Poster Sessions

MS66.P04

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)(OH))\_2NO\_2H\_2O]\_n (1), and [(Co(L)(NO\_3))\_2] (2), where L is the neutral N-donor ligand, 1,4-bis(triazol-ylmethyl)benzene. Remarkably, compound 1 is able to extrude the H\_2O 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\_3 anions to the metal centers, which implies a substantial change in the Co\_2\_ environment that has been monitored by EPR.


Keywords: MOF, flexible framework, molecular dynamics.

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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(thylenedithio)tetrathiafulvalene (ET) and it’s derivatives constitute a wide class of organic materials with transport properties ranging from insulating to superconducting.

![BMDT](image)

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’(7)-Cl\_2(1,2-C\_B\_H\_9\_)][3,3’-Co(1,2-C\_B\_H\_9\_)][3,3’-Co(1,2-C\_B\_H\_9\_)] (1) (ET)[8,8’-Br\_2(1,2-C\_B\_H\_9\_)][Cl\_2(3,3’-Co(1,2-C\_B\_H\_9\_)][3,3’-Co(1,2-C\_B\_H\_9\_)] (2) and (BMDT-TTF)[8,8’-Br\_2(1,2-C\_B\_H\_9\_)][3,3’-Co(1,2-C\_B\_H\_9\_)] (3).

The geometry of the [8,8’(7)-Cl\_2(1,2-C\_B\_H\_9\_)][3,3’-Co(1,2-C\_B\_H\_9\_)] (1)