Diffusion of Guests into Non-porous Crystals

Jerry L. Atwood[a], Leonard J. Barbour [b], Praveen K. Thallapally[a], [a]*Department of Chemistry, University of Missouri-Columbia, Columbia, MO 65211.* [b]*University of Stellenbosch, Department of Chemistry, 7602 Matieland, South Africa.* E-mail: atwoodj@missouri.edu

Crystals composed of purely organic compounds have largely been ignored as gas sorption substrates since such molecules usually pack with efficiencies in the narrow range of 60 to 67%. The host lattices of solvated inclusion compounds are often described as possessing zero-, one-, two- or three-dimensional solvent-accessible voids if the guest molecules are located in isolated cavities, channels, layers or networks of channels, respectively. It is therefore attractive to envision facile removal of the solvent molecules from these materials to yield highly porous host lattices analogous to those of zeolites. In reality, the process of desolvation almost always involves reassembly of the host molecules in the solid state to form one or more phases, where the pure compound is again efficiently packed. However, a few exceptions are known to exist. A low-density phase of sublimed p-*tert*-butylcalix[4]arene possesses lattice voids of *ca.* 235 $Å^3$ [1]. Despite an apparent lack of porosity, these crystals readily and reversibly absorb volatile gases [2,3] at room temperature and ambient pressures. In this presentation, new developments in the understanding of such gas absorption will be discussed.

[1] Atwood J. L., Barbour L. J., Jerga A., Schottel B. L., *Science*, 2002, **298**, 1000. [2] Atwood J. L., Barbour L. J., Jerga A., *Angew. Chem. Int. Ed. Engl.*, 2004, **43**, 2948. [3] Atwood J. L., Barbour L. J., Thallapally P. K., Wirsig T. B., *Chem. Comm*., 2005, 51.

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