HARMONIC DEGREE-BASED INDEX OF SPECIAL CHEMICAL MOLECULAR AND NANOTUBES

Wei GAO[1*], Mohammad R. FARAHANI[2], Jia-Bao LIU[3], Muhammad K. SIDDIQUI[4]

Let G be a simple molecular graph without directed and multiple edges and without loops, the vertex and edge-sets of which are represented by V(G) and E(G), respectively. Suppose G is a connected molecular graph and vertices u,v∈V(G). In this paper, we present explicit formulas for calculating the "general harmonic index, harmonic index and Harmonic polynomial" of a special chemical molecular graph "Cas(C)-CaR(C)[m,n,p] Nanotubes Junction" are given. The Cas(C)-CaR(C)[m,n,p] Nanotubes Junction is a new nano-structure that was defined by M.V. Diudea, on based the new graph operations (Leapfrog Le and Capra Ca) on the cycle graph C_n. In this paper, we compute the harmonic index vie two ways namely degree-based method and via polynomial method.

Keywords: Molecular graphs, Carbon Nanocones, Cas(C)-CaR(C)[m,n,p] Nanotubes Junction, Harmonic index, Harmonic polynomial, General harmonic index

1. Introduction

A graph is a collection of points and lines connecting a subset of them. The points and lines of a graph also called vertices and edges of the graph, respectively. The vertices and edges of a graph also correspond to the atoms and bonds of the molecular graph, respectively. If e is an edge/bond of G, connecting the vertices/atoms u and v, then we write $e=uv$ and say "u and v are adjacent". Mathematical chemistry is a branch of theoretical chemistry for discussion and prediction of the molecular structure using mathematical methods without necessarily referring to quantum mechanics.

Graph theory which is an important branch of applied mathematics has many applications to modelling real world problems from science to technology. Chemical graph theory which is a fascinating branch of graph theory has many

[1] School of Information Science and Technology, Yunnan Normal University, Kunming, China, *Corresponding author: Gaowei@ynnu.edu.cn

[2] Department of Applied Mathematics of Iran University of Science and Technology (IUST), Narmak, Tehran, Iran, e-mail: mrfarahani88@gmail.com

[3] School of Mathematics and Physics, Anhui Jianzhu University, Hefei, China, e-mail: liujiabaoad@163.com

[4] Department of Mathematics, COMSATS University Islamabad, Sahiwal Campus, Pakistan, e-mail: kamransiddiqui75@gmail.com

applications related to chemistry. Chemical graph theory provides many information about molecules and atoms by using pictorial representation (chemical graph) of these chemical compounds Chemical graph theory is an important branch of graph theory, which applies graph theory to mathematical modeling of chemical phenomena [1-4].

A novel topological index, named the General *Randić Index* in honor of Professor Milan *Randić*, has been introduced by *Bollobas and Erdos* [6]. It is derived from quantitative structure-property relationship (QSPR) makes a connection between the structures [5]. Fajtlowicz defined an invariant of the Randić index called the Harmonic index.

Topological indices, as numerical parameters of molecular structures, play a vital role in chemistry, and medicine science. It has been proved that topological indices reflect biochemical properties (such as the melting point, boiling point, toxicity and QSPR/QSAR study) of their corresponding compounds and drugs. Several articles contributed to determining the topological indices of special molecular graphs. There are many indices for a connected graph G.

The quantitative structure-property relationship (QSPR) makes a connection between the structure and the properties of molecules. In 1975, *Milan Randić* proposed the first degree based structural descriptor [5] named the *Randić Connectivity Index* χ(G), which is defined as:

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

where d_u and d_v are the degrees of the vertices *u* and *v*, respectively.

Later on, *Bollobas and Erdos* [6] replaced the exponent $-\frac{1}{2}$ by any real number *a* and defined the general *Randić* index as:

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

B. Zhou and *N. Trinajstić* [7,8] extended this concept to the general sum-connectivity index as

$$X_\alpha(G) = \sum_{uv \in E(G)} (d_u + d_v)^\alpha$$

where α is any real number and d_v denotes the degree of vertex v in G. *Li* and *Liu* [9] proposed the first three minimum general Randić indices of tree structure, and they also determined the corresponding extremal trees. *Liu* and *Gutman* [10] characterized several estimating on general Randić index. Throughout our paper, we always assume that α is a real number.

The *first Zagreb* index was formally introduced by *I. Gutman* and *N. Trinajstić* [11-13] on based structure descriptor about forty years ago (in 1972) as the sum of the squares of the degrees of all vertices/atoms in the molecules *G*, in

terms of bonds and the second Zagreb index M_2(G) was conceived somewhat later [19] and a new version of Zagreb indices named Hyper-Zagreb index was introduced by *Shirdel* et al. [14].

By setting $\alpha=1$ of the general Randić index and $\alpha=1$ and $\alpha=2$, respectively, then it becomes the second Zagreb index $M_2(G)$, the first Zagreb index $M_1(G)$ and the first Hyper-Zagreb index and Second Hyper-Zagreb index:

$$M_1(G)=\sum_{e=uv\in E(G)}\left(d_u+d_v\right),\ M_2(G)=\sum_{e=uv\in E(G)}\left(d_u\times d_v\right)$$

$$HM_1(G)=\sum_{e=uv\in E(G)}\left(d_v+d_v\right)^2\ ,\ HM_2(G)=\sum_{e=uv\in E(G)}\left(d_v d_v\right)^2$$

In 1980, Fajtlowicz defined an invariant of the Randić index called the harmonic index, as

$$H(G)=\sum_{e=uv\in E(G)}\frac{2}{d_u+d_v}$$

He examined the possible relations between countless graph invariants. With single exception H(G) did not attract anybody's attention, especially not chemists. Recently, Hosmani et al. [15] explored the chemical applications of the harmonic index. They revealed that harmonic index is also a useful tool in predicting the heats of vaporizations and critical temperatures of alkanes.

Iranmanesh et.al [16] were the first to introduce the harmonic polynomial of a caterpillar graph G of diameter 4 as follows:

$$H(G,x)=\sum_{e=uv\in E(G)}2x^{(du+dv-1)}$$

where $H(G)=\int_0^1 H(G,x)dx$.

Favaron et al. [17] manifested the relation between the eigenvalues and harmonic index of molecular graphs. *Zhong* [15] reported the minimum and maximum values of the harmonic index for connected molecular graphs and trees, and the corresponding extremal molecular graphs are also described. *Wu et al.* [16] derived the minimum value of the harmonic index with the minimum degree at least two. *Liu* [18] yielded the relationship between the diameter and the harmonic index of molecular graphs.

Very recently, *Yan et al.* [19] introduced the general harmonic index for extending harmonic index in more chemical engineering applications which can be stated as:

$$H_\alpha(G)=\sum_{uv\in E(G)}\left(\frac{2}{d_u+d_v}\right)^\alpha$$

where α is any real number and d_v denotes the degree of vertex v in G.

In this paper, we present explicit formulas for calculating the "general harmonic index, harmonic index and Harmonic polynomial" of a special chemical molecular graph "*Cas(C)-CaR(C)[m,n,p]* Nanotubes Junction" are given.

2. Applications of Topological Indices:

The Randić index is a topological descriptor that has related with a great deal of the synthetic qualities of the atoms and has been discovered parallel to processing the boiling point and Kovats constants of the particles. The first and second Zagreb index were found to be helpful for calculation of the aggregate π electron energy of the particles inside particular rough articulations. These are among the graph invariants who were proposed for estimation of skeleton of stretching of the carbon-atom.

During the most recent two decades, the analysts contemplated certain substance diagrams and arrange and processed their particular indices. W. Gao and M. R. Farahani figured degree-based indices of synthetic structures by utilizing an edge separated technique. Gao et al. in 2017 contemplated concoction structures in medications and some medication structures and processed the overlooked topological indices. As of late, Baig et al. in 2015 computed the topological descriptors of the concoction graphs of carbon graphite and precious stone cubic carbon structures and furthermore showed their graphical portrayal. These applications and writing survey inspired us to investigate some new substance diagrams and gem structures and process their topological records.

An information topological index based on Randic M. molecular connectivity index was constructed and calculated for 58 alkyl cycloalkanes. The information topological index, Randic connectivity index and number of carbon atoms were correlated with 11 kinds of thermodynamic and physico-chemical properties such as gaseous standard formation heat, gaseous standard entropy, gaseous standard formation free energy, boiling point, critical temperature, critical pressure, critical volume, evaporation heat, density, capacity and surface tension of the alkyl cycloalkanes.

3. Methods:

For the computation of our results we utilize the strategy for combinatorial registering, vertex partition strategy, edge partition technique, graph hypothetical instruments, scientific systems, degree counting strategy and entirety of degrees of neighbor's strategy. In addition, we utilize the matlab for scientific estimations and confirmations. We likewise utilize maple for plotting these numerical results.

4. Main Results

The aim of this section is to compute the general harmonic, harmonic indices and Harmonic polynomial for a special chemical molecular graph "*Cas(C)-CaR(C)[m,n,p]* Nanotubes Junction." The *Cas(C)-CaR(C)[m,n,p]* Nanotubes Junction is a new nano-structure that was defined by *M.V. Diudea* [20], on based the new graph operations on the cycle graph C_n, namely : Leapfrog Le and Capra Ca.

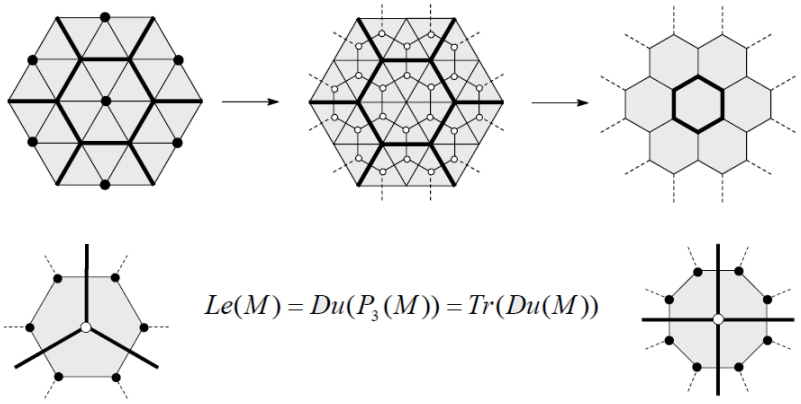

Fig. 1. An example of "Leapfrog Le(C_6)" graph operation.

Some examples of graph operations (Leapfrog Le and Capra Ca) are shown in Figs. 1 and 2 and readers can see the references [21-32].
Now, consider *Cas(C)-CaR(C)[m,n,p]* Nanotubes Junction $\forall m,n,p \in \mathbb{N}$, such that the 3-Dimensional lattice of *Cas(C)-CaR(C)[m,n,p]* Nanotubes Junction are shown in Fig. 3. In this paper we name the first member *Cas(C)[1,1,1]* or *Cas(C)* as the based unit (see Figs. 3 & 4), since all member of *Cas(C)[m,n,p]* Nanotubes are combine this unit.

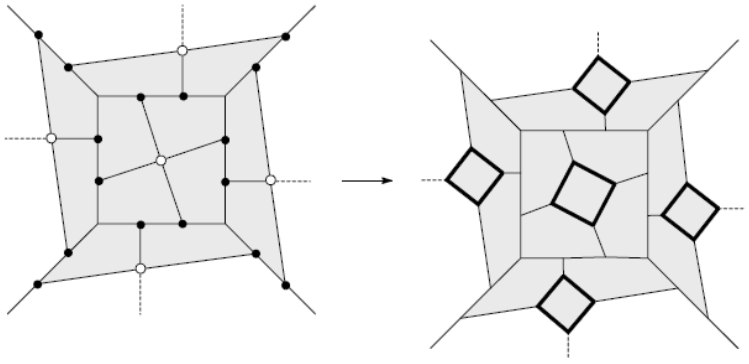

Fig. 2. An example of "Capra Ca(C_4)" graph operation.

From Fig. 3, one can see that 6 × 4=24 vertices/atoms of *Cas(C)* unit have degree 2 (red colored vertices in Fig. 3), and there are 2 × 4=8 vertices/atoms with degree 3 in any split of *Cas(C)* (yellow colored vertices in Fig. 3) and *Cas(C)* unit has 6 splits. Finally there are 8 common vertices between 3 joist splits of *Cas(C)* (obviously with degree 3 and colored by white). These imply that *Cas(C)* unit has 24+6×8+8=80 (|*V(Cas(C))*|)vertices/atoms and the number of edges/bonds of *Cas(C)* unit is equal to

$$|E(Cas(C))|=\frac{2\times|V_2|+3\times|V_3|}{2}=½[2\times24+3\times56]=216.$$

Thus following *M.V. Diudea* [24] we denote the number of *Cas(C)* units in the first rows and column in these Nanotubes by integer number *m*, *n* and *p*. Therefore, in general case of this nano-structure *Cas(C)-CaR(C)[m,n,p]*, there are *m*×*n*×*p Cas(C)* units and there exist
$|V(Cas(C)\text{-}CaR(C)[m,n,p])|=80\times m\times n\times p=80mnp$ number of vertices/atoms $(\forall m,n,p\in\mathbb{N})$.

Also, from the structure of *Cas(C)-CaR(C)[m,n,p]* Nanotubes Junction $\forall m,n,p\in\mathbb{N}$, in Fig. 4, one can see that the number of edges/bonds of *Cas(C)-CaR(C)[m,n,p]* is equal to

$|E(Cas(C)\text{-}CaR(C)[m,n,p])|=216\times m\times n\times p+4(m-1)(n-1)(p-1)=220mnp-4mn-4mp-4np+4m+4n+4p-4.$

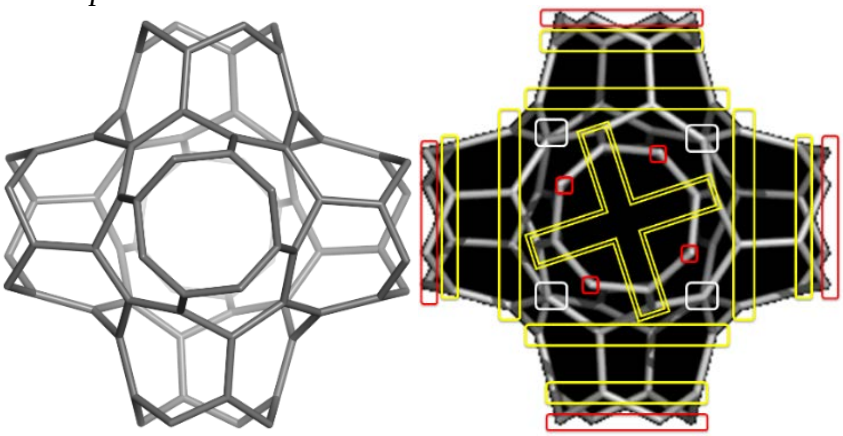

Fig. 3. The based unit Cas(C)-CaR(C)[1,1,1] of the Cas(C)-CaR(C)[m,n,p] Nanotubes Junction $\forall m,n\in\mathbb{N}$.

For computing these Degree-based indices and polynomial, let us to partition the vertex set and edge set of this Nanotubes, such that $\delta\leq k\leq\Delta$, $2\delta\leq i\leq2\Delta$, and $\delta^2\leq j\leq\Delta^2$ [33-35]:
$V_{k=}\{v\in V(G)|\ d_v=k\}$,

$E_i=\{e=uv \in E(G)|d_u+d_v=i\}$,
$E_j^*=\{uv \in E(G)|d_u \times d_v=j\}$.

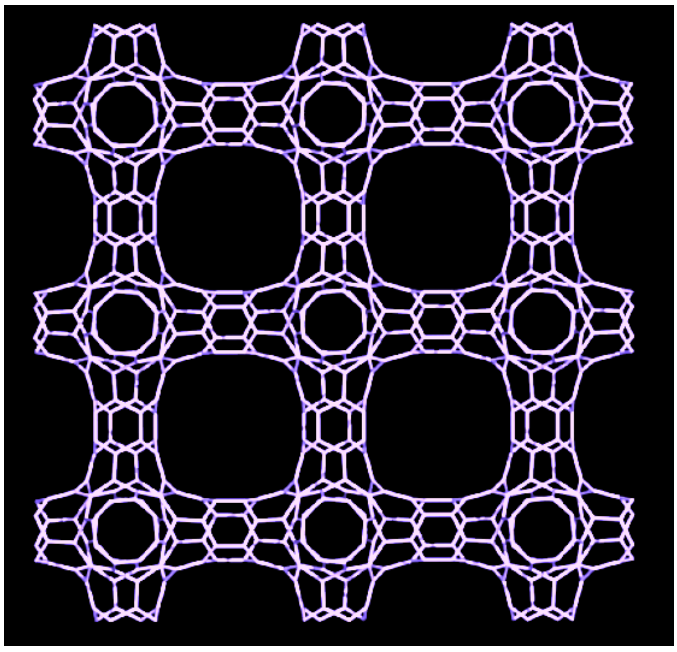

Fig. 4. A-Dimensional lattice of *Cas(C)-CaR(C)[m,n,p]* Nanotubes Junction $\forall m,n,p \in \mathbb{N}$.

Now, in this *Cas(C)-CaR(C)[m,n,p]* Nanotubes Junction , one can see that $\forall v \in V(Cas(C)$ $d_v=2$ or 3. So, we have the vertex partitions with their cardinalities as follows.

$V_3=\{v \in V(Cas(C))|\ d_v=3\}$
$V_2=\{v \in V(Cas(C))|\ d_v=2\}$.

Table: 1

Vertex partition for a small case

Vertex partition	V_3	V_2
Cardinality	56	24

And the edge partitions of *Cas(C)* unit with their cardinalities are as follows.

$E_5=E_6^{*=}\{uv \in E(Cas(C))|d_u=2$ & $d_v=3\}$
$E_6=E_9^{*=}\{uv \in E(Cas(C))|d_u=d_v=3\}$.

Table: 2

Edge partition for a small case

Edge partition	$E_5=E_6^*$	$E_6=E_9^*$
Cardinality	$2\times\|V_2\|=48$	168

In the general case G=*Cas(C)-CaR(C)[m,n,p]* Nanotubes Junction**,** one can see that ∀v∈ *V(Cas(C)-CaR(C)[m,n,p]) d_v=2* or 3, too and we have the vertex and edge partitions with their cardinalities as follows *(∀m,n,p∈ℕ)*.

$V_3=\{v \in V(Cas(C)\text{-}CaR(C)[m,n,p])|\ d_v=3\}$

$V_2=\{v \in V(Cas(C)\text{-}CaR(C)[m,n,p])|\ d_v=2\}$

Table: 3

Vertex partition for general case

Vertex partition	V_2	V_3
Cardinality	*4(2mp+2np+2mn)*	*8(10mnp-mp-np-mn)*

$E_5=E_6^*=\{uv \in E(Cas(C)\text{-}CaR(C)[m,n,p])|d_u=2\ \&\ d_v=3\}$

$E_6=E_9^*=\{uv \in E(Cas(C)\text{-}CaR(C)[m,n,p])|d_u=d_v=3\}$.

Table: 4

Edge partition for general case

Edge partition	$E_5=E_6^*$	$E_6=E_9^*$
Cardinality	*8(2mp+2np+2mn)*	*|E(Cas(C)-CaR(C)[m,n,p])|-16(mp+np+mn) =220mnp-20mn-20mp-20np+4m+4n+4p-4*

Now, according to the definitions of above mention degree-based indices of a molecular graph G, we see that

$$H_k(G)=\sum_{uv\in E(G)}\left(\frac{2}{d_u+d_v}\right)^k=2^kX_{(-k)}(G)=$$

$$H_k(Cas(C)\text{-}CaR(C)[m,n,p])=2^k6^{(-k)}\times 4(55mnp-5mn-5mp-5np+m+n+p-1)+2^k5^{(-k)}\times 16(mp+np+mn)$$

Also, this implies that the harmonic index of G=*Cas(C)-CaR(C)[m,n,p]* Nanotubes Junction is equal to

$$H(G)=\sum_{e=uv\in E(G)}\frac{2}{d_u+d_v}$$

$$=\sum_{uv\in E_5}\left(\frac{2}{d_u+d_v}\right)+\sum_{uv\in E_6}\left(\frac{2}{d_u+d_v}\right)$$

$$=\frac{2|E_5|}{5}+\frac{2|E_6|}{6}$$

$$=6.4(mp+np+mn)++\frac{4}{3}\ (55mnp-5mn-5mp-5np+m+n+p-1)$$

$$\approx 73.333mnp-0.2666(mp+np+mn)+1.333(m+n+p-1).\blacksquare$$

Finally, the harmonic polynomial of G=*Cas(C)-CaR(C)[m,n,p]* Nanotubes Junction is equal to

$$H(G,x)=2\sum_{uv\in E(TUC_4)}x^{d(u)+d(v)-1}$$
$$=2\sum_{uv\in E_5}x^{d(u)+d(v)-1}+2\sum_{uv\in E_6}x^{d(u)+d(v)-1}$$
$$=8\left(2mp+2np+2mn\right)\times 2x^{3+2-1}+4\left(55mnp-5mn-5mp-5np+m+n+p-1\right)\times 2x^{3+3-1}$$
$$=32\left(mp+np+mn\right)x^4+8\left(55mnp-5mn-5mp-5np+m+n+p-1\right)x^5.$$

Also, reader can see that

$$H(G)=\int_0^1 H(G,x)dx$$
$$=\int_0^1\left(32\left(mp+np+mn\right)x^4+8\left(55mnp-5mn-5mp-5np+m+n+p-1\right)x^5\right)$$
$$=\frac{32\left(mp+np+mn\right)x^5}{5}+\frac{4\left(55mnp-5mn-5mp-5np+m+n+p-1\right)x^6}{3}\Big|_x^1$$
$$=\frac{32\left(mp+np+mn\right)}{5}+\frac{4\left(55mnp-5mn-5mp-5np+m+n+p-1\right)}{3}$$
$$=\frac{4\left(55mnp+m+n+p-1\right)}{3}-\frac{4\left(mn+mp+np\right)}{15}.$$

$\approx 73.333mnp-0.2666(mp+np+mn)+1.333(m+n+p-1).$■

5. Comparison of H(G) for G=Cas(C)-CaR(C)[m,n,p]

Table: 5

Comparison for small values of n, m,p

[n,m,p]	[1,1,1]	[2,2,2]	[3,3,3]	[4,4,4]	[5,5,5]
H(G)	74.33	102.68	148.3	198.6	255.6

For the comparison of H(G) numerically for **Cas(C)-CaR(C)[m,n,p]**, we have computed for different values of m, n, p. Now from Table 5, we can easily see that all indices are in increasing order as the values of n, m, p are increasing.

6. Concluding remarks

In this paper we have computed harmonic index for different nanotubes. Also we compute the numerical value of index for different values of m,n,p. It is easy to see that the harmonic index is in increasing order.

The Harmonic index has many interesting properties. Among these is the property of fair discriminating power, but it is not a unique molecular descriptor. Pairs of graphs with identical values of the Harmonic index and Harmonic polynomial have been detected. The Harmonic index and its polynomial were also tested in the QSPR modeling of physical properties of the alkanes and molecular graphs and trees, and extremal molecular graphs. They revealed that harmonic

index is also a useful tool in predicting the heats of vaporizations and critical temperatures of alkanes.

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List of notations

$\chi(G)$	*Connectivity Index*
$R_k(G)$	general *Randić* index
$X_\alpha(G)$	general *Connectivity Index*
$M_1(G)$	the first Zagreb index
$M_2(G)$	the second Zagreb index
$HM_1(G)$	first Hyper-Zagreb index
$HM_2(G)$	Second Hyper-Zagreb index
$H(G)$	harmonic index
$H(G,x)$	the harmonic polynomial
$H_\alpha(G)$	the general harmonic index

R E F E R E N C E S

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