

s13.m35.p18 **A Molecule-Based Magnet Structure Above and Below the Critical Phase Transition Temperature.** Carlos Basílio Pinheiro<sup>a</sup>, Philip Pattison<sup>a,b</sup>, Humberto Stumpf<sup>c</sup> and Gervais Chapuis<sup>a</sup>, <sup>a</sup>Crystallography Laboratory - Swiss National Institute of Technology, Lausanne, Switzerland, <sup>b</sup>SNBL- ESRF, Grenoble Cédex, France, and <sup>c</sup>Chemistry Department, Federal University of Minas Gerais, Brazil. E-mail: carlos.pinheiro@epfl.ch

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The study of molecule-based magnets, *i.e.*, compounds with strong molecular character exhibiting spontaneous magnetization below a certain critical temperature ( $T_C$ ), involve synthesis of new compounds and studies of their physical properties. The goal is to produce compounds with pre-determined properties such as high coercive fields, remnant magnetization (memory effects) and optical properties. In this context it is of great relevance to know the 3D structure of these materials. We report the pioneering structural low temperature studies on  $[Pr-Rad]_2Mn_2[Cu(opba)]_3(DMSO)_{3.3} \cdot 5H_2O$  complex, where  $Pr-Rad^+$  is a radical cation propyl-nitronil nitroxide and DMSO is the solvent dimethyl-sulfoxide [1]. This compound presents a magnetic transition around 24 K [2]. X-ray diffraction experiments were performed at room temperature, 40 K and 15 K at SNBL-ESRF. The analysis of the reciprocal space at 293 K and 15 K does not indicate any symmetry change during the magnetic phase transition. The Mn ions form a hexagonal-like sub-lattice ( $Mn-Mn$ )=10.61(6) Å at 15 K and 10.6(1) Å at 293 K. The Cu atoms are placed in the middle of the face of the Mn hexagon and three of them are crystallographic independent ( $Cu-Cu$ )=5.37(2) Å at 15 K and 5.36(4) Å at 293 K. One Cu atom is bonded to the DMSO molecule. The other two Cu atoms are bonded to the  $Pr-Rad^+$  radical. The structural refinement shows that the  $Pr-Rad^+$  is not coordinated to the Cu atoms symmetrically. In addition to the different distances, the bonding angles are also different and as a result one  $Pr-Rad^+$  interacts more weakly with the neighboring Cu ions than the other. This asymmetry in the interactions seems to explain the increase of the total magnetic moment below 2 K [2].

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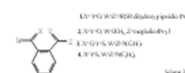
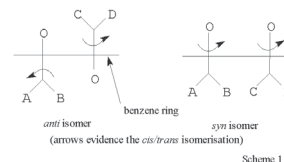
s13.m35.p19 ***o*-Phthalic Acid Derivatives: a Structural Investigation of Their Flexibility.** Patrizia Rossi<sup>a</sup>, Paolo Dapporto<sup>a</sup>, Annalisa Guerri<sup>a</sup>, Maria Altamura<sup>b</sup>, Francesco Cuda<sup>c</sup>, Antonio Guidi<sup>b</sup>, Cristina Nativi<sup>c</sup>, <sup>a</sup>Dept. of Energy Engineering, University of Florence, Italy, <sup>b</sup>Menarini Ricerche S.p.A., Italy, <sup>c</sup>Dept. Of Organic Chemistry, University of Florence, Italy. E-mail: prossi@ingfi1.ing.unifi.it

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*N,N',N'',N'''*-tetrasubstituted-*o*-phthalic acid diamides (4*N*-PADAs), are compounds potentially useful for the storage and handling of information at molecular level because of their peculiar structural features [1,2]. In fact with a proper exploitation of these latter, chemical libraries based on symmetry and on the control of the thermal flexibility can be obtained.

In this contribution, we report on a study focused on 4*N*-PADAs and closely related compounds in which internal rotations are the particular target.

In principle a 4*N*-PADA could exist as a set of interchanging stereoisomers arising from the syn or anti orientation of the two amide groups and the *cis/trans* amide isomerisation (Scheme 1). According to literature in solution of deuterated solvents the two amide groups prefer to stay *anti* parallel [1-3]. With these considerations in mind, we have performed a structural characterization (X-ray structure determination and quantum chemical calculation) of four derivatives of *o*-phthalic acid (Scheme 2).



Indeed, only compound **1** is a 4*N*-PADA amongst them and was selected because we decided to throw a glance to the combination of axial and s-bond based chirality in a chemical which could be itself a novel platform ready for combinatorial purposes. Compounds **2**, **3** and **4** were chosen for comparative purpose to assess the relative freedom of internal rotation in respect to **1**. Results were then discussed and validate in view of the the corresponding 3D features of analogous compounds retrieved from the Cambridge Structural Database [4].

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