

Poster Presentations

[MS38-P13] Further Studies on Ionic Co-Crystals: Dehydration and Hydration Behaviour.

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The use of ionic electrostatic interactions to produce new coordination compounds such as ICCs containing alkali metals and alkaline earth metals halides has been recently introduced in the field of molecular Crystal Engineering [1]. In this type of structures the interaction between inorganic ions and organic molecules must be seen as a special case of solvation, with the organic molecules acting as a solvent molecules (in competition with water if present) towards metal ions. As a matter of fact ICCs are generally hydrated at room conditions. The "solvating properties" of a number of molecules, mostly primary and secondary amides, have been studied, and their possible applications in the Pharmaceutical Industry depends on our knowledge of their properties, such as their stability at different temperature and/or relative humidity [2]. We present here the results of our investigations on two cases of study: (1) the thermal behaviour of barbituric acid ICCs with alkali bromides and the associated dehydration processes; (2) the preparation and characterization of the anhydrous, monohydrated, dihydrated and tetrahydrated ICCs of nicotinamide, an active pharmaceutical ingredient, with CaCl₂ by solid

state controlled humidity methods, and their behaviour with temperature. Four new crystal forms were solved from powder diffraction using simulated annealing procedures. The crystalline compounds were analyzed with differential scanning calorimetry (DSC), thermogravimetry (TG) and solid-state nuclear magnetic resonance (SS-NMR), which were crucial to resolve the ambiguities in the structure solutions.

[1] Braga D., Grepioni F., Maini L., Prosperi S., Gobetto R., Chierotti M.R. (2010). *Chem Commun*, **46(41)**, 7715-7717.

[2] Braga D., Grepioni F., Lampronti G.I., Maini L., Turrina A., (2011). *CrystEngComm*, **11**, 5621-5627

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