Spin Crossover Iron complexes in 2D and 3D frameworks

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A new ligand, trans-4,4`-azo-1,2,4-triazole (atr) was designed and synthesized to construct the possible candidates for spin crossover system. It could be served as a multi-dentate ligand or a good linkage ligand.[1] A series of Fe(II) polymeric compounds in 1D, 2D and 3D frameworks have been successfully synthesized and studied structurally and magnetically. The crystal structures of the ligand and the series of polymeric Fe(II) complexes will be presented. In all the complexes, each ligand atr serves as a bridge between two Fe(II) centers; There are water molecules and NCS ligand around each Fe(II) in the 1-D polymeric compound, $[Fe(\mu\text{-atr})(NCS)_2(H_2O)_2]$; An additional bridge ligand, pyz, is used to form a rectangular 2D framework, $[Fe(\mu\text{-atr})(\mu\text{-pyz})\ (NCS)_2]\ \ 4H_2O$. A cationic species with Fe to atr ratio of 1 to 3 is formed in a 3D framework with the perchlorate as the inclusion counter anions, $[Fe(\mu\text{-atr})_3](ClO_4)_2\ \ 2H_2O$, the structure shows a interlock network. The magnetic properties are quite interesting: It is paramagnetic for the 1D system but display spin transitions for both 2D and 3D systems. It exhibits an abrupt spin transition at T_c=225 K for $[Fe(\mu\text{-atr})(\mu\text{-pyz})\ (NCS)_2]\ \ 4H_2O$. However, it shows a two-step spin transition for the 3D frameworks $[Fe(\mu\text{-atr})_3](ClO_4)_2\ \ 2H_2O$.

[1] Kahn O., Martinez C.J., *Science,* 1998, **279**, 44.

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