Poster Presentation

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Novel LnMOFs based on tricarboxylate ligand: structures and topological representations

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Metal–organic frameworks (MOFs) are now a major topic of materials chemistry because of their actual and potential applications [1]. They are very interesting example of reticular chemistry as their frameworks are assembled by linking molecular units of well-defined shapes by strong bonds into periodic frameworks [2]. Furthermore, such structures can be deconstructed into their underlying nets (framework topology) to facilitate designed synthesis of materials with targeted porosity, pore size, and functionality [3]. Upon reacting tridentate ligand 1,3,5-tris(4-carboxyphenyl)benzene (H3BTB) with lanthanides cations under solvothermal conditions three novel series of metal-organic frameworks (MOFs) were obtained with the formulas [Ln2(BTB)2(CO)] (Ln=Y, Nd, Sm, Eu, Gd, Tb, Dy, and Er) (KO1-8), [Ln3(μ3-O)3(BTB)2(H2O)•(DMF)2] (Ln=Y, Tb, Dy, and Ho) (KO9-12), and [Ln(BTB)(H2O)2] (Ln=La, Ce, Pr, and Nd) (KO13-16). The X-ray crystal structural analysis reveals that the compounds of the first serie are a 3D structure composed of intercalated inorganic chains [(Ln2O14)–C–(Ln2O14)]∞ along [011], [101] and [110] directions, which are linked through BTB ligands. The structure of the second serie is formed up an inorganic chain that constructed from consequently edge-shared of dimeric cluster{Ln2O14} and tetranuclear cluster {Ln4O22}. These chains are linked by the BTB linkers generating the whole 3D structure, while the structure of the third serie is build up of an inorganic tetranucler chain (Ln(1)–Ln(2)–Ln(3)–Ln(2)) as SBU repeats along c axis forming an infinite zigzag inorganic chain. Each chain is in turn cross-linked to six adjacent chains through BTB bridges, forming a 3D framework with channels running along a axis. Their nets own different new topologies; the first one possess 3-nodal 3,5,6-connected nodes, while the second revels a 3-nodal network where the inorganic chain is formed by a combination of dimeric and tetranuclear cluster. Each cluster act as 8 and 12-connected nodes respectively and the ligand act as 3-connected node. The third one exhibits a 3,5-c network, in which the intermetallic positions in the chains are as a 5-connected nodal point and the ligand as a 3-connected node.

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