur. J. Inorg. Chem.*, 5-6 (2013) pp 984– 991.
- [4] Grunert M., Schweifer J., Weinberger P., Linert W., Mereiter K., Hilscher G., Müller M., Wiesinger G., van Koningsbruggen P.J., "Structure and physical properties of [ $\mu$ -tris(1,4-bis(tetrazol-1-yl)butane- *N*4,*N*4')iron(II)] bis(hexafluorophosphate), a new Fe(II) spin-crossover compound with a three dimensional threefold interlocked crystal lattice", *Inorg. Chem.*, 43, 1, (2004) pp 155-165.