

**FA4-MS02-P01****Synthetic, Structural and Luminescence Properties of a New Phosphorescent Cadmium Chloride Network with 2-aminopyrimidine.** Duane Choquesillo-Lazarte<sup>a</sup>, Juan Manuel García Ruiz<sup>a</sup>, Antonio Rodríguez-Diéguez<sup>b</sup>, Enrique Colacio<sup>b</sup>.<sup>a</sup>Laboratorio de Estudios Cristalográficos, IACT-CSIC. <sup>b</sup>Departamento de Química Inorgánica, Universidad de Granada.E-mail: [duanec@ugr.es](mailto:duanec@ugr.es)

In recent years the study on the self-assembly of organic and inorganic molecules in the solid state has become one of intense research activity [1] because it extends the range of new solids which can be designed to have particular physical and chemical properties. Hydro(solvo)thermal in situ metal/ligand reactions, as a new bridge between coordination chemistry and organic synthetic chemistry [2], are of great interest for the discovery of novel coordination architectures and organic reactions.[3] Although in situ metal/ligand reactions have been extensively investigated for many decades, only a few kinds of organic ligand in situ reactions have been found under hydro(solvo)thermal conditions. The exploration of new in situ metal/ligand reactions has remained a challenge for researchers in both coordination and organic chemistry. We report the hydrothermal reaction of CdCl<sub>2</sub> with 2-aminopyrimidine in water yielding one 2D metal-organic coordination framework [CdCl<sub>2</sub>(PymNH<sub>2</sub>)<sub>2</sub>] (PymNH<sub>2</sub> = 2-aminopyrimidine). This compound is a sheet coordination network, consisting of corner-sharing chains of Co<sub>2</sub>(μ-Cl)<sub>2</sub> bridged by PymNH<sub>2</sub> through ring nitrogen atoms. Additionally, this polymer exhibits strong phosphorescence at room temperature in the solid state.

[1] R. Robson, B. E. Abrahams, S. R. Batten, R. W. Gable, B. F. Hoskins and J. Lieu, *Supramolecular Architecture*, ACS publications, Washington, DC, **1992**. [2] A. Rodríguez-Diéguez and E. Colacio, *Chem. Commun.*, **2006**, 4140. [3] P. Vishweshwar, D. A. Beauchamp, M. J. Zaworotko, *Cryst. Growth Des.* **2006**, *6*, 2429.

**Keywords:** polymer structure; tetrazolate; luminescence

**FA4-MS02-P02****Structural and Magnetic Properties of Two Novel Fe(III) Schiff Base Complex.** Yasemin Yahsi<sup>a</sup>, Hulya Kara<sup>a</sup>, Orhan Buyukgungor<sup>b</sup>, Anastasia Iakovenko<sup>c</sup>, Lorenzo Sorace<sup>c</sup>. <sup>a</sup>Balikesir University, Faculty of Art and Science, Department of Physics, Balikesir, Turkey. <sup>b</sup>Ondokuz Mayıs University, Faculty of Art and Science, Department of Physics, Samsun, Turkey. <sup>c</sup>Dipartimento di Chimica and UdR INSTM, Università di Firenze, Firenze, Italy.E-mail: [yahsi@balikesir.edu.tr](mailto:yahsi@balikesir.edu.tr)

Two novel monomeric [C<sub>18</sub>H<sub>17</sub>Cl<sub>3</sub>N<sub>2</sub>O<sub>2</sub>Fe] (**1**) and dimeric [C<sub>38</sub>H<sub>36</sub>N<sub>4</sub>O<sub>4</sub>Cl<sub>6</sub>Fe<sub>2</sub>] (**2**) Fe(III) tetradentate schiff base complexes have been synthesized and their crystal structures have been determined by single crystal X-ray diffraction analysis. The compound **1** crystallizes in monoclinic space

group *P2<sub>1</sub>/c* with *a*= 8.740, *b*= 15.469, *c*= 14.564 Å, β= 107.045° and the X-ray structure analysis of monomeric Fe(III) complex shows that the Schiff base ligand coordinates toward one iron atom in a tetradentate mode and each iron atom is five coordinated. This monomeric Fe(III) complex is such like a dimeric iron complex with the 2.89 Å non-bonding interatomic Fe...O distances and the coordination geometry around iron atom can be described as a distorted square pyramid. In compound **1** the equatorial sites are occupied by the N<sub>2</sub>O<sub>2</sub> donor atoms of the schiff base ligand, with average bond distances of Fe–N=2.081 and Fe–O=1.894 Å, and the apical chloride atom, with Fe–Cl=2.237 Å. The compound **2** crystallizes in triclinic space group *P-1* with *a*=8.443, *b*=9.289, *c*= 12.600 Å, α= 82.085°, β= 79.107°, γ= 86.436° and the X-ray structure analysis of dimeric Fe(III) complex shows that the Schiff base ligand coordinates toward one iron atom in a tetradentate mode and each iron atom is six coordinated. The structure of **2** is a centrosymmetric dimer in which the iron (III) atoms are linked by μ-phenoxo bridges from one of the phenolic oxygen atoms of each Schiff base ligand to the opposite metal center and the two halves of the dimer are related by a crystallographic inversion center and the environment around each iron atom can be described as a distorted octahedral geometry. The variable-temperature (2–300 K) magnetic susceptibility (χ) data of the these two compounds have been investigated.

**Keywords:** magnetic properties; X-ray crystal structure analysis; iron complexes

**FA4-MS02-P03****Use of [Fe(dithiooxalate)<sub>2</sub>NO]<sup>2-</sup> as a Molecular Tecton in Crystal Engineering.** Hulya Kara<sup>a</sup>, Christopher J. Adams<sup>b</sup>, A. Guy Orpen<sup>b</sup>. <sup>a</sup>Department of Physics, Balikesir University, Balikesir, Turkey. <sup>b</sup>School of Chemistry, Department of Chemistry, Bristol University, Bristol, UK.E-mail: [hkara@balikesir.edu.tr](mailto:hkara@balikesir.edu.tr)

A series of crystalline salts based on the [Fe(dto)<sub>2</sub>NO]<sup>2-</sup> (dto = 1,2-dithiooxalate) dianion with hydrogen bond donor cations have been synthesised following a molecular tectonics approach. The chelating Fe(dto)⋯HN supramolecular synthon has been exploited in a systematic study of its robustness. The effects of competition between hydrogen-bond acceptors, of the shape and functionality of the cations are discussed. The preparation and structural characterisation of the new crystalline phases [4,4'-H<sub>2</sub>bipy][Fe(dto)<sub>2</sub>NO][H<sub>2</sub>O] (**1**), [3,3'-H<sub>2</sub>bipy][Fe(dto)<sub>2</sub>NO] (**2**), [H<sub>2</sub>Me<sub>4</sub>bipyz]<sub>2</sub>[Fe(dto)<sub>2</sub>NO][H<sub>2</sub>O]<sub>2</sub> (**3**) (Me<sub>4</sub>bipyz = 3,3',5,5'-tetramethyl-4,4'-bipyrazole) are reported. The charge-assisted NH⋯dto synthon is formed in each of compounds **1–3**. Cryomagnetic susceptibility measurements on these compounds from 3.6 K to room temperature indicated the operation of an antiferromagnetic interaction between Fe(III) atoms in each case. The best fit superexchange parameters are: J<sub>1</sub>= -12.47cm<sup>-1</sup> for **1**, J<sub>2</sub>= -15.20 cm<sup>-1</sup> for **2**, J<sub>3</sub>= -11.34 cm<sup>-1</sup> for **3** where H= -2JS<sub>1</sub>S<sub>2</sub>.

**Keywords:** iron complexes; magnetic properties; crystal engineering