Investigation of Spin Crossover Behaviours via Encapsulation of Xylene Isomers

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Metal-organic frameworks (MOFs) generated by the self-assembly of metal ions as the centre and bridging ligands through the facile formation of coordination bonds can form highly ordered, porous, crystalline materials by self-correction.[1–3] MOFs has attracted more attention due to their multifunctional properties and various applications, such as gas adsorption and separation, catalysis and sensors.[4–11]. Spin crossover (SCO) MOFs, an interesting subclass containing 3$d^{4–7}$ transition metal ions, exhibiting a reversible electronic state switching phenomenon between high spin (HS) and low spin (LS) states, can have potential applications in sensing, memory devices and magnetic devices.[12–14] However, rational design of SCO MOFs with controllable spin transition behaviours that can be used in precisely adsorbing and identifying guest molecules, especially isomers, are major challenges. Sensitively detecting xylene isomers is of particular interest in the chemical industry area, as their properties are very similar. Since SCO MOF has guest adsorption capacity and can perform various spin crossover phenomenon, it can be an excellent candidate to study on identification of isomers and further investigate the host-guest interactions within the framework structure. Herein, two SCO frameworks with similar topology $[Fe(Dz)Au(CN)_2)_2]\cdot 4(EtOH)$ (Dz = 3,6-bis(4-pyridyl)-1,2-diazine) and $[Fe(Tz)Au(CN)_2)_2]\cdot 2(EtOH)$ (Tz = 3,6-bis(4-pyridyl)-1,2,4,5-tetrazine) were synthesised as host and with different xylene isomers as guest within the materials. SCO behaviours are distinguished via varying xylenes and ratio of their mixtures likely due to different packing modes within the frameworks. Single crystal X-ray Diffraction, powder X-ray diffraction, variable temperature magnetic susceptibility, Raman Spectroscopy etc. have been conducted to understand the structural and magnetic properties and also the relationship between both in order to develop strategies of rational design of these materials and take advantage of their properties.

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