On Symmetry and Topological Indices of Fullerenes

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Abstract

It is well known to associate an Euclidean graph to a molecule. Balasubramanian computed the Euclidean graphs and their automorphism groups for benzene, eclipsed and staggered forms of ethane and eclipsed and staggered forms of ferrocene [see *Chem. Phys. Lett*. **232** (1995), 415].

In this paper, we present a simple algorithm for computing symmetry of molecules. We apply this algorithm to calculate the symmetry of some big fullerenes. The Wiener, Schultz and also Padmakar-Ivan(PI) indices of some big fullerenes are computed. Here the PI Index is a Szeged-like topological index developed very recently and defined as $PI(G) = \sum[n_{eu}(e|G)+ n_{ev}(e|G)]$, where $n_{eu}(e|G)$ is the number of edges of G lying closer to u than to v, $n_{ev}(e|G)$ is the number of edges of G lying closer to v than to u and summation goes over all edges of G. Finally, we pose some problems related to the symmetry and these topological indices for fullerenes.

Keywords: Fullerene, symmetry of molecules, Wiener index, PI index, Schultz index.

References

1. K. Balasubramanian, Graph-Theoretical Perception of Molecular Symmetry, *Chem. Phys. Letters*, **232**(1995) 415-423.
2**.** A.R. Ashrafi, On symmetry properties of molecules, *Chem. Phys. Letters*, **406** (2005) 75–80.
3. A.R. Ashrafi and M.R. Ahmadi, New computer program to calculate the symmetry of molecules, *Cent. Eur. J. Chem.,* **3**(4)(2005) 647–657.
4. A.R. Ashrafi, A. Loghman, PI Index of Zig-Zag Polyhex Nanotubes, Accepted in *Match Commun. Math. Comput. Chem*., 2005.
5. A.R. Ashrafi, On a new algorithm for computing symmetry of big fullerenes, in preparation.