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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

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$$M_1(H) = \sum_{u \in V(H)} d^2(u)$$
$$M_2(H) = \sum_{uv \in E(H)} d(u)d(v)$$

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 byjoining 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

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

where $m_{ij}(H)$, $i, j \geq 1$ be the number of edges uv of H suchthat 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	$f(x_1, x_2)$	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	$x_1 x_2$	$(D_{x_1} D_{x_2})M(H: x_1, x_2)_{x_1=x_2=1}$

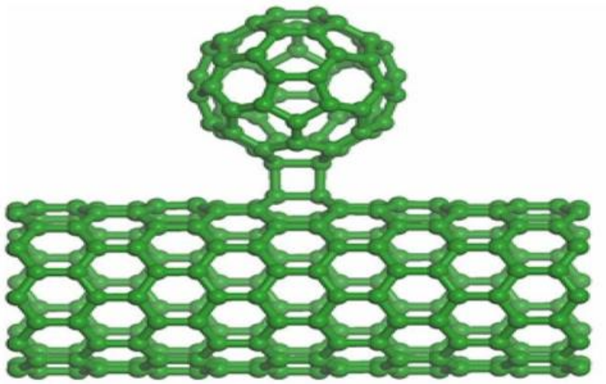

Figure 1. Swcnt Based Carbon Nanobud [2X 2]-HP ZIGZAG (10,0)
Remarks

Here we consider the molecular graph which corresponds totwo allotropes of carbon viz Carbon nanotube and Fullerene.

Research methodology

Methodology we used here is edge partition and analytical methods. We devised the number of edges based on the degree of its end vertices. Also, we used MATLAB to plot the graph of each index.

Results and Discussions

The different Link graphs such as R-Vertex Link graph, R- Edge Link graph, R-Vertex Neighborhood Link graph, R- Edge Neighborhood Link graph are obtained and established the popular first and second Zagreb indices through M-Polynomial. Throughout the paper, M represents M- polynomial, M_1 and M_2 denote the first and Second Zagreb indices.

I*. *R*- *graph of Single wall carbon nanotube

Let H_1 be the molecular graphs of single wall CarbonNanotube. Also let $(H1)$ be the R-graph of $H1$.

Theorem 1 - $(R(H_1))$ represents M-Polynomial of H and let $M_1(R(H1))$ and $M_2(R(H1))$ be the first and secondZagreb indices respectively, then

1. $(R(H_1)) = k(3n-2)x^6x^6_1 +_2 4kx^6x^4_1 +_2 [24k(3n-2) + 4k]x^6x^2 + 4kx^4x^2]$.
2. $M_1(R(H_1)) = 4k(21n + 110)$.
3. $M_2(R(H_1)) = 4k(45n + 14)$.

Proof – 1. Let $H1$ be the molecular graph of carbon nanotube and $(H1)$ be the R -graph of $H1$. All the edges of
$(H1)$ can be categorised under following partitions.

$E_{66} = \{uv \in (H)/du = 6, dv = 6\} \Rightarrow |m_{66}| = (3n-2).$
$E_{64} = \{uv \in (H)/du = 6, dv = 4\} \Rightarrow |m_{64}| = 4k.$
$E_{62} = \{uv \in (H)/du = 6, dv = 2\} \Rightarrow |m_{62}| = 2k(3n-2) + 4k.$
$E_{42} = \{uv \in (H)/du = 4, dv = 2\} \Rightarrow |m_{42}| = 4k.$

From definition of M-Polynomial

$(R(H_1)) = m_{66}x_1^6x_2^6 + m_{64}x_1^6x_2^4 + m_{62}x_1^6x_2^2 + m_{42}x_1^4x_2^2$
$= (3n-2)x_1^6x_2^6 + 4kx_1^6x_2^4 + [24k(3n-2) + 4k]x_1^6x_2^2 + 4kx_1^4x_2^2.$

2. $D_{x_1} = x_1\frac{\partial}{\partial x_1}[(R(H_1))] = x_1[(6k(3n-2)x_1^5x_2^6 + 24kx_1^5x_2^4 + [12(3n-2) + 24k]x_1^5x_2^2 + 16kx_1^3x_2^2)].$

$D_{x_2} = x_2\frac{\partial}{\partial x_2}[(R(H_1))] = x_1[(6k(3n-2)x_1^6x_2^5 + 16kx_1^6x_2^3 + [4(3n-2) + 8k]x_1^6x_2 + 8kx_1^4x_2)].$

$$(D_{x_1})_{x_1=x_2=1} = 6(3n-2) + 24k + 12k(3n-2) + 24k + 16k$$
$$= 54kn + 28k$$
$$(D_{x_2})_{x_1=x_2=1} = 6(3n-2) + 16k + 4k(3n-2) + 8k + 8k$$
$$= 30kn + 12k$$
$$M_1(R(H_1)) = (D_{x_1} + D_{x_2})(R(H_1))_{x_1=x_2=1}$$
$$M_1(R(H_1)) = 54kn + 28k + 30kn + 12k$$
$$M_1((H_1)) = 4k[21n + 10]$$

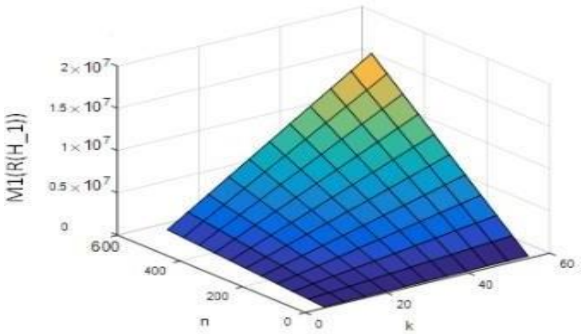

FIGURE II
First Zagreb Index Of R($H1$)

$3.\ D_{x_1}D_{x_2} = x_1 \frac{\partial}{\partial x_1}(D_{x_2})$

$= x_1x_2[(36k(3n-2)x_1^5x_2^5 + 96kx_1^5x_2^5 + [24k(3n-2) + 48k]x_1^5x_2 + 32kx_1^5x_2)]$

$(D_{x_1}D_{x_2})M_2(R(H_1))_{x_1=x_2=1} = 36(3n-2)96k + 24k(3n-2)48k + 32k$

$M_2((H_1)) = 180kn + 56k$

$M_2((H_1)) = 4k(45n + 14).$

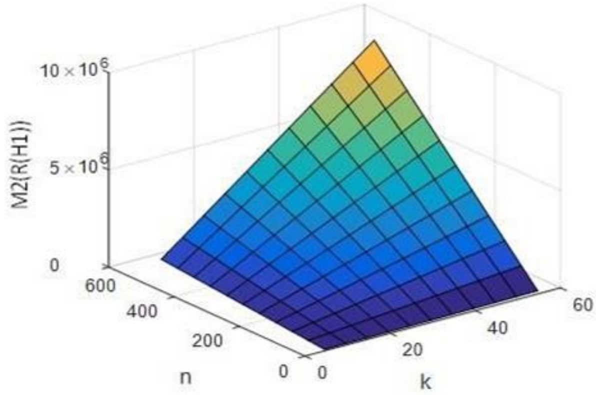

FIGURE III
Second Zagreb Index Of R($H1$)

R-Vertex Link graph of Single Wall Carbon Nanotube and Fullerene

Let H_1 and H_2 are the molecular graphs of single wall Carbon Nanotube and Fullerene respectively. Also let $R(H)$ be the R-Vertex link graph of $H1$ and $H2$.

Theorem 2 -Let $(Rv(H))$, $M1(Rv(H))$ and $M2(Rv(H))$ be the M-Polynomial, First Zagreb index and Second Zagreb index respectively. Then,

1. $(R(H)) = [k(3n-2)-3]x_1^6x_2^6 + 3x_1^6x_2^7 + 4kx_1^4x_2^6 + 87x_1^5x_2^5 + 3x_1^5x_2^4 + x_1^4x_2^7 + (2(3n-2)+4k-3)^2x_1^6x_2^6 + 3x_1^2x_2^7 + 4kx_1^2x_2^4.$
2. $M_1(R_v(H)) = 2k(42n + 13) + 581.$
3. $M_2(R_v(H)) = 12k(15n + 2) + 866.$

Proof – 1. Let $R(H)$ be the molecular graph of R- Vertex Link graph of H_1 and H_2. All the edges of graph $(R(H))$ can be categorised under following partitions

$E_{66} = \{uv \in (H)/du = 6, dv = 6\} \Rightarrow |m_{66}| =$
$(3n-2) - 3.$
$E_{67} = \{uv \in (H)/du = 6, dv = 7\} \Rightarrow |m_{67}| = 3.$
$E_{46} = \{uv \in (H)/du = 4, dv = 6\} \Rightarrow |m_{46}| = 4k.$
$E_{33} = \{uv \in (H)/du = 3, dv = 3\} \Rightarrow |m_{33}| = 87.$
$E_{34} = \{uv \in (H)/du = 3, dv = 4\} \Rightarrow |m_{34}| = 3.$
$E_{47} = \{uv \in (H)/du = 4, dv = 7\} \Rightarrow |m_{47}| = 1.$
$E_{26} = \{uv \in (H)/du = 2, dv = 6\} \Rightarrow |m_{26}| = 6kn - 3.$
$E_{27} = \{uv \in (H)/du = 2, dv = 7\} \Rightarrow |m_{27}| = 3.$
$E_{24} = \{uv \in (H)/du = 2, dv = 4\} \Rightarrow |m_{24}| = 4k.$

From definition of M-Polynomial

$(H: x_1, x_2) = \sum_{i \le j} m_{ij}(H) x_1^i x_2^j.$

M-Polynomial is derived as:

$$(R_v(H): x_1, x_2) = m_{66}x_1^6x_2^6 + m_{67}x_1^6x_2^7 + m_{46}x_1^4x_2^6 + m_{33}x_1^3x_2^3 + m_{34}x_1^3x_2^4 + m_{47}x_1^4x_2^7 + m_{26}x_1^2x_2^6 + m_{27}x_1^2x_2^7 + m_{24}x_1^2x_2^4$$

$(R_v(H)) = [k(3n-2) - 3]x_1^6x_2^6 + 3x_1^6x_2^7 + 4kx_1^4x_2^6 + 87x_1^3x_2^3 + 3x_1^3x_2^4 + x_1^4x_2^7 + (2(3n-2) + 4k - 3)x_1^2x_2^6 + 3x_1^2x_2^7 + 4kx_1^2x_2^4.$

2. First Zagreb index of $R(H)$ is defined as
$M_1(R_v(H)) = (D_{x_1} + D_{x_2})M(R_v(H); x_1, x_2)_{x_1=x_2=1}$

$D_{x_1} = x_1 \frac{\partial}{\partial x_1}[(R_v(H); x_1, x_2)]$
$= x_1[(k(3n-2) - 3)6x_1^5x_2^6 + 18x_1^5x_2^7 + 16kx_1^3x_2^6 + 87 \times 3x_1^2x_2^3 + 6x_1^2x_2^4 + 4x_1^3x_2^7 + (6kn-3) \times 2x_1x_2^6 + 6x_1x_2^7 + 8kx_1x_2^4]$

$D_{x_2} = x_2 \frac{\partial}{\partial x_2}[M(R_v(H); x_1, x_2)]$
$= x_2[(k(3n-2) - 3)6x_1^6x_2^5 + 21x_1^6x_2^6 + 24kx_1^4x_2^5 + 87 \times 3x_1^3x_2^2 + 12x_1^3x_2^3 + 7x_1^4x_2^6 + (6kn-3) \times 6x_1^2x_2^5 + 21x_1^2x_2^6 + 16kx_1^2x_2^3]$

$$(D_{x_1})_{x_1=x_2=1} = 6[(3n-2) - 3] + 18 + 16k + 261 + 6 + 4 + 2(6kn-3) + 6 + 8k$$
$= 30kn + 22k + 271$
$= 2(15n + 11) + 271$

$$(D_{x_2})_{x_1=x_2=1} = 6[(3n-2) - 3] + 21 + 24 + 261 + 12 + 7 + 6(6kn-3) + 21 + 16k$$
$= 54kn + 4k + 310$
$= 2(27n + 2) + 310.$

$M_1(R_v(H)) = (D_{x_1} + D_{x_2})M(R_v(H); x_1, x_2)_{x_1=x_2=1}$
$M_1(R_v(H)) = 2k(15n + 11) + 271 + 2k(27n + 2) + 310$
$M_1(R_v(H)) = 2k(42n + 13) + 581$

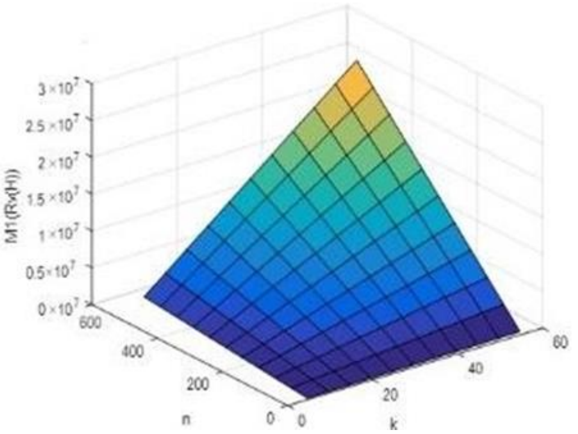

FIGURE IV
First Zagreb Index Of $R(H)$

3. Second Zagreb index of $R_v(H)$ is defined as

$M_2(R_v(H)) = (D_{x_1} D_{x_2}) M(R_v(H); x_1, x_2)_{x_1=x_2=1}$

$D_{x_1} D_{x_2} = x_1 \frac{\partial}{\partial x_1}(D_{x_2})$

$= x_1 x_2 [(k(3n-2)-3)36x_1^3x_2^3 + 18x_1^3 \times 7x_2^6 + 16kx_1^3 \times 6x_2^3 + 87 \times 3x_1^2 \times 3x_2^2 + 6x_1^2 \times 4x_2^3 + 4x_1^3 \times 7x_2^6 + (6nk-3) \times 2x_1 \times 6x_2^3 + 6x_1 \times 7x_2^6 + 8kx_1 \times 4x_2^3]$

$(D_{x_1} D_{x_2})(R_v(H); x_1, x_2)_{x_1=x_2=1}$

$$= 36((3n-2)-3) + 18 \times 7 + 16 \times 6k + 87 \times 9 + 24 + 28 + 24(3n-2) + 48k - 36 + 42 + 32$$

$M_2(R_v(H)) = 180kn + 24k + 866$

$M_2(R_v(H)) = 12k(15n + 2) + 866.$

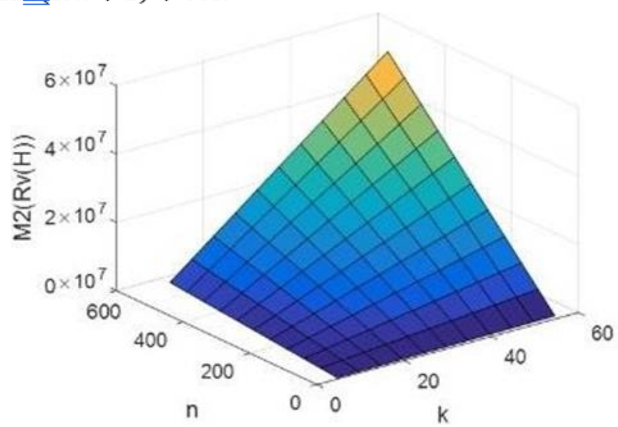

FIGURE V
Second Zagreb Index Of $R(H)$

R-Edge Link graph of Single Wall Carbon Nanotube and Fullerene

Let $H1$ and $H2$ be the molecular graphs of single wall Carbon Nanotube and Fullerene respectively. Also let
$R(H)$ be the R-Edge link graph of $H1$ and $H2$
Theorem 3 - If M , M1(Re(H)) and M2(Re(H)) are M- polynomial, First and Second Zagreb indices of Re(H) respectively, Then

1. $M(R_e(H); x_1, x_2) = k(3n-2)x_1^6x_2^6 + 4kx_1^4x_2^6 + (6kn-2)x_1^2x_2^6 + 2x_1^3x_2^6 + 4kx_1^2x_2^4 + 87x_1^3x_2^3 + 4x_1^3x_2^4.$
2. $M_1(R_e(H)) = 4k(21n+10) + 552.$
3. $M_2(R_e(H)) = 4k(45n+32) + 771.$

Proof – 1. Let $(R(H))$ be the molecular graph of R-Vertex Link graph of H_1 and H_2. All the edges of graph $R(H)$ can be categorised under following partions.

$E_{66} = \{uv \in (R_e(H))/du = 6, dv = 6\} \Longrightarrow |m_{66}| = (3n-2).$

$E_{46} = \{uv \in (R_e(H))/du = 4, dv = 6\} \Longrightarrow |m_{46}| = 4k.$

$E_{26} = \{uv \in (R_e(H))/du = 2, dv = 6\} \Longrightarrow |m_{26}| = 6kn - 2.$

$E_{36} = \{uv \in (R_e(H))/du = 3, dv = 6\} \Longrightarrow |m_{36}| = 2.$

$E_{24} = \{uv \in (R_e(H))/du = 2, dv = 4\} \Longrightarrow |m_{24}| = 4k.$

$E_{33} = \{uv \in (R_e(H))/du = 3, dv = 3\} \Longrightarrow |m_{33}| = 87.$

$E_{34} = \{uv \in (R_e(H))/du = 3, dv = 4\} \Longrightarrow |m_{34}| = 4$

From definition of M-Polynomial

$$M(H: x_1, x_2) = \sum_{i \le j} m_{ij}(H)x_1^i x_2^j.$$

M-Polynomial is derived as:

$$M(R_e(H): x_1, x_2) = m_{66}x_1^6x_2^6 + m_{46}x_1^4x_2^6 + m_{26}x_1^2x_2^6 + m_{36}x_1^3x_2^6 + m_{24}x_1^2x_2^4 + m_{33}x_1^3x_2^3 + m_{34}x_1^3x_2^4$$

$$= (3n-2)x_1^6x_2^6 + 4kx_1^4x_2^6 + (6kn-2)x_1^2x_2^6 + 2x_1^3x_2^6 + 4kx_1^2x_2^4 + 87x_1^3x_2^3 + 4x_1^3x_2^4.$$

2. First Zagreb index of $R_e(H)$ is defined as

$$M_1(R_e(H)) = (D_{x_1} + D_{x_2})M(R_e(H); x_1, x_2)_{x_1=x_2=1}$$

$D_{x_1} = x_1 \frac{\partial}{\partial x_1}[(R_e(H); x_1, x_2)] = x_1 [k(3n-2) \times 6x_1^5x_2^6 + 16kx_1^3x_2^6 + 2(6kn-2) \times x_1x_2^6 + 6x_1^2x_2^6 + 8kx_1x_2^4 + 261x_1^2x_2^3 + 12x_1^2x_2^4]$

$D_{x_2} = x_2 \frac{\partial}{\partial x_2}[(R_e(H); x_1, x_2)] = x_2 [k(3n-2) \times 6x_1^6x_2^5 + 24kx_1^4x_2^3 + 6(6kn-2) \times x_1^2x_2^5 + 12x_1^3x_2^5 + 16kx_1^2x_2^3 + 261x_1^3x_2^2 + 16x_1^3x_2^3]$

$$(D_{x_1})_{x_1=x_2=1} = 18kn - 12k + 16k + 12kn - 4 + 6 + 8k + 261 + 12$$

$=30kn + 12k + 275$

$=26(5n + 2) + 275$

$$(D_{x_2})_{x_1=x_2=1} = 18kn - 12k + 24k + 36kn - 12 + 12 + 16k + 261 + 16$$

$=54kn + 28k + 277$

$=2(27n + 14) + 277$

$(D_{x_1} + D_{x_2})(R_e(H); x_1, x_2)_{x_1=x_2=1}$

$M_1(R_e(H)) = 26k(5n + 2) + 275 + 54kn + 28k + 277$

$M_1(R_e(H)) = 4k(21n + 10) + 552.$

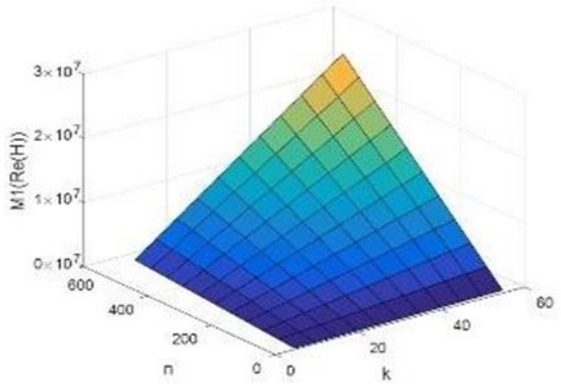

FIGURE VI
First Zagreb Index Of $R(H)$

3.Second Zagreb index of $R_e(H)$ is defined as

$$M_2(R_e(H)) = (D_{x_1}D_{x_2})M(R_e(H); x_1, x_2)_{x_1=x_2=1}$$

$$D_{x_1}D_{x_2} = x_1 \frac{\partial}{\partial x_1}(D_{x_2})$$

$$= x_1x_2[k(3n-2) \times 6x_1^5 \times 6x_2^5 + 24k \times 4x_1^3x_2^3 + (36kn-12) \times 2x_1x_2^5 + 36x_1^2x_2^5 + 32kx_1x_2^3 + 261 \times 3x_1^2x_2^2 + 16 \times 3x_1^2x_2^3]$$

$(D_{x_1}D_{x_2})(R_e(H); x_1, x_2)_{x_1=x_2=1}$

$$= 108kn - 72 + 96k + 72kn - 24 + 36 + 32k + 783 + 48$$

$$M_2(R_e(H)) = 180kn + 128k + 771$$

$M_2(R_e(H)) = 4k(45n + 32) + 771.$

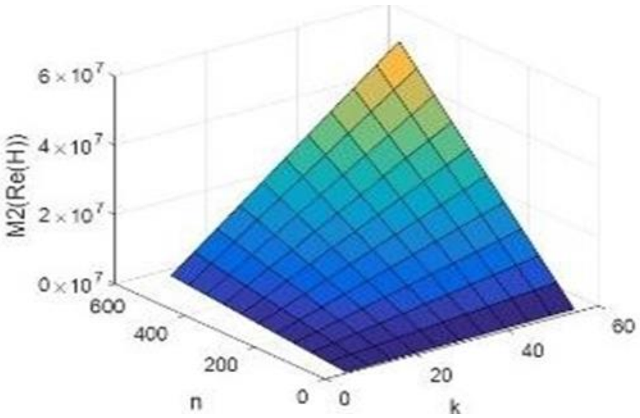

FIGURE VII
Second Zagreb Index Of $R(H)$

R-Vertex Neighborhood Link graph of Single Wall Carbon Nanotube and Fullerene

Let H_1 and H_2 are the molecular graphs of single wall Carbon Nanotube and Fullerene respectively. Also let $RV_n(H)$ be the R-Vertex Neighbourhood link graph of H_1 and H_2.

Theorem 4 - If M , $M_1(RV_n(H))$ and $M_2(RV_n(H))$ are M-polynomial, First and Second Zagreb indices of $RV_n(H)$ respectively, then

1. $(R_V(H); x_1, x_2) = [k(3n-2) - 9]x_1^6x_2^6 + 9x_1^6x_2^7 + 4kx_1^4x_2^6 + 522x_1^3x_2^3 + 9x_1^4x_2^7 + 15x_1^3x_2^4.$
2. $M_1(R_{V_n}(H)) = 4(9n+4) + 3345.$
3. $M_2(R_{V_n}(H)) = 12(9n+2) + 5184.$

Proof - Let $R_{V_n}(H)$ be the molecular graph of R-Vertex Neighborhood Link graph of H_1 and H_2.All the edges of graph $R_{V_n}(H)$ can be categorised under following partions

$E_{66} = \{uv \in E(R_{V_n}(H)) / du = 6, dv = 6\} \Rightarrow |m_{66}|$
$= (3n-2) - 9.$

$E_{67} = \{uv \in E(R_{V_n}(H)) / du = 6, dv = 7\} \Rightarrow |m_{67}| = 9.$

$E_{46} = \{uv \in E(R_{V_n}(H)) / du = 4, dv = 6\} \Rightarrow |m_{46}| = 4k.$

$E_{33} = \{uv \in E(R_{V_n}(H)) / du = 3, dv = 3\} \Rightarrow |m_{33}|$
$= 522.$

$E_{34} = \{uv \in E(R_{V_n}(H)) / du = 3, dv = 4\} \Rightarrow |m_{34}|$
$= 12 + 3 = 15.$

$E_{47} = \{uv \in E(R_{V_n}(H)) / du = 4, dv = 7\} \Rightarrow |m_{47}|$
$= 6 + 3 = 9.$

From definition of M-Polynomial
$M(H: x_1, x_2) = \sum_{i \leq j} m_{ij}(H) x_1^i x_2^j.$

M-Polynomial is derived as:

$M(R_{V_n}(H): x_1, x_2) = m_{66}x_1^6x_2^6 + m_{67}x_1^6x_2^7 + m_{46}x_1^4x_2^6 + m_{33}x_1^3x_2^3 + m_{47}x_1^4x_2^7 + m_{34}x_1^3x_2^4$

$= [k(3n-2)-9]x_1x_2 + 9x_1^6x_2^6 + 4kx_1^4x_2^6 + 87 \times 6x_1^3x_2^3 + 9x_1^4x_2^7 + 15x_1^3x_2^4$

$(R_{V_n}(H); x_1, x_2) = [(3n-2)-9]x_1^6x_2^6 + 9x_1^6x_2^7 + 4kx_1^4x_2^6 + 522x_1^3x_2^3 + 9x_1^4x_2^7 + 15x_1^3x_2^4.$

2. First Zagreb index of $R_{V_n}(H)$ is defined as

$M_1(R_V(H)) = (D_{x_1} + D_{x_2})M(R_{V_n}(H); x_1, x_2)_{x_1=x_2=1}$

$D_{x_1} = x_1 \frac{\partial}{\partial x_1}[(R_{V_n}(H); x_1, x_2)]$

$= x_1[(k(3n-2)-9)6x_1^5x_2^6 + 54x_1^5x_2^7 + 16kx_1^3x_2^6 + 87 \times 18x_1^2x_2^3 + 36x_1^3x_2^7 + 45x_1^2x_2^4]$

$D_{x_2} = x_2 \frac{\partial}{\partial x_2}[M(R_{V_n}(H); x_1, x_2)]$

$= x_2[(k(3n-2)-9)6x_1^6x_2^5 + 63x_1^6x_2^6 + 24kx_1^4x_2^5 + 522 \times 3x_1^3x_2^2 + 63x_1^4x_2^6 + 60x_1^3x_2^3]$

$(D_{x_1})_{x_1=x_2=1} = 6[(3n-2)-9] + 54 + 16k + 1566 + 36 + 45$

$= 18kn + 4k + 1647$

$= 2(9n+2) + 1647$

$(D_{x_2})_{x_1=x_2=1} = 6[(3n-2)-9] + 63 + 24k + 1566 + 63 + 60$

$= 18kn + 12k + 1698$

$= 6(3n+2) + 1698$

$(D_{x_1} + D_{x_2})M(R_{V_n}(H); x_1, x_2)_{x_1=x_2=1}$

$M_1(R_{V_n}(H)) = 2(9n+2) + 1647 + 6k(3n+2) + 1698$

$M_1(R_{V_n}(H)) = 4(9n+4) + 3345.$

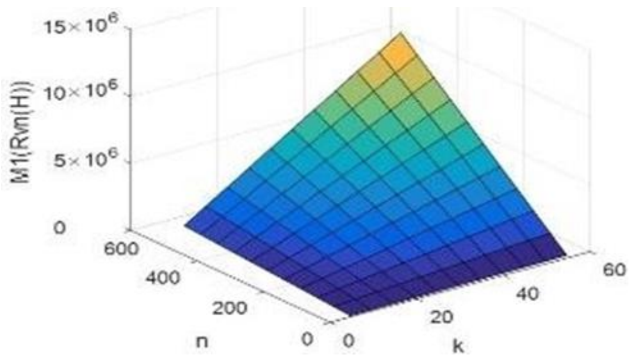

FIGURE VIII
First Zagreb Index Of $RVn\ (H)$

3. Second Zagreb index of $R_{V_n}(H)$ is defined as

$M_2(R_{V_n}(H)) = (D_{x_1}D_{x_2})(R_{V_n}(H); x_1, x_2)_{x_1=x_2=1}$

$D_{x_1}D_{x_2} = x_1 \frac{\partial}{\partial x_1}(D_{x_2})$

$$= x_1x_2|(k(3n-2)-9) \times 36x_1^5x_2^5 + 378x_1^5x_2^6 + 96kx_1^5x_2^5 + 4698x_1^4x_2^4 + 252x_1^5x_2^6 + 180x_1^4x_2^5|$$

$$(D_{x_1}D_{x_2})(R_{V_n}(H); x_1, x_2)\Big|_{x_1=x_2=1} = 108kn - 72k - 324 + 378 + 96k + 4698$$

$M_2\,(R_{V_n}(H)) = 108kn + 24k + 5184$

$M_2\,(R_V(H)) = 12k(9n + 2) + 5184$

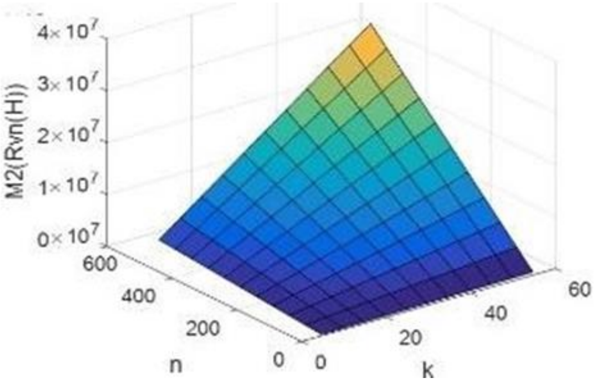

FIGURE IX
Second Zagreb Index Of $RV_n\,(H)$

R-Edge Neighborhood Link graph of Single Wall Carbon Nanotube and Fullerene

Let H_1 and H_2 be the molecular graphs of single wall Carbon Nanotube and Fullerene respectively. Also let $R_E(H)$ be the R-Vertex Neighborhood link graph of H_1 and H_2.

Theorem 5 - If $M\,(R_{E_n}(H))$, $M_1\,(R_{E_n}(H))$ and $M_2\,(R_{E_n}(H))$ are M-polynomial, First and Second Zagreb indices of $R_{E_n}(H)$ respectively, then

1. $(R_E\,(H); x_1, x_2) = [k(3n-2)-5]x_1^6x_2^6 + 5x_1^6x_2^7 + 4kx_1^4x_2^6 + (6nk-2)x_1^6x_2^6 + 2x_1^6x_2^7 + 4kx_1^4x_2^4 + 174x_1^6x_2^6 + 6x_1^6x_2^4 + 2x_1^4x_2^7$.
2. $M_1\,(R_E(H)) = 4k(21n + 8) + 1123.$
3. $M_2\,(R_E(H)) = 54k(5n + 2) + 1284.$

Proof – 1. Let $R_E(H)$ be the molecular graph of R-Vertex Neighbourhood Link graph of H_1 and H_2.All the edges of graph $R_{E_n}(H)$ can be categorized under following partitions.

$E_{66} = \{uv \in E\,(R_E(H))\,/du = 6, dv = 6\} \Rightarrow |m_{66}| = (3n-2) - 5.$

$E_{67} = \{uv \in E\,(R_E(H))\,/du = 6, dv = 7\} \Rightarrow |m_{67}| = 5.$

$E_{46} = \{uv \in E\,(R_{E_n}\,(H))\,/du = 4, dv = 6\} \Rightarrow |m_{46}| = 4k.$

$E_{26} = \{uv \in E\,(R_E(H))\,/du = 2, dv = 6\} \Longrightarrow |m_{26}|$
$= 6nk - 2.$

$E_{27} = \{uv \in E\,(R_E(H))\,/du = 2, dv = 7\} \Longrightarrow |m_{27}| = 2.$

$E_{24} = \{uv \in E\,(R_E(H))\,/du = 2, dv = 4\} \Longrightarrow |m_{24}| = 4k.$

$E_{33} = \{uv \in E\,(R_E(H))\,/du = 3, dv = 3\} \Longrightarrow |m_{33}|$
$= 174.$

$E_{34} = \{uv \in E\,(R_E(H))\,/du = 3, dv = 4\} \Longrightarrow |m_{34}| = 6.$

$E_{47} = \{uv \in E\,(R_E(H))\,/du = 4, dv = 7\} \Longrightarrow |m_{47}| = 2.$

From definition of M-Polynomial

$$M(H: x_1, x_2) = \sum_{i \le j} m_{ij}(H) x_1^i x_2^j$$

$$(R_{E_n}(H): x_1, x_2) = m_{66}x_1^6x_2^6 + m_{67}x_1^6x_2^7 + m_{46}x_1^4x_2^6 + m_{33}x_1^3x_2^3 + m_{34}x_1^3x_2^4 + m_{47}x_1^4x_2^7$$

$(R_{E_n}(H); x_1, x_2) = [k(3n-2) - 5]x_1^6x_2^6 + 5x_1^6x_2^7 + 4kx_1^4x_2^6 + (6nk-2)x_1^2x_2^6 + 2x_1^2x_2^7 + 4kx_1^2x_2^4 + 174x_1^3x_2^3 + 6x_1^3x_2^4 + 2x_1^4x_2^7.$

2. First Zagreb index of $R_E(H)$ is defined as

$M_1\,(R_E(H)) = (D_{x_1} + D_{x_2})M(R_{E_n}(H); x_1, x_2)_{x_1 = x_2 = 1}$

$D_{x_1} = x_1 \frac{\partial}{\partial x_1}[(R_{E_n}(H); x_1, x_2)]$

$= x_1[(k(3n-2) - 5)6x_1^5x_2^6 + 30x_1^5x_2^7 + 16kx_1^3x_2^6 + (6nk-2) \times 2x_1x_2^6 + 4x_1x_2^7 + 8kx_1x_2^4 + 522x_1^2x_2^3 + 18x_1^2x_2^4 + 8x_1^3x_2^7]$

$D_{x_2} = x_2 \frac{\partial}{\partial x_2}[M(R_{E_n}(H); x_1, x_2)]$

$= x_2[(k(3n-2) - 5)6x_1^6x_2^5 + 35x_1^6x_2^6 + 24kx_1^4x_2^5 + (6nk-2) \times 6x_1^2x_2^5 + 14x_1^2x_2^6 + 16kx_1^2x_2^3 + 522x_1^3x_2^2 + 24x_1^3x_2^3 + 14x_1^4x_2^6]$

$(D_{x_1})_{x_1 = x_2 = 1} = 18kn - 12k - 30 + 30 + 16k + 12nk - 4 + 4 + 8 + 522 + 18 + 8$

$= 30kn + 4k + 556$

$= 2(15n + 2) + 556$

$(D_{x_2})_{x_1 = x_2 = 1} = 18kn - 12k - 30 + 35 + 244 + 36nk - 12 + 14 + 16k + 522 + 24 + 14$

$= 54kn + 28k + 567$

$= 2(27n + 14) + 567$

$(D_{x_1} + D_{x_2})(R_{E_n}(H); x_1, x_2)_{x_1 = x_2 = 1}$
$= 30kn + 4k + 556 + 54kn + 28k + 567$

$M_1\,(R_E(H)) = 84kn + 32k + 1123$

$$M_1\,(R_E(H)) = 4(21n + 8) + 1123.$$

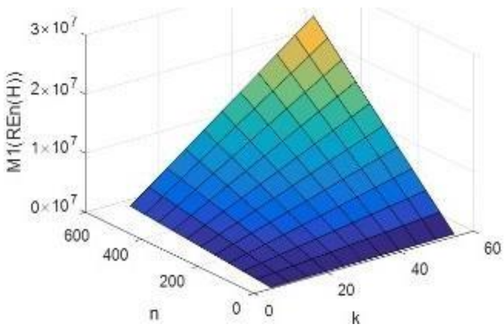

FIGURE X
First Zagreb Index OF$RE(H)$

3.Second Zagreb index of $R_{E_n}(H)$ is defined as

$$M_2\,(R_E(H)) = (D_{x_1}D_{x_2})M(R_{E_n}(H); x_1, x_2)_{x_1=x_2=1}$$

$$= x_1x_2\,[((3n-2)-5)\times 30x_1^6x_2^4 + 210x_1^6x_2^5 + 120kx_1^4x_2^4 + (6nk-2)\times 30x_1^2x_2^4 + 84x_1^2x_2^5 + 48kx_1^2x_2^2 + 1044x_1^3x_2^2 + 72x_1^3x_2^2 + 84x_1^4x_2^3]$$

$$(D_{x_1}D_{x_2})(R_{E_n}(H); x_1, x_2)_{x_1=x_2=1} = 90kn - 60k - 150 + 210 + 120k + 180nk - 60 + 84 + 48k + 1044 + 72 + 84$$

$$M_2\,(R_E(H)) = 270kn + 108k + 1284$$

$$M_2\,(R_E(H)) = 54(5n+2) + 1284.$$

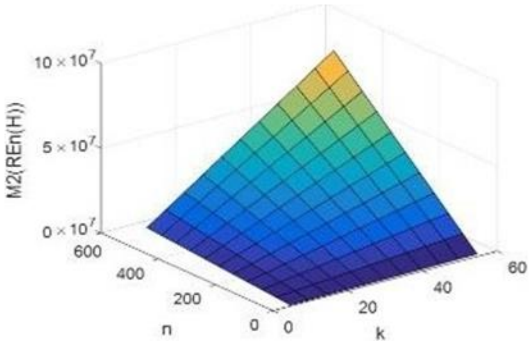

FIGURE XI
Second Zagreb Index OF$RE(H)$

Conclusion

In this paper, we obtained different Link graphs of Carbon Nanotube and Fullerene through graph operations such as R-graph, R-Vertex join graph, R-edge join graph, R-vertex neighborhood and R-Edge neighborhood graphs and derived the M-polynomial for each graph. We established First and Second Zagreb indices of all these link graphs through M- Polynomial method. From the plots of the variation of indices with molecular structure parameters, we observe that the behavior of all indices is very close.

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