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Redefined Zagreb, Randic, Harmonic and GA Indices of Graphene

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Abstract

Graph theory has provided chemist with a variety of useful tools, such as topological indices. A topological index $Top(G)$ of a graph G is a number with the property that for every graph H isomorphic to G, $Top(H) = Top(G)$. Graphene is one of the most promising nanomaterials because of its unique combination of superb properties,which opens away for its exploitation in a wide spectrum of applications ranging from electronics to optics, sensors, and biodevices. In this article, we present exact expressions for some topological indices of carbon compound graphene. We compute, Re-defined version of Zagreb indices, General Randic index, General version of harmonic index, Ordinary geometric-arithmetic index of Graphene.

Mathematics Subject Classification: 05C12, 05C90

Keywords: Re-defined version of Zagreb indices, General Randic index, General version of harmonic index, Ordinary geometric-arithmetic index, Graphene

1 Introduction

Graphene is an atomic scale honeycomb lattice made of carbon atoms. Graphene is 200 times stronger than steel, one million times thinner than a human hair, and world's most conductive material. So it has captured the attention of scientists, researchers, and industrialists worldwide. It is one of the most promising nanomaterials because of its unique combination of superb properties, which opens a way for its exploitation in a wide spectrum of applications ranging from electronics to optics, sensors, and biodevices. Also it is the most effective material for electromagnetic interference (EMI) shielding. In this paper, we determine Re-defined version of Zagreb indices, General Randic index, General version of harmonic index, Ordinary geometric-arithmetic index of Graphene.

Topological indices are the molecular descriptors that describe the structures of chemical compounds and they help us to predict certain physicochemical properties like boiling point, enthalpy of vaporization, stability, etc. All molecular graphs considered in this paper are finite, connected, loop less, and without multiple edges. Let $G = (V, E)$ be a graph with vertex set V and edge set E. The degree of a vertex $u \in E(G)$ is denoted by d_u and is the number of vertices that are adjacent to u. The edge connecting the vertices u and v is denoted by uv. Now we focus on computation of topological indices of Graphene [4, 5, 6, 8]

Redefined Zagreb indices

In chemistry much studied and applied graph invariants are the pair of molecular descriptors (or topological index), known as the First Zagreb index $M_1(G)$ and Second Zagreb index $M_2(G)$. They first appeared in the topological formula for total φ-energy of conjugated molecules that has been derived in 1972 by I. Gutman and N.Trinajstić [6]. Later the Zagreb indices found applications in QSPR and QSAR studies. Zagreb indices are included in a number of programs used for the routine computation of topological indices, such as POLLY, OASIS, DRAGON, CERIUS, TAM, DISSIM etc. $M_1(G)$ and $M_2(G)$ are, in fact, measures of branching of the molecular carbonatom skeleton [8] and can thus be viewed as molecular structure descriptors. The Zagreb indices and their variants have been used to study molecular complexity, chirality, ZE-isomerism and heterosystems, etc. Overall, Zagreb indices exhibited a potential applicability for deriving multi-linear regression models. Details on the chemical applications of the two Zagreb indices can be found in the books [13, 14]. Further studies on Zagreb indices can be found in [1, 16, 20].

Ranjini et al. [11] re-defined the Zagreb indices, i.e., the redefined first, second and third Zagreb indices for a graph G and these are manifested as

Definition 1.1. *Let $G = (V, E)$ be a molecular graph and d_u is the degree of the vertex u, similarly d_v is the degree of the vertex v. Now the Re-defined version of Zagreb indices are defined as follows,*

$$ReZG_1(G) = \sum_{e=uv\in E(G)} \frac{d_u + d_v}{d_u d_v}$$

$$ReZG_2(G) = \sum_{e=uv\in E(G)} \frac{d_u d_v}{d_u + d_v}$$

$$ReZG_3(G) = \sum_{e=uv\in E(G)} (d_u d_v)(d_u + d_v).$$

General Randic index

There are several degree based indices introduced to test the properties of compounds and drugs, which have been widely used in chemical and pharmacy engineering. Bollobas and Erdos [2] introduced the general Randic index.

Definition 1.2. *Let $G = (V, E)$ be a molecular graph and d_u is the degree of the vertex u, then $R_k(G)$ index of G is defined as,* $R_k(G) = \sum_{e=uv\in E(G)} (d_u d_v)^k$.

General Harmonic index

The Harmonic index was introduced by Zhong [19]. It has been found that the harmonic index correlates well with the Randic index and with the π-electron energy of benzenoid hydrocarbons. Very recently, in order to extend harmonic index for more chemical applications, Yan et al. [18] introduced the general version of harmonic index.

Definition 1.3. $H_k(G) = \sum_{e=uv\in E(G)} \left(\frac{2}{d_u + d_v}\right)^k.$

Ordinary Geometric-Arithmetic index

Eliasi and Iranmanesh [4] proposed the ordinary geometric-arithmetic index as the extension of geometric-arithmetic index which was stated as

Definition 1.4. $OGA_k(G) = \sum_{e=uv\in E(G)} \left(\frac{2\sqrt{d_u d_v}}{d_u + d_v}\right)^k.$

2 Main results

Theorem 2.1. *The First Re-defined version of Zagreb index of Graphene with 't' rows of benzene rings and 's' benzene rings in each row is given by,*

$$ReZG_1(G) = \begin{cases} 4s + 2 & \text{if } t = 1 \\ 2t + 2s + ts & \text{if } t \neq 1 \end{cases}$$

Proof. Consider a Graphene with 't' rows and 's' benzene rings in each row. Let $|m_{i,j}|$ denotes the number of edges connecting the vertices of degrees d_i and d_j. Two dimensional structure of graphene with t rows and s benzene rings in each row is as shown in Figure 1. It contains only $m_{2,2}$, $m_{2,3}$ and $m_{3,3}$ edges. In the below figure $m_{2,2}$, $m_{2,3}$ and $m_{3,3}$ edges are colored in green, red and black respectively.

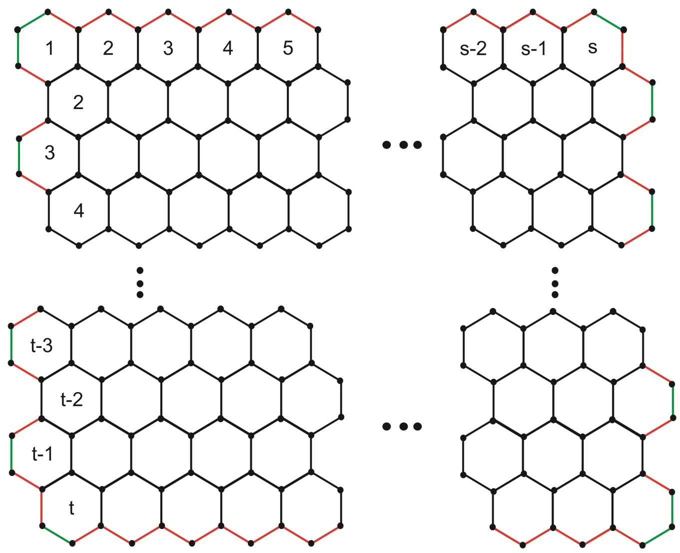

Figure : 1

The number of $m_{2,2}$, $m_{2,3}$ and $m_{3,3}$ edges in each row is mentioned in the following table.

Row	$\lvert m_{2,2}\rvert$	$\lvert m_{2,3}\rvert$	$\lvert m_{3,3}\rvert$
1	3	2s	3s−2
2	1	2	3s−1
3	1	2	3s−1
4	1	2	3s−1
. . .	. . .	. . .	. . .
t	3	2s	s−1
Total	t+4	4s+2t−4	3ts−2s−t−1

$\therefore$ Graphene contains $|m_{2,2}| = (t+4)$ edges, $|m_{2,3}| = (4s+2t-4)$ edges and $|m_{3,3}| = (3ts-2s-t-1)$ edges.

CASE 1. The First Re-defined version of Zagreb index of Graphene for $t \neq 1$ is

$$ReZG_1(G) = \sum_{e=uv\in E(G)} \frac{d_u + d_v}{d_u d_v}$$
$$= |m_{2,2}|\Big(\frac{2+2}{4}\Big) + |m_{2,3}|\Big(\frac{2+3}{6}\Big) + |m_{3,3}|\Big(\frac{3+3}{9}\Big)$$
$$= (t+4)(1) + (4s+2t-4)\Big(\frac{5}{6}\Big) + (3ts-2s-t-1)\Big(\frac{2}{3}\Big)$$
$$= 2t + 2s + ts$$
$\therefore\ ReZG_1(G) = 2t + 2s + ts$, for $t \neq 1$

CASE 2. For $t = 1$, $|m_{2,2}| = 6$ edges, $|m_{2,3}| = (4s-4)$ edges and $|m_{3,3}| = (s-1)$ edges as shown in the following Figure 2.

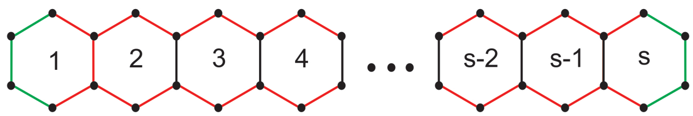

Figure : 2

The First Re-defined version of Zagreb index of Graphene for $t = 1$ is

$$ReZG_1(G) = \sum_{e=uv\in E(G)} \frac{d_u + d_v}{d_u d_v}$$
$$= |m_{2,2}|\Big(\frac{2+2}{4}\Big) + |m_{2,3}|\Big(\frac{2+3}{6}\Big) + |m_{3,3}|\Big(\frac{3+3}{9}\Big)$$
$$= 6(1) + (4s-4)\Big(\frac{5}{6}\Big) + (s-1)\Big(\frac{2}{3}\Big)$$
$\therefore\ ReZG_1(G) = 4s + 2$, for $t = 1$.

□

Theorem 2.2. *The Second Re-defined version of Zagreb index of Graphene with 't' rows of benzene rings and 's' benzene rings in each row is given by,*

$$ReZG_2(G) = \begin{cases} \Big(\frac{63}{10}\Big)s - \Big(\frac{3}{10}\Big) & \text{if } t = 1 \\ \Big(\frac{19}{10}\Big)t + \Big(\frac{9}{5}\Big)s + \Big(\frac{9}{2}\Big)ts - \Big(\frac{23}{10}\Big) & \text{if } t \neq 1 \end{cases}$$

Proof. CASE 1. The Second Re-defined version of Zagreb index of Graphene for $t \neq 1$ is

$$ReZG_2(G) = \sum_{e=uv\in E(G)} \frac{d_u d_v}{d_u + d_v}$$
$$= |m_{2,2}|(1) + |m_{2,3}|\Big(\frac{6}{5}\Big) + |m_{3,3}|\Big(\frac{9}{6}\Big)$$
$$= (t+4)(1) + (4s+2t-4)\Big(\frac{6}{5}\Big) + (3ts-2s-t-1)\Big(\frac{3}{2}\Big)$$
$$= \Big(\frac{19}{10}\Big)t + \Big(\frac{9}{5}\Big)s + \Big(\frac{9}{2}\Big)ts - \Big(\frac{23}{10}\Big)$$

$\therefore ReZG_2(G) = \left(\frac{19}{10}\right)t + \left(\frac{9}{5}\right)s + \left(\frac{9}{2}\right)ts - \left(\frac{23}{10}\right)$, for $t \neq 1$.

CASE 2. The Second Re-defined version of Zagreb index of Graphene for $t = 1$ is

$$ReZG_2(G) = \sum_{e=uv\in E(G)} \frac{d_u d_v}{d_u + d_v}$$

$= |m_{2,2}|(1) + |m_{2,3}|\left(\frac{6}{5}\right) + |m_{3,3}|\left(\frac{9}{6}\right)$

$= 6(1) + (4s-4)\left(\frac{6}{5}\right) + (s-1)\left(\frac{3}{2}\right)$

$\therefore ReZG_2(G) = \left(\frac{63}{10}\right)s - \left(\frac{3}{10}\right)$, for $t = 1$.

□

Theorem 2.3. *The third Re-defined version of Zagreb index of Graphene with 't' rows of benzene rings and 's' benzene rings in each row is given by,*

$$ReZG_3(G) = \begin{cases} 174s - 78 & \text{if } t = 1 \\ 22t + 12s + 162ts - 110 & \text{if } t \neq 1 \end{cases}$$

Proof. *CASE 1.* The third Re-defined version of Zagreb index of Graphene for $t \neq 1$ is

$$ReZG_3(G) = \sum_{e=uv\in E(G)} (d_u d_v)(d_u + d_v)$$

$= |m_{2,2}|(4.4) + |m_{2,3}|(6.5) + |m_{3,3}|(9.6)$

$= (t+4)(16) + (4s+2t-4)(30) + (3ts-2s-t-1)(54)$

$= 22t + 12s + 162ts - 110$

$\therefore ReZG_3(G) = 22t + 12s + 162ts - 110$, for $t \neq 1$.

CASE 2. The third Re-defined version of Zagreb index of Graphene for $t = 1$ is

$$ReZG_3(G) = \sum_{e=uv\in E(G)} (d_u d_v)(d_u + d_v)$$

$= |m_{2,2}|(16) + |m_{2,3}|(30) + |m_{3,3}|(54)$

$= 6(16) + (4s-4)(30) + (s-1)(54)$

$\therefore ReZG_3(G) = 174s - 78$, for $t = 1$.

□

Theorem 2.4. *The General Randic index of Graphene with 't' rows of benzene rings and 's' benzene rings in each row is given by,*

$$R_k(G) = \begin{cases} (2^{2+k}3^k - 3^{2k})s + (2^{2k+1}3 - 2^{2+k}3^k - 3^{2k}) & \text{if } t = 1 \\ (2^{2k} + 2^{k+1}3^k - 3^{2k})t + (2^{2+k}3^k - 2(3)^{2k})s + (3^{2k+1})ts - (2^{2k+2} - 2^{2+k}3^k - 3^{2k}) & \text{if } t \neq 1 \end{cases}$$

Proof. *CASE 1.* The General Randic index of Graphene for $t \neq 1$ is

$$R_k(G) = \sum_{e=uv\in E(G)} (d_u d_v)^k$$

$= |m_{2,2}|4^k + |m_{2,3}|6^k + |m_{3,3}|9^k$

$= (t+4)(4^k) + (4s+2t-4)(6^k) + (3ts-2s-t-1)9^k$
$= 4^k t + 4^{k+1} + 4(6^k)s + 2(6^k)t - 4(6^k) + 3ts((9^k) - 2s(9^k) - t(9^k) - 9^k$
$\therefore R_k(G) = (2^{2k} + 2^{k+1}3^k - 3^{2k})t + (2^{2+k}3^k - 2(3)^{2k})s + (3^{2k+1})ts - (2^{2k+2} - 2^{2+k}3^k - 3^{2k}),$
for $t \neq 1$.

CASE 2. The General Randic index of Graphene for $t = 1$ is
$R_k(G) = \sum_{e=uv\in E(G)} (d_u d_v)^k$
$= |m_{2,2}|4^k + |m_{2,3}|6^k + |m_{3,3}|9^k$
$= 6(4^k) + (4s-4)(6^k) + (s-1)9^k$
$= 2^{2k+1}(3) + 4(6)^k s - 4(6^k) - s(9^k) - (9^k)$
$= (2^{2+k}3^k - 3^{2k})s + (2^{2k+1}3 - 2^{2+k}3^k - 3^{2k})$
$\therefore R_k(G) = (2^{2+k}3^k - 3^{2k})s + (2^{2k+1}3 - 2^{2+k}3^k - 3^{2k})$, for $t = 1$. □

Theorem 2.5. *The General Harmonic index of Graphene with 't' rows of benzene rings and 's' benzene rings in each row is given by,*

$$H_k(G) = \begin{cases} (2^{2+k}5^{-k} + 3^{-k})s + (2^{1-k}3 - 2^{2+k}5^{-k} - 3^{-k}) & \text{if } t = 1 \\ (2^{-k} + 2^{k+1} - 3^{-k})t + (2^{2+k} - 2(3)^{-k})s + (3^{1-k})ts + (2^{2-k} - 4(5)^{-k} - 3^{-k}) & \text{if } t \neq 1 \end{cases}$$

Proof. CASE 1. The General Harmonic index of Graphene for $t \neq 1$ is
$H_k(G) = \sum_{e=uv\in E(G)} \left(\frac{2}{d_u + d_v}\right)^k$
$= |m_{2,2}|4^k + |m_{2,3}|6^k + |m_{3,3}|9^k$
$= |m_{2,2}|\left(\frac{2}{4}\right)^k + |m_{2,3}|\left(\frac{2}{5}\right)^k + |m_{3,3}|\left(\frac{2}{6}\right)^k$
$= (t+4)\left(\frac{1}{2}\right)^k + (4s+2t-4)\left(\frac{2}{5}\right)^k + (3ts-2s-t-1)\left(\frac{1}{3}\right)^k$
$= (t+4)2^{-k} + (4s+2t-4)2^k 5^{-k} + (3ts-2s-t-1)3^{-k}$
$H_k(G) = (2^{-k} + 2^{k+1} - 3^{-k})t + (2^{2+k} - 2(3)^{-k})s + (3^{1-k})ts + (2^{2-k} - 4(5)^{-k} - 3^{-k})$, for $t \neq 1$.

CASE 2. The General Harmonic index of Graphene for $t = 1$ is
$H_k(G) = \sum_{e=uv\in E(G)} \left(\frac{2}{d_u + d_v}\right)^k$
$= |m_{2,2}|2^{-k} + |m_{2,3}|2^k 5^{-k} + |m_{3,3}|3^{-k}$
$= (6)2^{-k} + (4s-4)2^k 5^{-k} + (s-1)3^{-k}$
$= 2^{2k+1}(3) + 4(6)^k s - 4(6^k) - s(9^k) - (9^k)$
$= (2^{2+k}3^k - 3^{2k})s + (2^{2k+1}3 - 2^{2+k}3^k - 3^{2k})$
$\therefore H_k(G) = (2^{2+k}5^{-k} + 3^{-k})s + (2^{1-k}3 - 2^{2+k}5^{-k} - 3^{-k})$, for $t = 1$. □

Theorem 2.6. *The Ordinary Geometric-Arithmetic index of Graphene with 't' rows of benzene rings and 's' benzene rings in each row is given by,*

$$OGA_k(G)=\begin{cases} (2^{k+2}\sqrt{6}^k5^{-k}+1)s+(5-2^{k+2}\sqrt{6}^k5^{-k}) & \textit{if} \ \ t=1 \\ (2^{1+k}(\sqrt{6})^k5^{-k})t+(2^{2+k}(\sqrt{6})^k5^{-k}-2)s+(3)ts+(3-2^{2+k}\sqrt{6}^k5^k) & \textit{if} \ \ t\neq 1 \end{cases}$$

Proof. CASE 1. The Ordinary Geometric-Arithmetic index index of Graphene for $t \neq 1$ is $OGA_k(G)$

$$=\sum_{e=uv\in E(G)}\Big(\frac{2\sqrt{d_ud_v}}{d_u+d_v}\Big)^k.$$

$$=|m_{2,2}|\Big(\frac{2(2)}{4}\Big)^k+|m_{2,3}|\Big(\frac{2\sqrt{6}}{5}\Big)^k+|m_{3,3}|\Big(\frac{2(3)}{6}\Big)^k.$$

$$=(t+4)1^k+(4s+2t-4)\Big(\frac{2^k\sqrt{6}^k}{5^k}\Big)+(3ts-2s-t-1)\ .$$

$\therefore$

$OGA_k(G) = (2^{1+k}(\sqrt{6})^k5^{-k})t+(2^{2+k}(\sqrt{6})^k5^{-k}-2)s+(3)ts+(3-2^{2+k}\sqrt{6}^k5^k)$, for $t \neq 1$.

CASE 2. The Ordinary Geometric-Arithmetic index index of Graphene for $t = 1$ is $OGA_k(G)$

$$=\sum_{e=uv\in E(G)}\Big(\frac{2\sqrt{d_ud_v}}{d_u+d_v}\Big)^k.$$

$$=|m_{2,2}|+|m_{2,3}|2^k\sqrt{6}^k5^{-k}+|m_{3,3}|.$$

$$=(6)+(4s-4)2^k\sqrt{6}^k5^{-k}+(s-1).$$

$\therefore OGA_k(G) = (2^{k+2}\sqrt{6}^k5^{-k}+1)s+(5-2^{k+2}\sqrt{6}^k5^{-k})$, for $t = 1$.

□

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