

s13.m38.o2 **New Molecular Materials Using TTF's and Pc's as Building Blocks.** Silvio Decurtins, Shi-Xia Liu, *Department of Chemistry and Biochemistry, University of Bern, Freiestrasse 3, CH-3012 Bern, Switzerland. E-mail: decurtins@iac.unibe.ch*

**Keywords: Tetrathiafulvalene; Phthalocyanine; Molecular Magnetism**

Our strategy involves the covalent attachment of metal ion binding groups to bis(ethylenedithio)tetrathiafulvalene (BEDT-TTF)<sup>[1]</sup> or Phthalocyanine (Pc)<sup>[2]</sup> derivatives and their linkage into supramolecular systems. Thereby, some BEDT-TTF or Pc derivatives symmetrically and asymmetrically functionalized by polypyridines or polypyrazines have been synthesized. The binding abilities to transition metal ions are investigated. A goal is to achieve  $\pi$ -d interactions in such multifunctional molecular materials.

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s13.m38.o3 **Vapochromic behaviour of the solid Ni(BME-DACH) in the presence of SO<sub>2</sub> : Structural characterization by single crystal and powder diffraction.** Joseph Reibenspies,<sup>a</sup> Nattamai Bhuvanesh,<sup>a</sup> Marcetta Darensbourg,<sup>a</sup> Missy Golden,<sup>a</sup> Peter Lee<sup>b</sup> and Yuegang Zhang<sup>b</sup>, <sup>a</sup>*Department of Chemistry, Texas A & M University, College Station, TX, USA, and* <sup>b</sup>*Argonne National Laboratory, Argonne ILL, USA. E-mail: j-reibenspies@tamu.edu*

**Keywords: Vapochromic; Powder Diffraction; Solid State Reaction**

The Nickel coordination complex of BME-DACH [*N,N'*-Bis(2-mercaptoethyl)-1,4-diazacycloheptane] has proven to be an effect vapochromic solid-state sensor for SO<sub>2</sub>. In the presence of SO<sub>2</sub> the solid Ni(BME-DACH) powder turns from a light brown to a bright orange and when placed in air the orange powder reverts back to the brown solid. The crystal structure and the thermal gravimetric analysis (TGA) of the orange powder indicates the presence of two molecules of SO<sub>2</sub> per molecule of Ni(BME-DACH). The TGA also indicates that at 60°C one molecule of SO<sub>2</sub> is lost and an intermediate containing one molecule of SO<sub>2</sub> per molecule of Ni(BME-DACH) is formed. Finally a molecule of SO<sub>2</sub> is lost at 100°C to form the light brown Ni(BME-DACH) powder. Micro powder diffraction techniques have been employed to follow the loss of SO<sub>2</sub> over time. The diffraction experiment shows that at room temperature, there is a gradual loss of the SO<sub>2</sub> from the orange Ni(BME-DACH)·2SO<sub>2</sub> complex to form the dark brown Ni(BME-DACH)·1SO<sub>2</sub> complex and finally the appearance of the light brown Ni(BME-DACH) complex. At any given time a mixture of at least two of these complexes is seen at room temperature. The crystal structure of the dark brown powder, which was isolated from the TGA experiment at 70°C, was solved by SDPD (Structure Determination from Powder Data) methods and consists of Ni(BME-DACH)·1SO<sub>2</sub>. Based on the crystal structures of the of Ni(BME-DACH)·2SO<sub>2</sub>, Ni(BME-DACH)·1SO<sub>2</sub>, Ni(BME-DACH), the TGA and the dynamic X-ray powder diffraction studies, a mechanism will be presented for the effusion of SO<sub>2</sub> from the orange powder [Ni(BME-DACH)·2SO<sub>2</sub>].