New Porphyrin Hosts for Supramolecular Fullerene Binding

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The attraction of curved fullerene surfaces to the planar pi surfaces of porphyrin and metalloporphyrins has been demonstrated in both the solid state and solution. We present here new linked bis-porphyrin hosts, both acyclic and cyclic, designed for the supramolecular binding of fullerenes using this intermolecular interaction. Design criteria for these hosts are based on the observed packing motifs found in the X-ray crystal structures of porphyrin-fullerene cocrystallates. Molecular modelling has been used to guide the poprhyrin host design.

A range of porphyrin connections involving both covalent and coordinate linkages have been prepared. The fullerene binding properties of these hosts have been explored using NMR, mass spectroscopy and
X-ray studies. Several hosts show selectivity of binding for higher fullerenes and the formation of insoluble host-guest fullerene-porphyrin complexes. Evidence is discussed for the importance of electrostatic contributions to the porphyrin-fullerene interaction energy in host-guest complexes involving fullerene derivatives or endohedral fullerenes.