MS37-P4 Synthesis, Structures and Luminescence Properties of Metal-Organic Frameworks Based on Lithium- Lanthanide and Terephthalate

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Lanthanide MOFs (LnMOFs), as an important subclass of advanced functional materials, which can be synthesized using a wide range of lanthanide cations and organic ligands, they have been investigated in the fields of coordination chemistry, not only for their diverse architectures due to high coordination numbers and big ionic radii of lanthanide cations, but also for the potential applications in field of luminescence [1]. Among these compounds, the lithium-based MOFs [2] are attracting particular interest in being the promising candidates for replacing the conventional electrode in Li-ion batteries, exhibiting a high reversible specific capacity and excellent cyclability [3]. Novel metal-organic frameworks assembled from Ln(III), Li(I) and rigid dicarboxylate ligand, formulated as [LiLn(BDC)₂(H₂O)•2(H₂O)] (MS1-6,7a) and [LiTb(BDC)₂] (MS7b) ($L\ddot{n} = Tb$, Dy, Ho, Er, Yb, $Y_{0.96}Eu_{0.04}$, $Y_{0.93}Tb_{0.07}$ and H,BDC = terephthalic acid), were obtained under hydrothermal conditions. The isostructural MS1-6 crystallize in monoclinic P2₁/c space group. While, in the case of Tb³⁺ a mixture of at least two phases was obtained, the former one (MS7a) and a new monoclinic C2/c phase (MS7b). All compounds have been studied by single-crystal and and the bulk characterized by powder X-ray diffraction (PXRD). The structures of MS1-6 and MS7a are built up of inorganic-organic hybrid chains. While, the structure of MS7b is constructed from double inorganic chains. Both MS1-6,7a and MS7b structures possess a 3D framework with 1D trigonal channels running along the a and c axis, containing water molecules and anhydrous, respectively. Topological studies revealed that MS1-6 and MS7a have a new 2-nodal 3,10-c net, while **MS7b** generates a 3D net with unusual β-Sn topology. The photoluminescence properties Eu- and Tb-doped compounds (MS5-6) are also investigated, exhibiting strong red and green light emissions, respectively, which are attributed to the efficient energy transfer process from the BDC ligand to Eu3+ and Tb3

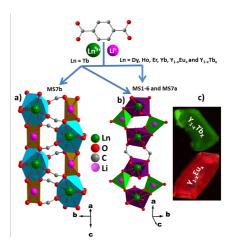


Figure 1. Perspective view of the infinite chains along the c and a axis for MS7b (a) and MS1-6 (b). The optical microscopic images under UV-light of single-crystals of Eu- and Tb-dopped compounds (c).

Keywords: lanthanide-organic frameworks, dicarboxylate, hydrothermal, crystal structure, topology, photoluminescence