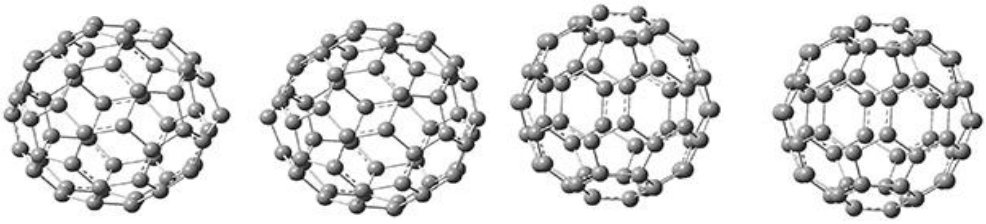
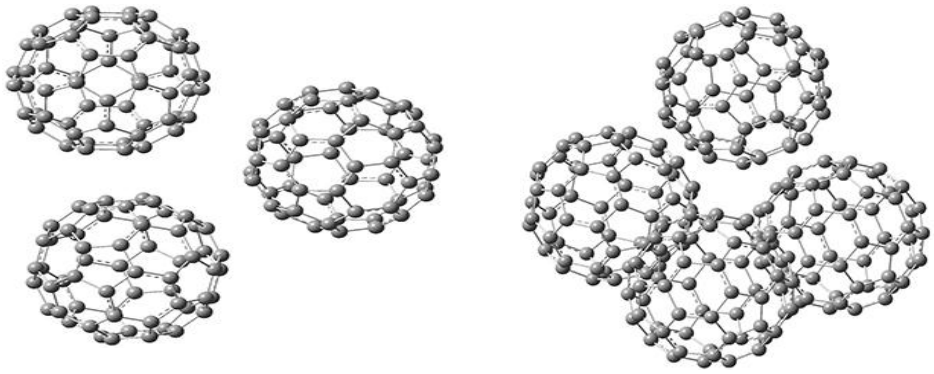
FULLERENE OLIGOMERS AS ELECTRON TRAPS

Clark and co-workers have examined small fullerene clusters for their ability to capture electrons.[1] They first looked at the fullerene dimer, comparing the electron affinity of the dimer having a C-C bond between the two cages (about 1.6-1.7 Å between the two cages) **1** and where the two cages are interacting only through van der Waals attractions (around 2.6 Å) **2**. The structures and their radical anions were computed at RI-BP86/TZV. The structures of the two radical anions are shown in Figure 1. Interestingly, the radical anion of **2** is actually lower in energy that the radical anion of **1**. Comparisons with some other methods are discussed, including a CASSPT2(5,4)/ANO-L-VDZ, computation, that support this result.



1 **2**



3 **4**

Figure 1. RI-BP86/TZV optimized geometries of the radical anions of **1-4**.

(Be sure to click on these images to be able to manipulate these structures in 3-D!)

This suggests that the added electron is being held between the cages, in an interstitial region. That suggested looking at the trimer and tetramer structures **3** and **4**. The radical anions of these two oligomers are also shown in Figure 1. These oligomers show electron affinities of 1 eV greater than for fullerene itself, along with the ability to stabilize the dianion and even the trianion, what the authors call “deep electron traps”.

Source: http://comporgchem.com/blog/?p=3243