Porosity in Molecular Crystals
Leonard J. Barbour, Liliana Dobrzeńska, Gareth O. Lloyd,
Department of Chemistry, University of Stellenbosch. Stellenbosch, South Africa. E-mail: ljbarbour@sun.ac.za.

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%. Consequently, void spaces larger than 25 Å³ are seldom encountered in organic solids. 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 is almost always accompanied by reassembly of the host molecules in the solid state to form one or more so-called apohost phases, where the pure compound is once again efficiently packed. However, a few exceptions to this phenomenon are known to exist.

We are interested in using the principles of crystal engineering to design and construct new solids for applications such as gas sorption. Although the availability of vacant lattice voids is essential, these solids are apparently not required to be “porous” in the classical sense when considering the van der Waals surfaces of the constituent host molecules. This contribution will focus very generally on the concept of porosity in molecular crystals, and on the phenomenon of guest transport within a solid host framework.

Keywords: porous materials, self assembly supramolecular chemistry, crystal engineering