

Poster Presentation

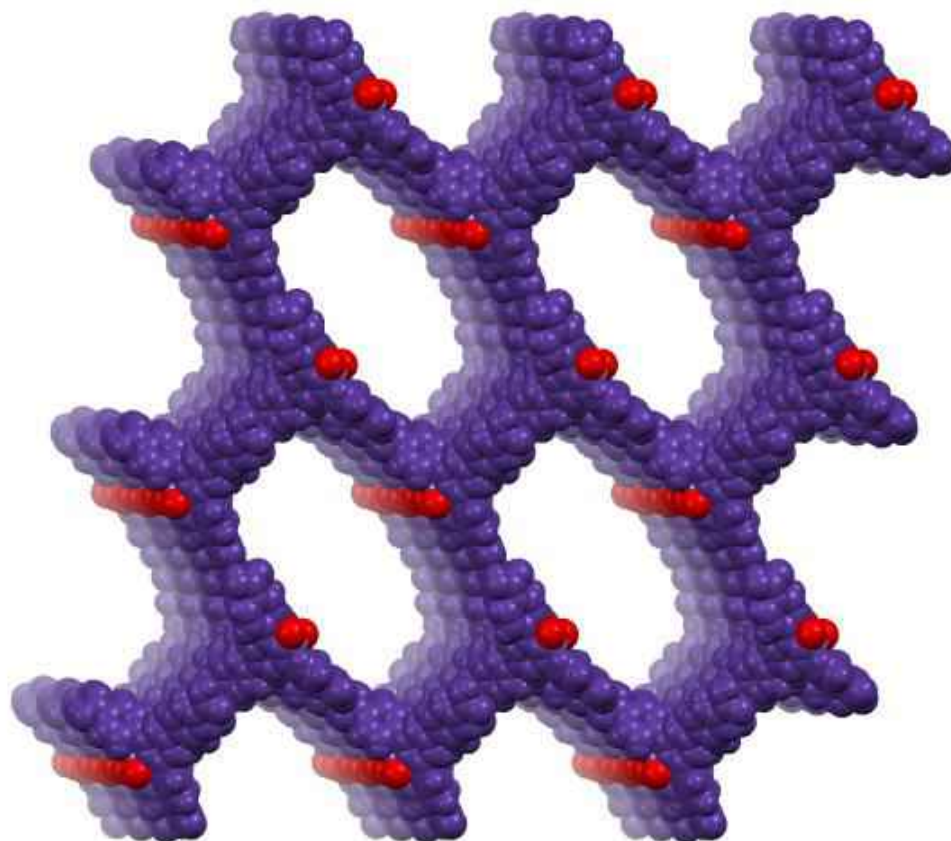
MS35.P14

Triphenylarenes: a New Family of Tunable Porous Organic Crystals

H. Lai¹, C. Zentner¹, R. Wiscons¹, M. Zeller², J. Rowsell¹

¹Oberlin College, Department of Chemistry and Biochemistry, Oberlin, Ohio, USA, ²Youngstown State University, Department of Chemistry, Youngstown, Ohio, USA

Porous organic molecular crystals are of particular interest to crystal engineers because of their potential applications in small molecule storage, separation and catalysis. Compared to network solids, molecular solids present advantages for processing related to their solubility and ease of derivatization. Our research group recently established the microporosity of a carboxylated triphenylbenzene crystal structure, which retains crystallinity even after solvent evaporation. The extrinsically porous structure of this compound is largely directed by two intermolecular interactions: aromatic stacking, and hydrogen bonding in the familiar R22(8) motif. We have synthesized new derivatives bearing various functional groups to probe their steric and electronic effects on the molecular packing and the surface polarity of the pores. The structures of two solvated quasi-polymorphs of the nitro-substituted derivative have been determined using single-crystal X-ray diffraction methods. These structures provide insight into the interplay between the two important synthons, while exhibiting different catenation modes of hexagonal hydrogen-bonded sheets. In both packings, the nitro functional group points towards the interior of solvent-filled channels, suggesting that the installation of other functional groups at the same position is a viable method for tailoring the interactions between guest molecules and the host framework.



Keywords: porous material, organic molecular crystal