Poster Presentation

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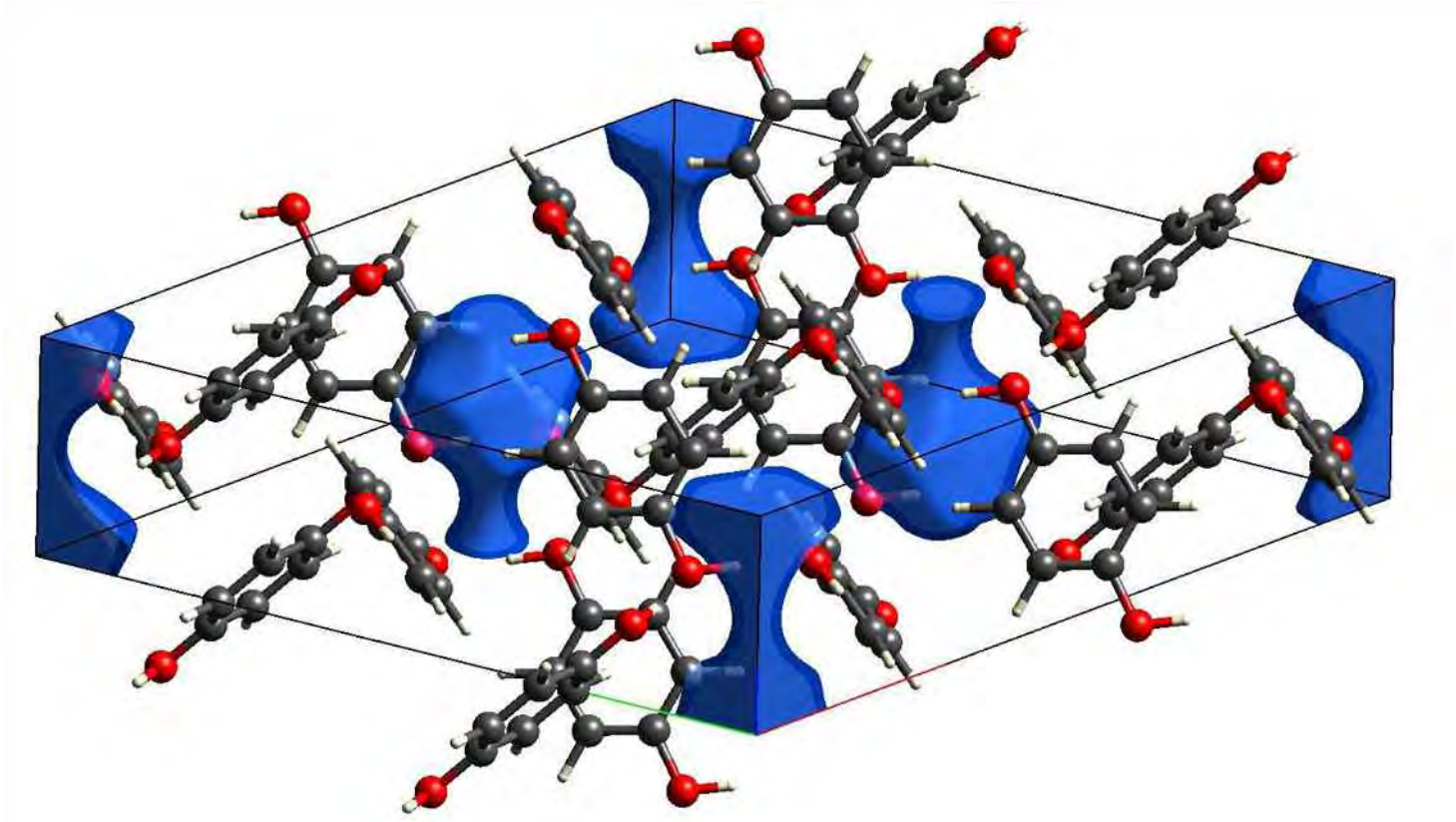
Exploring Host-Guest Interactions: a Single Crystal High-Pressure study

E. Eikeland[1], S. Madsen[1], J. Overgaard[1], M. Spackman[2], B. Iversen[1]

[1]*Aarhus University, Center for Materials Crystallography, Department of Chemistry and iNANO, Aarhus C, Denmark,* [2]*University of Western Australia, School of Chemistry and Biochemistry, Crawley WA, Australia*

Single crystal X-ray diffraction data from several Hydroquinone clathrate systems, with various small guest molecules (e.g. HCOOH, MeOH), have been obtained up to a pressure of 10 GPa, using a diamond anvil cell (DAC). Hydroquinone clathrates are key examples of supramolecular aggregates, having a diverse structural chemistry controlled, to a large extent, by the detailed intermolecular interactions between the host and the guest molecules. Although supramolecular chemistry is the foundation for the design and development of advanced materials (e.g. for catalysis, targeted drug delivery, chemical separation and nonlinear optics) the basic understanding leading to such complex systems are often lacking. High pressure (HP) crystallography is an excellent method of systematically increasing host-guest interactions by forcing the molecules closer together, often leading to interesting and unexpected results. At ambient pressure smaller guest molecules are often disordered inside the clathrate cavities. As the external pressure increases the cavities shrink, and it seems likely that guest molecules will order inside the cavity breaking the host symmetry. Guest ordering transitions are also found upon cooling. In this work, results from HP studies of the hydroquinone – formic acid system reveal that the structure is stable up to 10 GPa, at which pressure the guest cavity volume is reduced by more than 50 % without ordering of the guest atoms. Earlier studies have shown that the empty Hydroquinone clathrate undergoes a phase transition into a nonporous structure already at 0.4 GPa. [1] This indicates that formic acid stabilizes the host framework through strong intermolecular host-guest interactions, but without lowering the host symmetry.

[1] *Kim, B., J. Phys. Chem. B, 2013. 117(25): p. 7621-7625.*



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