

s13.m37.o2 **Physical chemistry of lanthanide coordination polymers.** Susan A Bourne and Lesego J Moitsheki, *Department of Chemistry, University of Cape Town, Rondebosch 7701, South Africa. E-mail: xraysue@science.uct.ac.za*

Keywords: Coordination Polymer; Crystal Engineering; Thermal Analysis

Coordination polymers and 0D frameworks, built up of metal centres linked by organic ligands, have been extensively studied in recent years with especial interest in their utility for molecular recognition, non-linear optical properties or for catalytic purposes.[1] As part of a study on the crystal engineering of network solids, a series of coordination polymers have been prepared using lanthanide salts and bridging ligands derived from pyridyl or sulfonate molecules. Crystal structures of these materials reveal well-ordered network structures, similar in some cases to those previously reported by Schröder *et al.* [2] The thermal decomposition behaviour of the coordination polymers has been studied using Differential Scanning Calorimetry (DSC), Thermogravimetry (TG) and Hot Stage Microscopy (HSM). The kinetics of decomposition have been studied for $[\text{Gd}(\text{L}^1)(\text{MeOH})(\text{NO}_3)_3]$ (where L^1 is 4,4'-bipyridine- N,N' -dioxide) and for $[\text{Tl}(\text{L}^2)(\text{NO}_3)_3]$ (where L^2 is 1,5-naphthalenedisulfonate). In some cases the coordination polymers act as host networks, encapsulating organic guest molecules. In these cases the kinetics of guest desorption can be studied and results correlated with the crystal structures. Absorption of guest molecules from the vapour phase can also be effected in some cases, and followed using a vacuum balance.

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s13.m37.o3 **Thermogravimetric and IR spectroscopic hints of structure validated by X-ray crystallography.** János Madarász,^a Petra Bombicz^b and György Pokol^a, ^a*Institute of General and Analytical Chemistry, Budapest University of Technology and Economics, H-1521 Budapest, Hungary, and* ^b*Institute of Chemistry, Chemical Research Centre, Hungarian Academy of Sciences, P.O. Box 17, H-1525 Budapest, Hungary. E-mail: madarasz@tki.aak.bme.hu*

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The molecular moieties, their arrangement and intermolecular interactions within a crystal strongly affect its thermal stability and FTIR absorption. Usually we try to explore the building blocks in a set of related substances applying combustion analysis, thermal analysis (thermogravimetry and coupled techniques) FTIR-spectroscopy, in combination before single crystal X-ray diffraction. The former methods may provide initial information on stoichiometry, ionic states and binding strengths of the constituents. Sometimes the results give also a hint of the structure. *Vice versa* the knowledge of the structure and especially of the H bonds from single crystal X-ray diffraction helps to explain decomposition behavior and FTIR absorption spectra of the materials. This complex application of the methods helps us to reveal structure-property relationships and based on the gained implications we can conclude on related polycrystalline samples, even on a clearing up of reaction pathway.

One of our investigated systems is a set of amine complexes of Cu(II) containing theophyllinate anions, for modeling chelating of DNA-bound guanine [1-3]. The other is a set of lattice compounds of theophylline with compounds related to ethylenediamine for collecting information on the possible structure of anti-asthmatic drug aminophylline [4-6]. The third system [7-9] contains various thiourea-metal precursors of semiconductive sulfide thin films. They are Cu(I), Sn(II), Zn(II) complexes containing thiourea ligands in various stoichiometric composition

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