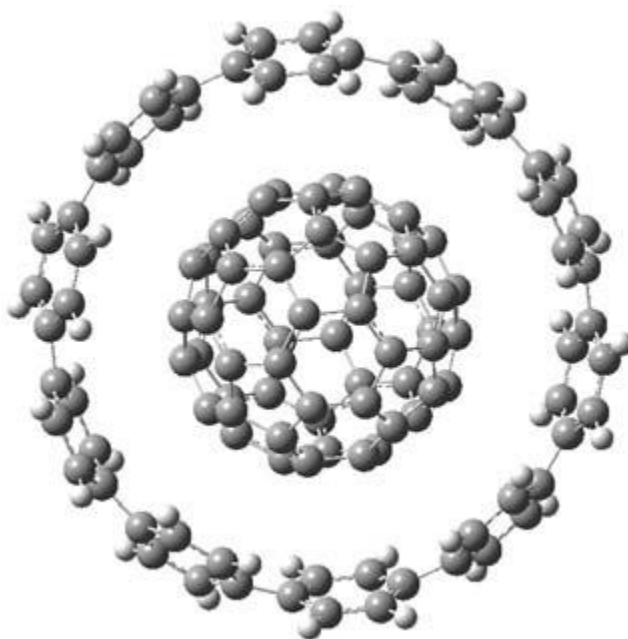


FANTASTIC HOST-GUEST COMPLEX

Check out this an incredibly cool host guest complex: the [10]-cycloparaphenylene ([10]CPP) hoop encapsulating C₆₀!¹



(Be sure to click on this image to bring up the 3-D interactive structure – as with all structures in my blog!)

¹H and ¹³C NMR and fluorescence quenching spectrometry clearly indicate that this complex is formed when [10]CPP is mixed with C₆₀ in toluene.

In fact, when C₆₀ is mixed with a mixture of nanohoops ranging from 8 to 12 phenyl ring, only the [10]CPP hoop complexes with the fullerene. The experimental binding energy is between 38 and 59 kJ mol⁻¹.

M06-2x/6-31G* computations give the structure shown above. The computed binding energy is 173 kJ mol⁻¹, but the computations do not include solvent. So this overestimation might be somewhat due to the difference in gas phase vs. solution complexation.

Source: <http://comporgchem.com/blog/?p=1819>