Molecular hosts from benzocyclotrimers for inclusion of small molecules

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Syrm-benzocyclotrimers are polycyclic structures, usually obtained from cross-coupling reactions of bicyclic olefins. These compounds are concave molecules suitable for many supramolecular applications.\textsuperscript{1,2} We have recently reported on the functionalization with hydroxylamine of the enantiopure, highly symmetric benzocyclotrimer 1 derived from (-)-borneol. Trioxime 2 self-condenses to capsule 5, able to guest small molecules of gas. The condensation of 1 with diamines of different length leads to molecular cages of various size 3. These are hosting compounds well suited to guest molecules of gas, especially small hydrocarbons.

The inclusion of methane, ethane, ethylene and acetylene was studied with the aid of NMR spectroscopy. The results show that these molecular cages are rigid hosts, where the size determines the efficiency to accept and hold the molecular guest.