MS34-O4 Inclusion chemistry: Guest species determining properties of multi-component crystals

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The humble solvate has been a crystal form for as long as crystals have been recognised. Solvates, a type of multi-component crystal, have produced many scientific studies and important industrial materials. Examples include the hydrated “boiling stones” known as zeolites and the pharmaceutical solvates, their stability towards hydrate formation being incredibly important to modern lifestyles. Often banished to the supplementary information, the removal or exchange of solvents (guests) from multi-component crystals is a necessary step to produce a “porous” material and often is not as simple as just “boiling” the material. In this presentation we shall show how the use of different solvates can allow for the production of different desirable properties within a material. Even though you can remove most solvents from multi-component crystals leaving at least one component behind, this often leads to a non-porous “collapsed” phases [1]. Careful selection of the “right” solvent can lead to metastable porous materials as will be shown utilising solvates of metallocycles and metallocages (also known as metal-organic polyhedral, MOPs) in which the interplay between intrinsic and extrinsic cavities results in porosity [2]. When crystal engineering these molecular porous materials the “interactions” between the molecular building blocks can be overly focused on, but the guest can play a keystone role in determining the desired property [3]. The “solvation” of the molecular building blocks within the solid periodic structures means the inclusion of solvents in the solid is an important aspect of crystal engineering all porous materials. Finally, with porosity shown, inclusion chemistry is utilised to generate interesting physical properties in the form of gas storage and separation [4], fluorescence tuning [5] and paramagnetism from diamagnetic building blocks [6].

References

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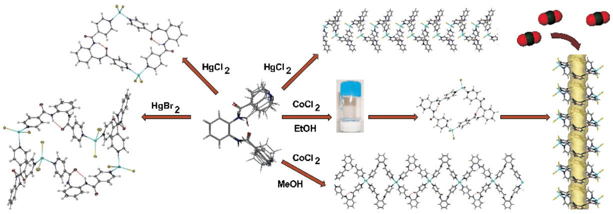

Figure 1. Solvent effects and solvent inclusion contribute to a large variety of phases, only some of which show porous properties and inclusion chemistry.

Keywords: Porous, Metallocycle, Molecular Cages, Solvates, Inclusion Chemistry