Prediction of acenes electron affinity energy using TIM

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Abstract

Manufacturing the nanoscale components has faced some limitations, which is virtually impossible in many cases. Acenes are organic molecules that have received considerable attention in molecular electronics and nanoscale. Due to the important electronic properties of the family, many studies have been conducted on them. A molecular graph is a simple graph whose vertex is mainly made up of atoms in a molecule and the bonds between atoms are the graph edges. In chemical graphs, hydrogen atoms were removed and excluded. Moreover, the degree of each vertex is a maximum of 4 and all bonds between atoms are considered as single. Topological indices are defined based on graph theory. The first Zagreb index is one of the topological indices, which is defined as follows $M_1(G) = \sum_{u \in V(G)} d^2(u)$

Where u is a member of the graph vertices and d is its degree. The Electron Affinity Energy was calculated using Gaussian 09 software and the experimental data of references were compared with those mentioned in valid papers. Prediction of electron affinity energy has a very high accuracy through the first Zagreb index with $R^2 = 0.9988$.

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