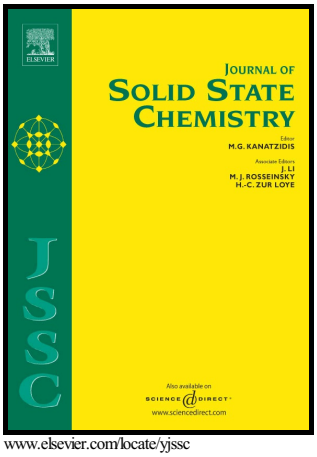

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Abstract

Design and synthesis of Lanthanide based metal organic framework is a frontier area of research owing to their structural diversity enabling specific applications. The luminescence properties of rare earths, tuned by the structural features of Ln-MOFs are investigated extensively. Rare earth oxalates which can be synthesized in a facile method, ensuring the structural features of MOFs with excellent photoluminescence characteristics deserves much attention. This work is the first time report on the single crystal structure and Judd-Ofelt (JO) theoretical analysis – their correlation with the intense and sharp green luminescence of Terbium oxalate crystals. The intense green luminescence observed for Terbium oxalate crystals for a wide range of excitation from DUV to visible region despite the luminescence limiting factors are discussed. The absence of concentration quenching and lifting up of forbidden nature of f-f transitions, allowing direct excitation of Terbium ions is analysed with the help of JO theory and single crystal structure analysis. The JO analysis predicted the asymmetry of Terbium sites, allowing the electric dipole transitions and from the JO intensity parameters, promising spectroscopic parameters – emission cross section, branching ratio, gain band width and gain coefficient of the material were calculated. The single crystal structure analysis revealed the asymmetry of Tb sites and structure of Terbium oxalate is formed by the hydrogen bonded stacking of overlapped six Terbium membered rings connected by the oxalate ligands. The molecularly thick layers thus formed on the crystal surface are imaged by the atomic force microscopy. The presence of water channels in