MS42-05 **When Small Molecules Get Large – A Journey into the Unknown.** Amber L. Thompson,[a]*Chemical Crystallography, University of Oxford, UK.*
E-mail: amber.thompson@chem.ox.ac.uk

As small molecules get larger [1], determining their structures becomes increasingly challenging. Initially, the problem is growing suitable crystals; while this can be a problem for even very small molecules, for bigger molecules it can be particularly challenging. Once that hurdle has been overcome data collection is the next difficulty, where solvent loss, and poor diffraction can be serious impediments. Synchrotron radiation can make the impossible possible, but can also introduce new problems for example, radiation damage. Finally, structure refinement is always difficult due problems including a paucity of data, the large number of parameters and often, large regions of poorly defined solvent. In the last 10 years, the author's view of what constitutes a large structure has changed significantly. Starting in a world where a unit cell contains only a handful of atoms, small pharmaceutical compunds could seem quite large. More recently, collaborators have found increasingly large molecules to study, the most recent being 11.5 Kda! Some of the stops on this Journey into the Unknown will be presented along with some of the pit-falls, obstacles, detours and cul-de-sacs: the Final Destination is unknown.

Some examples of BIG molecules [1]!

[1] See for example Frey *et al.*, (2008), *J. Am. Chem. Soc.*, 130(33), 11013–11022; Davis, *et al.* (2010), *Org. Lett.*, 12(19), 2124–2127; Davis, *et al.* (2010), *J. Am. Chem. Soc.*, 133(1), 30-31; *Sprafke et al.*, (2011), *J. Am. Chem. Soc.*, 133(43), 17262–17273.

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MS43-01 **Host-guest interactions in cyclodextrin inclusion complexes at extreme conditions.** Francesca P. A. Fabbiani,[a] Gernot Buth,[b] Rubén Granero García,[ac] Fernando J. Lahoz,[c] Carsten Paulmann,[de] Sofiane Saouane,[a] *[a]GZG, Abt. Kristallographie, Georg-August-Universität Göttingen, Germany, [b]Karlsruhe Institute for Technology, ISS, Germany, [c] ISQCH, Facultad de Ciencias, Universidad de Zaragoza - CSIC, Spain, [d]Mineral. Petrog. Inst., Universität Hamburg, Germany, [e]DESY, Hasylab, Hamburg, Germany*
E-mail: ffabbia@gwdg.de

Since their discovery in the 1950s, the formation of inclusion complexes of cyclodextrins (CDs) in the solid and liquid states continues to be the subject of numerous studies.[1] CDs have found some useful applications in the pharmaceutical industry, for example as complexing agents for sparingly water-soluble drug molecules, or as stabilisers.[2] The ability of hydrated CDs and their inclusion complexes to form different physical forms under conditions of ambient pressure has been previously reported in the literature but has not been widely investigated.[3,4] Apart from recent solution NMR experiments and molecular dynamic simulations, the high-pressure behaviour of CDs remains virtually unexplored to date.[5,6] Through a series of case studies, we present new structural evidence, obtained by single-crystal X-ray diffraction, in support of the great structural variation and polymorphic behaviour exhibited by CDs under conditions of low temperature and high-pressure. In particular, we focus on a) the experimental conditions under which the new structures were obtained, b) the comparison of host-guest interactions in the new and known forms, and c) the role of water for structure stability.

[1] See for example: Cramer, F. (1954). Einschlussverbindungen. Springer-Verlag, Berlin.
[2] Loftsson, T. & Duchęne, D. (2007). *Int. J. Pharm.* **329**, 1-11. Hall.
[3] Saenger, W. & Steiner, T. (1998). *Acta Cryst.* A**54**, 798-805.
[4] Caira, M. R., de Vries, E. J. C. & Nassimbeni, L. R. (2003). *Chem. Commun.* 2058-2059.
[5] Ivanova, G. I., Văo, E. R., Temtem, M., Aguiar-Ricardo, A., Casimiro, T. & Cabrita, E. J. (2009). *Magn. Reson. Chem.* **47**(2), 133-141.
[6] Altarsha, M., Ingrosso, F. & Ruiz-Lopez, M. F. (2012). *J. Phys. Chem. B* **116**(13), 3982-3990.

Keywords: inclusion complexes; water; polymorphism