Molecular Soccer Ball Inclusion Capsules and Clusters

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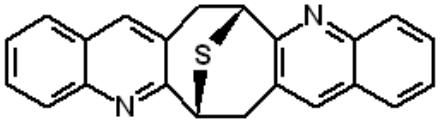
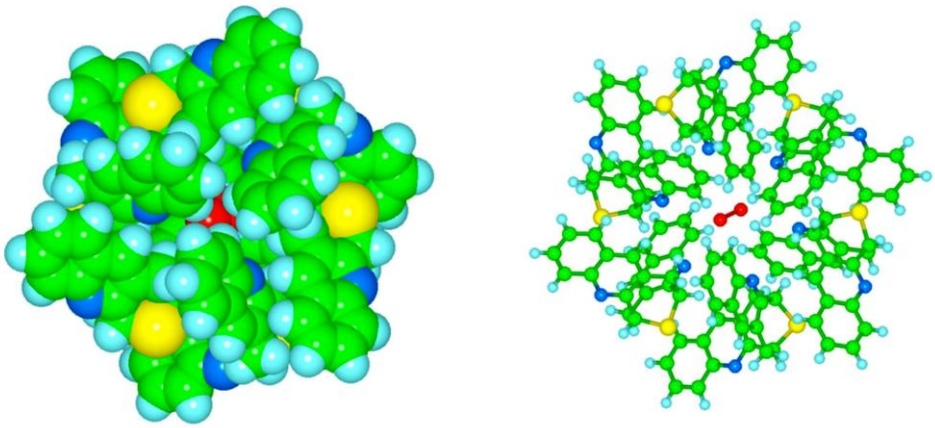
The racemic diheteroaromatic host molecules **1** and **2** exhibit the unusual property of aggregating into molecular soccer ball inclusion structures. Three molecules of each enantiomer undergo self-assembly into a spheroidal hexamer and these spheroids then pack to yield crystal structures in space group *R*3bar with concomitant guest inclusion.

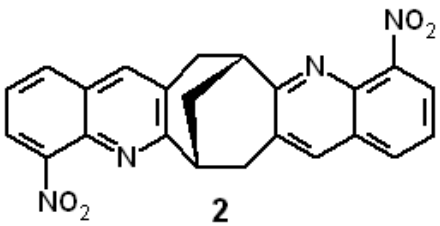


1

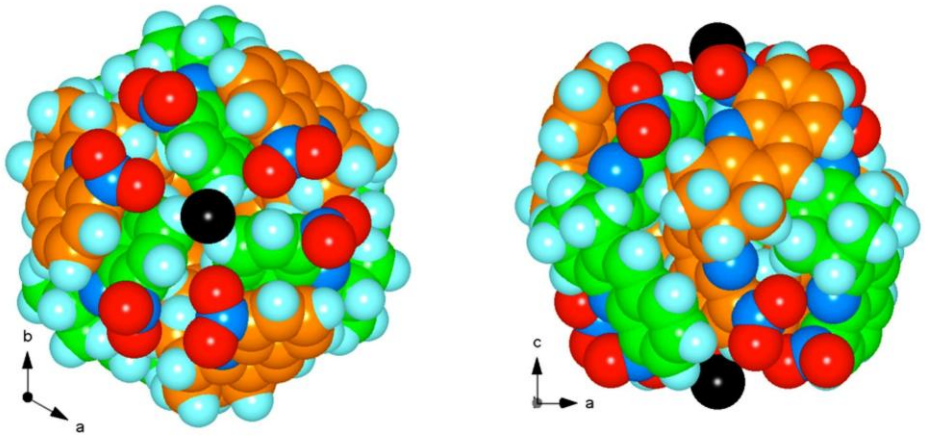
The sulphur-bridged compound 1 yields molecular capsules of composition (1)6.(guest), in which the guest enclosed at the centre of the spheroid (3 bar site) can be water, or methanol (as illustrated here).



In contrast, the dinitro derivative **2** forms clusters in which the central region is too small for guest inclusion. Instead, a series of hydrates are formed where the water molecules associate with the outer surface of the spheroid at a region of high polarity. Two orthogonal views of this arrangement are illustrated, with the guest water molecules represented as black spheres, and with the opposite host enantiomers coloured green or orange.



2



A continuous series of hydrates is produced across the entire range of compositions between $(\mathbf{2})_6$ and $(\mathbf{2})_6$.(water) with essentially no change to the crystal structure produced.

The assembly of the spheroids in solution can be regarded as a series of 3bar symmetry operations (a 120 degree rotation combined with inversion provided by the opposite enantiomer). This is illustrated here for compound **2**. Further details of the construction of these unusual inclusion compounds will be presented.