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Zagreb indices of link graphs related to carbon nanotube and fullerene

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Abstract---A Link graph ***H*** is obtained by connecting ***p*** number of Fullerenes to a single wall carbon nanotube using covalent bonds. R-graph, R-Vertex, R-Edge, R- Vertex neighborhood, R-Edge neighborhood of these Link graphs are obtained in this paper. First Zagreb Index and Second Zagreb index of these graphs are derived using M-Polynomial method.

Keywords---Zagreb indices, link graphs, carbon nanotube, fullerene.

Introduction

Topological indices are numerical terms popular in mathematical chemistry and these quantities are widely used for predicting properties of chemical compounds from its molecular structure [1], [2]. It must be a structural invariant, means that every graph automorphism preserves it. There have been defined several topological indices, and many of them are used to model chemical, pharmacological, and other aspects of molecules. Among different types of indices degree-based indices are derived from the degrees of the vertices of a molecular graph. Firstly, Wiener index, is introduced by the Chemist Harold Wiener in 1947 and is defined as

$$W(H) = \sum_{uv \in V(H)} d_u + d_v$$

Gutman and Trinajstc'[3]-[5] looked into the dependence of an alternant hydrocarbon's total π-electron energy, and they came across the terms denoted by M_1 and M_2, commonly known as Zagreb indices of the first and second kinds, and are defined as

$$M_1(H) = \sum_{u \in V(H)} d^2(u)$$

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

In this paper, First and second Zagreb indices are developed on some graph operations[6], [7]) of two molecular graphs. The molecular structure considered here are allotropes of Carbon, known as Carbon nanotube and Fullerene. We use the following definitions:

Definition 1 – The R -graph[8] of a graph H is represented by $R(H)$ and is obtained from H by linking a vertex $w_e \notin V(H)$ corresponding to each edge $e = uv \in (H)$ andjoining w_e to end vertices u and v for each edge e.

Definition 2 - R -Vertex join [9] of H_1 and H_2 is represented by $R(H)$ is obtained from $R(H_1)$ and H_2 by linking every vertex of $V(H_1)$ and $V(H_2)$ by an edge.

Definition 3 - R -Edge join [9] of H_1 and H_2 is represented by $R(H)$ is obtained from $R(H_1)$ and H_2 by joining every new vertex of $R(H_1)$ and $V(H_2)$ by an edge.

Definition 4 - R -Edge neighborhood link graph [10] between H_1 and H_2 is represented by $R_E(H)$ is obtained by joining the neighbourhood separated vertices of newly added vertices of $R(H_1)$ to each copy of H_2 by an edge.

Definition 5 - R -Vertex neighborhood link graph [10] between H_1 and H_2 is represented by $R_{V_n}(H)$ is obtained by joining the neighborhood separated vertices of an existing vertex of (H_1) are connected to each copy of H_2 by an edge.

Definition 6 - Let H be a graph. Then M-Polynomial [11] of H is defined as

$$M(H: x, y) = \sum_{i \leq j} m_{ij}(H) x^i y^j$$

where $m_{ij}(H)$, $i, j \geq 1$ be the number of edges uv of H such that $d_u, d_v = \{i, j\}$.
Some degree based topological indices were derived from M-Polynomial and are given below:

Table I
EXPRESSION OF M_1 AND M_2 WITH M-POLYNOMIAL

Topological Index	$f(x1, x2)$	Expression with M-Polynomial
M_1	$x_1 + x_2$	$(D_{x_1} + D_{x_2})M(H: x_1, x_2)_{x_1=x_2=1}$
M_2	$x_1 x_2$	$(D_{x_1} D_{x_2})M(H: x_1, x_2)_{x_1=x_2=1}$