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ORIGINAL PAPER

A new organically templated magnesium sulfate: structure, spectroscopic analysis, and thermal behaviour

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A new magnesium sulfate templated by 2-methylpiperazine, $(C_5H_{14}N_2)[Mg(H_2O)_6](SO_4)_2$, was prepared by the slow evaporation method. The obtained crystals were investigated by the Raman and FTIR spectroscopy and crystallographically characterised by single-crystal X-ray diffraction. The compound crystallises in the monoclinic system, space group $P2_1/n$. Supramolecular network of this hybrid material consists of Mg^{2+} cations octahedrally coordinated by six water molecules, sulfate tetrahedra and protonated and disordered diamine linked together by two types of hydrogen bonds: OW—H···O and N—H···O. Dehydration of the title compound takes place in three steps. Thermal decomposition of the anhydrous phase consists in the loss of the organic moiety and one sulfate group leading to the formation of magnesium sulfate.

Keywords: amine magnesium sulfate, supramolecular network, crystal structure, thermal decomposition, dehydration

Introduction

Organic/inorganic hybrid materials continue to be of great interest because of their structural diversity and potential application in many fields such as mechanical resistance, optics, electric, and solid state electronics (Kagan et al., 1999; Hill, 1998). Transition metal sulfates templated by protonated amines are a well-known family of such materials. A large number of hybrid sulfates containing a divalent metal and amine has been recently reported (Rekik et al., 2006a, 2006b, 2008; Naïli et al., 2006; Yahyaoui et al., 2007; Rujiwatra & Limtrakul, 2005; Healy et al., 1984; Chaabouni et al., 1996; Held, 2003; Ben Ghozlen et al., 1994; Hajlaoui et al., 2012). Despite the richness of the crystal chemistry of open framework metal sulfates, the synthesis of organically templated magnesium sulfates is a rarely studied area. The difficulty of obtaining good quality crystals with this element can be the main reason. Recently, three magnesium sulfates templated by ethylenediamine, piperazine, and 1,4-diazabicyclo[2.2.2]octane (DABCO) have been reported (Rekik et al., 2012). In this type of compounds, organic diamines are often used as the structure-directing agent. The choice of an organic amine has usually a profound influence on the final structure of the material and leads to the formation of a novel inorganic framework. In this paper, chemical preparation, crystal structure, spectroscopic analyses, and thermal behaviour of the 2-methylpiperazinediium hexaaquamagnesium(II) bis(sulfate), $(C_5H_{14}N_2)[Mg(H_2O)_6](SO_4)_2$ (I), are reported.

Experimental

FTIR spectra (in KBr pellets) were obtained using a Perkin–Elmer FTIR spectrometer Model 100 in the range of 400–4000 cm^{-1}. Raman spectra were recorded on a Jobin Yvon Horiba HR800 LabRAM spectrometer in the range of 50–4000 cm^{-1}.

DTA-TG measurements were performed using a

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