



Structural, thermal decomposition and luminescent studies on gel grown crystals of poly[tetraaquadinicotinatostrontium(II)] containing 'χ'-shaped hydrophobic channels

R. Drisya¹ · U. S. Soumyamol¹ · P. R. Satheesh Chandran¹ · M. R. Sudarsanakumar¹ · M. R. Prathapachandra Kurup²

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Abstract

Single crystals of the polymeric title complex tetraaquadinicotinatostrontium (SPYC) were successfully grown by a simple and efficient method—the gel encapsulation technique. Sodium metasilicate was used as the gel medium for this purpose. The crystal structure of the complex indicates that it belongs to triclinic system with space group $P\bar{1}$. The packing diagram of the complex shows uniformly arranged 'χ'-shaped hydrophobic channels. The thermal decomposition of the crystals have been studied by thermogravimetric analysis at four different heating rates and kinetic parameters including apparent activation energy (E_a), and pre-exponential factor ($\log A$) were calculated by Kissinger, Ozawa and Flynn–Wall–Ozawa methods. Analytical techniques including FT-IR, CHN, powder and single-crystal X-ray diffraction were also carried out to characterize the grown crystals. The solid-state luminescent properties of free ligand and complex were also investigated at room temperature.

Keywords Metal–organic frameworks · Thermal analysis · Non-isothermal kinetic studies · Flynn–Wall–Ozawa method

Introduction

Metal–organic frameworks (MOFs) are a class of crystalline materials constructed from inorganic–organic building units that have numerous applications in the field of catalysis, energy storage, drug delivery systems, luminescence and gas storage. MOFs have gained a lot of traction over the past few years owing to their interesting framework architecture, topology and optical properties. An important category belonging to MOFs are the metal carboxylates which can form a lot of hybrid structures [1–5]. Aromatic dicarboxylic acids containing N and O acceptors show copious coordination modes for the construction of variety of metal–organic compounds [6–8].

Dinicotinic acid or pyridine-3,5-dicarboxylic acid (H_2pydc) is an important symmetrical and rigid organic ligand because of its multitopic binding sites with various metal ions. The rigidity is attributed by the presence of pyridine backbone in the structure. These types of ligands can self-assemble metal ions to higher dimensional supramolecular frameworks through hydrogen bonding and π – π stacking interactions. The metal complexes of pyridine dicarboxylic acids have applications in catalysis, biological activities, magnetism and fluorescence [9–13]. The absence of d orbital controlled coordination chemistry in alkaline earth metals results in higher coordination numbers from six to nine [14]. Hence the geometry of the compound is difficult to control and creates steric saturation within the structure.

The nature of thermally stimulated processes and the physico-chemical properties of materials can be monitored by thermogravimetric and differential thermal analysis. Kinetic studies from thermal analysis are helpful for evaluating the Arrhenius parameters [activation energy (E_a) and pre-exponential factor (A)] and thereby explaining the mechanism of decomposition reactions. In order to investigate the kinetic parameters, multiple heating rate method is recommended by the International

✉ M. R. Sudarsanakumar
sudarsanmr@gmail.com

¹ Department of Chemistry, Mahatma Gandhi College, Thiruvananthapuram, Kerala 695 004, India

² Department of Chemistry, School of Physical Sciences, Central University of Kerala, Riverside Transit Campus, Padenakad, Nileshwar, Kerala 671 314, India