

Prediction of acenes Gibbs energy using TIM

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Abstract

Parts manufacturing has some limitations at the nano scale that is practically impossible in many cases. Therefore, scientific interests to smithereens in the natural scale have led to creation of nanostructures field in recent years. The acenes with the chemical formula $C_{4n+2}H_{2n+4}$ is a family of organic molecules that are highly regarded at the nano scale, but an investigation on their thermodynamic properties require spending a high price especially when the number of loops is higher than six. This paper seeks to provide a model to predict acenes' thermodynamic properties by applying the topological indices method (TIM). 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 second Zagreb index is one of the topological indices, which is defined as follows:

$$M_2(G) = \sum_{uv \in E(G)} d(u)d(v)$$

where u is a member of the graph vertices and d is its degree. The Gibbs energy was calculated using Chem. Office 2015 software and the experimental data of references were compared with those mentioned in valid papers. Prediction of Gibbs Energy has a very high accuracy through the second Zagreb index with

$$R^2 = 1$$

$$E_{gibbs} = 3.9606(M_2) + 26.625$$

Biography

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