Poster

Structure Determinations and Phase Transition Study on New One-dimensional Fe(II) Coordination Polymers Using Tetrazole Derivatives

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Materials with phase transition phenomenon often lead to build switches, sensors, cantilever and so on. In this work, a novel ligand, 2-(2-(4- fluorobenzyl)-2H-tetrazol-5-yl) pyridine (2-PFBTP) was used to synthesize one-dimensional coordination polymers, $[Fe^{II}(2\text{-PFBTP})_2(4,4'\text{-bpy})](ClO_4)_2 \cdot 0.5\ C_2H_5OH$ (**1**) and $[Fe^{II}(2\text{-PFBTP})_2(\text{bpea})](ClO_4)_2$ (**2**), hereinafter referred as Complex **1** and Complex **2**, respectively. Both structures were determined by powder x-ray diffraction (PXRD) data via simulated annealing algorithm (SA) in real space. The results indicate that the local structure of Fe site sits in $\{FeN_6\}$ core with the pseudo-octahedral geometry. In Complex **1**, there are two bidentate 2-PFBTP ligands in equatorial positions, where a 4,4'- bipyridine ligand bridges across two Fe(II) ions in axial manner to form a one-dimensional polymeric structure. For complex **2**, the local structure of the Fe site is the same as that of Complex **1**, but the axial bridge ligand was replaced by 1,2-Bis(4-pyridyl)ethane (bpea). At room temperature, the average bond distances of Fe-N in Complex **1** and **2** are approximately 2.00(2) Å and 2.02(2) Å, respectively. The distance between two irons for Complex **1** is 11.054 Å while 13.318 Å can be found in Complex **2**. Based on TGA results, there is 0.5 ethanol molecule in a unit cell but no solvent molecules in Complex **2**. The measurements of Differential Scanning Calorimetry (DSC) express a reversible endothermic broad peak appeared around 92°C (365K) and 55°C (328K) for Complex **1** and **2**, respectively. In order to illustrate how the bridge ligand imposes the cooperative effect and further changes on the phase transition temperature, the investigations of variable temperature via PXRD and Fe $L_{II,III}$-edge x-ray absorption spectroscopy (XAS) will be performed to pinpoint the geometric and electronic structures of Fe site in both complexes. Thereafter, the magnetic measurements of both complexes will be performed by SQUID to verify whether the phase transition is related to spin transition phenomenon.