Proceedings of the Jangjeon Mathematical Society
25 (2022), No. 4, pp. 455 - 465

www.jangjeon.or.kr
http://dx.doi.org/10.17777/pjms2022.25.4.455

INVESTIGATION ON SOME TOPOLOGICAL INDICES OF CARBON NANOBUD THROUGH M-POLYNOMIAL

DEEPASREE S KUMAR, P.S.RANJINI AND V. LOKESHA

Abstract. Topological indices are popular descriptors used in chemical graph theory. These are basically numerical values that correlate the topology of chemical compounds to its different physical properties and synthetic reactivities. Among different classes of topological indices, degree based topological indices have prominent role in characterising the topology of molecular graph and are widely used in quantitative structure property relationship (QSPR) and quantitative structure activity relationship (QSAR) studies. Carbon Nanobud exhibits superior properties compared to both Nanotubes and Fullerene. Structure of Carbon nanobud is achieved by fusion of fullerene and Nanotubes with carbon-carbon covalent bond connections between them. Some of the popular degree based topological indices of a typical Nanobud molecular structure is estimated in this article. Here we considered a single fullerene (C_{60}), attached on the surface of a zigzag Single Walled Carbon Nanotube (SWNT) by a [2 x 2] cyclo-addition.

Keywords: Zagreb indices, Link graphs,Carbon Nanobuds

Mathematics Subject Classification: 05C35; 05C07; 05C40

Submission Date: 11 November 2021

1. Introduction

In mathematical chemistry, topological indices have become a very valuable tool for predicting properties of a compound from its molecular structure. It is possible to correlate the physical, chemical or biological properties of a compound to its molecular structure through numerical values called topological indices, which are derived from the Molecular graph of the compound. Topological indices can be easily used for chemical modeling with the help of software packages. Graph theory has growing applications in different Science and Engineering fields. The QSAR and QSPR studies, which relate biological or chemical features, are the most common uses of Topological index[2,3,17,18,19]. Topological Index was introduced by Wiener in 1947, called Wiener index [13], which correlates the topology of alkanes with its boiling points. A subclass of these descriptors called Adriatic indices [20] are widely used by researchers in chemical characterisation. In the upcoming sections, some of the popular topological indices are discussed and they are computed for a simple Carbon nanobud structure. M-Polynomial of the structure is derived first and then the indices are estimated using M Polynomial.

1.1. **Definition.** Among different types of topological indices, degree based topological indices are very popular because of its applications in chemical graph theory.

Some of the important degree based topological indices are considered in this paper and its definitions are given in this section. Molecular graph $G(V, E)$,where the vertex set is represented by V and edge set is represented by E of a molecular structure. The molecular structure is formed by atoms serve as vertices and chemical bonds between atoms serve as edges. The degree refers to the total number of vertices attached to each vertex. The degree of a vertex v is represented by dv. We followed the book [9] for definitions and notations in the graph theory.

Gutman and Trinajstić [8] established the Zagreb index , which was verified in a research of total π-electron energy structure -dependence. Kulli [11] studied Zagreb index for Carbon nanotubes in detail.

The terms denoted by M_1 and M_2 commonly known as Zagreb indices of the first and second kind and defined as follows[15] :

$$M_1(G) = \sum_{v \in V} (d_v)^2 = \sum_{uv \in E(G)} (d_u + d_v).$$

Second Modified Zagreb index [13] is defined as

$${}^{m}M_2(G) = \sum_{uv \in E(G)} \frac{1}{d_u d_v}.$$

The Randic index, which is widely utilised in the realm in the field of drug design, is another popular index. This was introduced by Milan Randic [14] in 1974.

$$R(G) = \sum_{uv \in E(G)} \frac{1}{\sqrt{d_u d_v}}.$$

Ernesto Estrada[5] later adjusted the Randic index to relate with the thermodynamic features of alkanes, specifically formation of heats. Atom-bomb connectivity index(ABC-index) is a new version of the Randic index that is defined as

$$ABC(G) = \sum_{uv \in E(G)} \sqrt{\frac{d_u + d_u - 2}{d_u d_v}}.$$

ABC index was further elaborated by Kulli [12, 20] and applied in certain nanostructures compounds. The Augmented Zagreb index, which is derived from the ABC index, was introduced by Furtula et al[7]. The enhanced Zagreb index is defined as

$$A(G) = \sum_{uv \in E(G)} \left(\frac{d_u d_v}{d_u + d_v - 2}\right)^3.$$