Sandwiches and Cavities: The Supramolecular Chemistry of Hemimellitic Acid

Sophie H. Dale^a, Augusta E. L. Coombs^a, William Clegg^a, Mark R. J. Elsegood^b, Sarita Kainth^b, ^aSchool of Natural Sciences, University of Newcastle-upon-Tyne, Newcastle-upon-Tyne, UK. ^bChemistry Department, Loughborough University, Loughborough, UK. E-mail: S.H.Dale@newcastle.ac.uk

Prior to our investigations of its potential contribution to supramolecular chemistry, and despite its commercial availability as a crystalline dihydrate, hemimellitic acid (H₃HMA; benzene-1,2,3-tricarboxylic acid) appeared in only 8 crystal structures recorded in the Cambridge Structural Database (CSD; Version 5.26, November 2004). The presence of carboxylic acid functionality in H₃HMA facilitates the formation of both organic-based hydrogen bonding arrays and metal-organic coordination frameworks, as has been previously demonstrated using trimesic and terephthalic acids.

 H_3HMA forms solvent-inclusion clathrates with solvent molecules capable of hydrogen bonding, often with rectangular solvent-filled cavities running through the structure [1]. Co-crystallisation with molecules containing *N*-heterocycles has also led to hydrogen bonded structures, often with accompanying proton-transfer [2]. The most interesting findings undoubtedly result from a systematic study of the coordination of H_3HMA to monopositive (Group 1 metals) and dipositive (Group 2 and transition metals) cations [3]. Significant structural diversity has been observed within this series of complexes; trends within the series will be analysed.

[1] Dale S. H., Elsegood M. R. J., Coombs A. E. L., *CrystEngComm*, 2004, 328-335. [2] Dale S. H., Elsegood M. R. J., Kainth S., *manuscripts in preparation*. [3] Dale S. H., Elsegood M. R. J., Kainth S., *manuscripts in preparation*.

Keywords: supramolecular chemistry, hydrogen bonding, carboxylic acids