b = 9.6565(5), c = 23.2828(11) Å,  $\beta = 111.637(8)^\circ$ , V = 4759.6(4) Å<sup>3</sup>, space group *C2/c*. The 3.3% reduction in unit cell volume is explained in terms of water loss, rearrangement of the water structure and coordination about the mobile Co atom.

Keywords: cubane, modulation, magnetism

### MS66.P03

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# Semiconducting triindoles: Crystallographic packing vs electrical performance

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The field of organic electronics has experienced an enormous development over the past ten years and today we can consider it a mature field. Devices such as OLEDs, OFETS or photovoltaic cells are already reaching the market. These devices have in common that their performance depends on how efficiently charge carriers move in the organic active layers. Important advances achieved in this field have been therefore connected to the enhancement of the charge carrier mobility of the organic molecules which have reached values that can already compete with amorphous silicium.

In close relation with the supramolecular order, the highest charge carrier mobility is

susually obtained in organic single crystals. Furthermore, organic single crystals offer an excellent opportunity to investigate structure-properties relationships and to elucidate charge transport mechanisms in organic materials, not yet fully understood.



introduced heptacyclic 10,15-dihydro-5*H*-diindolo[3,2-*a*:3',2'-*c*]carbazole (triindole) as an interesting new organic semiconductor.

This molecule is an electron-rich heptacyclic platform with a high tendency to aggregate both in solution and in crystalline state. We have recently found that CH- $\pi$  interactions have an important role in the self assembly of triindole-based molecules[2],[3]. Triindole-based single crystalline materials have been found to exhibit high hole mobilities (up to  $\mu = 0.4$  cm<sup>2</sup> V<sup>-1</sup> s<sup>-1</sup>) since they combine intrinsic electron donor properties with a highly ordered columnar packing that paves the way for increased charge carrier mobility due to favorable intermolecular  $\pi$ -orbitals overlap [1].

In this communication, we present how through an adequate functionalization we can modulate both the intermolecular interactions and the crystallographic packing, as could be determined through single crystal analysis of different derivatives. It will be shown how the crystallographic packing influences the electrical performance and the processability of these materials essential parameters towards their incorporation in devices.

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## Solid state transformation in coordination polymers with flexible ligands

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There is a growing interest in the nature of flexible and dynamic metal–organic frameworks (MOFs) owing to their potential applications as functional materials. Several examples of 'breathing' MOFs are known, in which structural changes occur without bond cleavage. In turn, few examples of MOFs in which the solid state transformation involves covalent bond breaking and formation are also known [1].

Herein, we report two new coordination polymers,  $\{[Co(L)_2(OH_2)_2].2NO_3.2H_2O\}_n$  (1), and  $\{[Co(L)_2(NO_3)_2]\}_n$  (2), where L is the neutral N-donor ligand, 1,4-bis(triazol-ylmethyl)benzene. Remarkably, compound 1 is able to extrude the H<sub>2</sub>O molecules (both solvated and coordinated) and transforms into compound 2 in the solid state. This process occurs on heating, with a consequent rearrangement of the 1D chains present in 1 into 2D layers. It is accompanied by a change in conformation of the flexible ligand, which implies breaking and formation of Co-N bonds. Such a change in conformation has been followed by spectroscopic techniques. Additionally, conversion of 1 into 2 also requires coordination of the NO<sub>3</sub> anions to the metal centers, which implies a substantial change in the Co<sup>II</sup> environment that has been monitored by EPR.

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# New molecular conductors with halogen substituted cobalt bis(dicarbollide) anions

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Radical cation salts and charge transfer complexes based on bis(e thylenedithio)tetrathiafulvalene (ET) and it's derivatives constitute a wide class of organic materials with transport properties ranging from insulating to superconducting.



Recently we started study of effect of different substituents in the iron group metal bis(1,2-dicarbollide) complexes on crystal packing and physical properties of their salts with radical cations – ET derivatives. In this report we describe synthesis, crystal structure and electrical conductivity of ET and BMDT salts of halogen substituted cobalt bis(dicarbollide) anion:  $(ET)[8,8^{\circ},(7)-Cl_2(Cl_{0.09})-3,3^{\circ}-Co(1,2-C_2B_9H_{10})(1,2-C_2B_9H_{9.91})]$  (1)  $(ET)[8,(7),8^{\circ}-Br_{0.75}(Cl_{0.25})Cl-3,3^{\circ}-Co(1,2-C_2B_9H_{10})_2]$  (2) and  $(BMDT-TTF)_4[8,8^{\circ}-Br_{1.16}(OH)_{0.72}-3,3^{\circ}-Co(1,2-C_2B_9H_{10.06})_2]$  (3).

The geometry of the  $[8,8',(7)-Cl_2(Cl_{0.09})-3,3'-Co(1,2-C_2B_9H_{10})(1,2-C_2B_9$ 

