Stability Indicators of Hydrogenated Fullerenes

Tomislav Došlić,^a Manuel Martinović^b and Nađa Došlić^b

mmartin@irb.hr

^aFaculty of Civil Engineering, University of Zagreb, Zagreb, Croatia ^bRuđer Bošković Institute, Zagreb, Croatia

In predicting stability of hydrogenated fullerenes, the Isolated Pentagon Rule successfully correlates with stable fullerenes, but fails to differentiate among stable isoforms. Various graph-theory originating descriptors and topological descriptors have been developed over the years to describe fullerene stability, with moderate success and with implementation in a range of software programs [1]. Fullerene stability doesn't correlate with the number of resonant or Kekulé structures either, which is the case in benzenoid hydrocarbons: among the 1812 isomers of C_{60} , the most energetically stable one is 20th, while the most unstable one is 1st in the ranking by number of resonance structures [1]. Certain hydrogenated forms of C_{60} fullerenes, including $C_{60}H_{36}$ and $C_{60}H_{60}$, have been experimentally observed as stable. In the context of Kekulé structures of buckminsterfullerene, hydrogenation of bonds can be thought of as reduction of numbers of resonant structures at certain locations [2]. In our preliminary findings, based on DFT energies of variously hydrogenated buckminsterfullerenes, stability of partially hydrogenated structures surprisingly correlates with the number of resonant structures. The most energetically stable hydrogenation patterns, seem to be when hydrogen atoms are added in pairs. The correlation is present across various level of theory. Current preliminary TDDFT data [3], is the starting point for upcoming calculations that explore excited states of hydrogenated fullerenes at higher levels of theory.

References:

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