Chiral Channels in Molecular Co-Crystals: Structures on the Path to Tris(carboxyphenyl)arenes

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Porous molecular crystals that retain their structure in the absence of trapped solvent molecules are rare, given the flexibility of most non-covalent interactions. The crystal structure of microporous 1,3,5-tris(4-carboxyphenyl)benzene (tcpb) is notable for its large void volume and thermal stability, which stems from a complex polycatenation of its hydrogen-bonded network. Our group is exploring the crystallography of derivatives of this model compound with an eye towards tuning the dimensions and polarity of its pore structure. In one synthetic pathway, tritolylarenes are prepared as intermediates. We have discovered that even these molecules, which have no hydrogen-bond forming groups, tend towards complex crystal packings that exhibit disorder, aperiodicity, and solvent-filled voids. Additional exploration of co-crystals of these propeller shaped entities produced a pseudohexagonal columnar structure assembled from π-stacked helices. These helices enclose channels containing disordered tetrafluoroborate counterions, suggesting the possibility of ion exchange properties.

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