MS36-O5

The structure of copper(II)-hydroxypiridinecarboxylic acid derivatives in both solid and solution phases

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Metal complexes of small biomolecules are frequently used as bioactive compounds in diverse fields of clinical practices. The structure and physico-chemical properties such as solubility and stability of these functional metal complexes are usually fine-tuned in order to optimize the bioavailability and bioactivity. Single crystal X-ray diffraction (SXRD) is one of the most powerful technique for the investigation of the structures of these organic compounds and their complexes in solid phase. However, this method has some weaknesses in case of biologically relevant compounds. Firstly, the preparation of a good quality and suitable size crystal, in many cases, requires sophisticated techniques. Secondly, a number of complexes with different compositions and structures are generally formed in aqueous solution, and so the coexistence of various species is rather typical. This means that the majority of complexes cannot be obtained and studied in crystalline form. Another question is whether the structure of the complex obtained as a single crystal is identical with the one was observed in the solution. These problems warrant the use of another technique in combination with SXRD in which the equilibrium systems of biologically relevant metal complexes can be investigated in solution. In case of paramagnetic metal complexes (such as copper(II)) electron paramagnetic resoncance (EPR) spectroscopy is an extremely sensitive technique to detect the chemical surrounding of the unpaired electron and provides unique local structural information. In the present work we use pH-dependent EPR spectroscopy in combination with SXRD to investigate the complexation properties of a series of substituted hydroxypyridinecarboxylic acids (HPCs)[1,2] with copper(II). The solution equilibrium system of their copper(II) complexes were investigated by EPR and their bis-ligand [CuL_2] complexes were crystallized then investigated by SXRD technique resulted in complementary outcome of the solid and liquid phases.

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MS37 Mechanochemistry: structure and reaction

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MS37-O1

Is a mechanochemical reaction always truly mechanochemical?

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Mechanochemistry has surged in popularity, and is now commonplace in many chemical and materials sciences laboratories. Successful examples of mechanochemical techniques being used in multi-component crystallisation, chemical and bio-chemical synthesis and in the field of supramolecular chemistry are now widely known. However, while many of these examples employ mechanochemical techniques, are they truly *mechano*chemical in nature? This talk will explore a variety of examples where mechanical energy has been used to induce a chemical or physical change in solid-state systems. A variety of effects that result from the mechanical treatment of solids will be discussed, encompassing both single and multi-phase systems. Particular emphasis will be placed on distinguishing between processes that are directly driven by mechanical energy (e.g. mechanically induced chemical reactions), indirectly driven by mechanical energy (e.g. driven by a product of the mechanical energy), and those that are facilitated by it (e.g. those that would proceed in the absence of mechanical energy).

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