Structural and Thermochemical Studies of Lattice Inclusion Hosts

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Lattice inclusion hosts are molecules that form cage or channel type frameworks in the solid-state having Å to nanometer-sized voids [1]. Recent crystal engineering strategies for the design of open-framework solids, inclusion of small guest/solvent molecules in the voids, and thermo-chemical behavior of host-guest complexes will be discussed. Significant structural and functional differences in channel and cage type host structures are due to differences in hydrogen bonding / intermolecular interactions, van der Waals close packing, and the strength of host lattice in trapping guest species. Structural control of the cage/channel lattice and modification of pore size/shape through functional group and guest selection is illustrated in robust organic host systems. Certain volatile guests are tightly enclathrated in the host framework as measured by high T_{onset} values in DSC measurements. Selective guest inclusion is monitored by TG-IR and explained through hydrogen bonding in X-ray crystal structures. Some host scaffolds assembled via O-H…O, N-H…O hydrogen bonds and halogen…halogen, pi-pi stacking interactions based on T-shaped, H-shaped and trigonal tectons have appeared in recent publications from our group [2-4].

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