

## MS32-P18

### Hydrogen bonding in organic salt hydrates

Laszlo Fabian<sup>1</sup>

1. School of Pharmacy, University of East Anglia, Norwich, United Kingdom

**email:** [l.fabian@uea.ac.uk](mailto:l.fabian@uea.ac.uk)

About half of the drugs currently on market are salts. Salt based formulations are often preferred to those using neutral molecules, because they provide higher solubility. However, salts are prone to form hydrates, which may lead to stability problems with the drug product. The aim of this work is to investigate how specific hydrogen bonding interactions influence hydrate formation and whether the different propensities of ions towards hydrate formation [1] can be related to hydrogen bonding preferences.

The hydrogen bond coordination [2] of ammonium, chloride and carboxylate ions will be discussed using data from the Cambridge Structural Database [3]. Comparisons between hydrate and anhydrous structures of the same ion pair reveal how water–ion hydrogen bonding competes with direct anion–cation hydrogen bonds. For example, the average coordination number of ions is larger in hydrates, but the frequency of direct anion–cation bonds is reduced in hydrates relative to anhydrous structures. Similarly, the average number of ammonium ions bonding to a single anion is lower in hydrates than in anhydrous structures. Analysis of the hydrogen bonding environment of water in these structures shows clear differences between the anions and cations, e.g. in ammonium carboxylate salts water–carboxylate bonds are much more frequent than ammonium–water bond.

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## MS32-P19

### Magnetic properties of highly symmetrical compounds of cobalt(II) and nickel(II)

Marcin Koziel<sup>1</sup>, Klaudia Nowakowska<sup>1</sup>, Marlena Gryl<sup>1</sup>, Dawid Pinkowicz<sup>1</sup>, Wiesław Lasocha<sup>1</sup>

1. Faculty of Chemistry, Jagiellonian University, Kraków, Poland

**email:** [marcin.koziel@uj.edu.pl](mailto:marcin.koziel@uj.edu.pl)

The proper symmetry of crystal lattice determines the presence of many physical properties like piezo- or pyroelectricity, or nonlinear optical behaviour. [1] On the other hand the local symmetry of transition metal ions influences the energy of electron orbitals and, as a consequence, absorption of electromagnetic radiation as well as luminescent and magnetic properties. Therefore directing the synthesis towards particular symmetry of the solid product can allow control over the properties of resulting material. The aim of our current research includes the deeper understanding of the relation between the symmetry of the used building blocks and the symmetry of the products obtained in the self-assembly process. We also attempt to obtain products with high symmetry of the crystal lattice. It is quite a challenge for crystal engineering because highly symmetrical building blocks do not often yield highly symmetrical products. Such phenomena as partial dissociation, solvation, intermolecular interactions or improper stoichiometry may render all efforts unsuccessful. Apart from inorganic compounds, where cubic system is quite common, in all other compounds the monoclinic and triclinic systems dominate. The most common orthorhombic group is adapted by c.a. 10% of structures, mostly chiral compounds, and the trigonal, tetragonal and hexagonal systems are the most rare.

In order to obtain the required features of the products we combined highly symmetrical organic molecules with various salts of 3d-elements. The inorganic component is introduced to improve stability of the compound as well as interesting electronic properties. We successfully obtained several new compounds, some of them belonging to high-symmetry space groups. The methodology, the structures and some interesting properties of the products will be presented.

References:

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