C_{98} IPR Isomers: Computed Relative Stabilities

Zdeněk Slanina[1] and Xiang Zhao[2]

[1]Department of Theoretical Studies
Institute for Molecular Science
Myodaiji
Okazaki, J 444-8585
Japan

[2]Laboratory of Computational Chemistry
Department of Knowledge-Based Information Engineering
Toyohashi University of Technology
Toyohashi, J 441-8580
Japan

The complete set of 259 isolated-pentagon-rule (IPR) isomers of C_{98} has been treated by full geometry optimizations with the SAM1, PM3, AM1, and MNDO quantum-chemical semiempirical methods. All the applied methods point out a C_2 species (FM code - 248:C_2) as the lowest-energy structure in the IPR set. In order to predict the relative stabilities at elevated temperatures, entropy contributions are also computed and thus, evaluations in terms of the Gibbs function are possible for this system for the first time. Interesting stability interchanges in the isomeric set are found so that not only the ground-state structure 248:C_2 but also other structures (108:C_s, 113:C_2, 109:C_1) are significantly populated at high temperatures. The results are placed into a wider context of higher fullerenes and their computations.