Poster

Characterization of phase transition behaviors of iron complexes based on pyridyl-tetrazole ligands

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Compounds with phase transition characters are possible to prepare materials with controllable properties for application of nanotechnology nowadays. Among of them, spin-crossover (SCO) compounds represent a class of switchable coordination complexes which can change their electronic configurations between low spin (LS) and high spin (HS) states by different stimuli such as temperature, light, pressure, intense magnetic field and electric field. In this work, a series of spin crossover complexes, [Fe(II) $(2BTP)_2(bpy)](ClO_4)_2 \cdot C_2H_5OH$ (**1**), $[Fe(II)(2BTP)_2(bpy)](ClO_4)_2$ (**2**), and $[Fe(II)(2BTP)_2(bpea)](ClO_4)_2$ (**3**), (2BTP= 2-(2-benzyl-2H-tetrazol-5-yl) pyridine, bpy= 4,4'-bipyridine, bpea= 1,2-bis(4-pyridyl)ethane) were synthesized and their structures were determined by single crystal x-ray diffraction (SXRD) or powder x-ray diffraction (PXRD) data. The local structure of Fe site is in $\{FeN_6\}$ core which the central Fe(II) ion is bonded by two bidentate ligands and two monodentate bis-pyridyl bridging ligands to form an octahedral environment. The bridging ligand further connects two Fe(II) ions to form one-dimensional polymeric structure. The magnetic measurements indicated that complex **1** exhibits hysteresis loop ~ 30K ($T_{1/2}\uparrow$=350K, $T_{1/2}\downarrow$=320K). Complex **2** and **3** show $T_{1/2}$ around 380K and 320K, respectively. The average Fe-N bond distances at LS and HS are 1.988(7) Å and 2.20(1) Å, respectively. At LS state, the Fe---Fe distance is around 11.15 Å in **1** and **2**, but increases to 13.17 Å in **3**. The variable temperature x-ray absorption spectroscopy (VT-XAS) of Fe K-edge and $L_{III,II}$ -edge were used to study the electronic structures of these three complexes. The differences of magnetic measurements will be discussed in terms of the inter- and intramolecular interactions, VT-XAS, and differential scanning calorimetry (DSC) results.