

m28.o04**Inclusion compounds from a Diol Host**Gaelle Ramon¹, Luigi R. Nassimbeni¹, E. Weber²¹Chemistry Dept, UCT, South Africa, ²Institute for Organic Chemistry, Freiberg, Germany**Keywords: supramolecular assemblies, host-guest structures, inclusion complexes**

The host 9,9'-(ethyne-1,2-diyl)difluorene-9-ol (**WEB22**) was crystallised with the 3 isomers of picoline and with pyridine by slow evaporation at room temperature. The structures of all inclusion compounds were solved. The inclusion compound of 4-picoline, despite different cell parameters and a different space group, displays a similar packing to the other compounds. The four inclusion compounds were of the same host:guest ratio of 1:2 and were nearly isostructural with respect to the host molecules positions. They all exhibit wide channels in which the guest molecules are located. We examined the selectivity of the host molecules towards the included solvents by carrying out 2- and 3-component competition experiments, which were studied by Gas Chromatography. Singular results were obtained from some 2-component experiments and were discussed. To complement the competition experiment results, lattice energy calculations were performed on these inclusion compounds of **WEB22**.

m28.o05**Structures of iron(II) and copper(II) coordination polymers with α,ω -bis(tetrazol-1-yl)di(ethylene glycol)**Yves Boland,^a Bernard Tinant,^b Anne Attout^a, Yann Garcia^a^aUnité de Chimie des Matériaux Inorganiques et Organiques. ^bUnité de Chimie Structurale et des Mécanismes Réactionnels, Université catholique de Louvain, Place L. Pasteur 1, 1348 Louvain-la-Neuve, Belgium. E-mail: boland@chim.ucl.ac.be**Keywords: coordination polymers, spin crossover, Jahn-Teller effect**

Spin crossover (SCO) materials are compounds wherein the spin state can be switched by external stimuli [1]. In the present work, 3D SCO iron(II) coordination polymers [2] have been obtained with bis(tetrazol-1-yl)di(ethylene glycol) (btz₁O) as bis-monodentate ligand. These materials of formula [Fe(btz₁O)₃]₂A₂ crystallize in the Rspace group (A = ClO₄⁻, PF₆⁻, AsF₆⁻). Structural changes triggered by the SCO from high-spin (HS) to low-spin (LS) or the counter anion will be presented. The structural changes associated with the SCO originate from the increase of the Fe-N bond length and subsequent rearrangements of the structure. Indeed, the Fe-N bond length varies from 1.985(2) Å in the LS state to 2.185(4) Å in the HS state. Besides, the Fe...Fe distance increases from 11.64 to 11.82 Å as the SCO proceeds. The structure of [Cu(btz₁O)₂(H₂O)₂](BF₄)₂ differs from the one described above. Indeed, due to the tendency of copper(II) to exhibit a Jahn-Teller distortion, two coordination sites around the copper in *trans* position are occupied by water molecules (Cu-N = 2.013(4) and 2.016(4) Å; Cu-O = 2.278(6) and 2.387(5) Å). The subsequent blocking of the network propagation along one direction results in a 2D material which crystallizes in the C2/c group. The hydrogen bonding network involving the coordinated water molecules and non-coordinated tetrafluoroborate anions pushes the coppers together resulting in metal...metal distances rather shorter than in [Fe(btz₁O)₃]₂A₂ (8.27 Å) and a much more distorted ligand conformation. The metal nature is therefore responsible for a change in dimensionality through its coordination preference.

[1] Gütllich P., et al., *Chem. Soc. Rev.*, 2000, 29, 419.[2] Garcia Y., et al., *Top. Curr. Chem.*, 2004, 233, 229.