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Topological Indices of H-Naphtalenic Nanosheet

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Abstract: In chemical graph theory, a single numeric number related to a chemical structure is called a topological descriptor or topological index of a graph. In this paper, we compute analytically certain topological indices for H-Naphtalenic nanosheet like Randic index, first Zagreb index, second Zagreb index, geometric arithmetic index, atom bond connectivity index, sum connectivity index and hyper-Zagreb index using edge partition technique. The first multiple Zagreb index and the second multiple Zagreb index of the nanosheet are also discussed in this paper.

Keywords: topological indices; chemical graphs; degree of vertices; nanosheet; drug designing.

1 Introduction

A topological index is a numeric quantity associated to molecular graph, which contains information about the physicochemical properties of a compound and also helps in the mathematical modeling of biological reactivity of chemicals. Topological indices remain invariant under isomorphism of graphs. Most of the topological indices depend on the degree of vertices of chemical graph or distance between the vertices. They are being widely used in QSAR/ QSPR studies in chemistry and drug designing. We refer to [1,2] for readers interested in applications of topological indices in structural activity relations and drug modeling.

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A graph with edge set *E(G)* and vertex set *V(G)* is connected, if there exist an association between any two vertices in *G*. A chemical graph is a simple graph i.e undirected, without loops and multiple edges, whose vertices represent atoms and edges represent bonds between those atoms of any chemical structure. Edges may be labeled as 1 and 2 to emphasize the single and double bonds between atoms, respectively. Number of vertices attached to a given vertex, say, *v* is called the degree of *v*, denoted by d_v and $s_u=\sum_{(vN_u)} d_v$ where $N_u=\{v\in V(G) \mid uv\in E(G)\}$. The first degree based topological index is Randic index *χ(G)* introduced by Milan Randic[3] in 1975 and is defined as:

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

The general Randic index was proposed by Bollobás and Erdös[4] in 1998, defined as

$$R_\alpha(G) = \sum_{uv\in E(G)} (d_u d_v)^\alpha \quad (2)$$

Obviously, Randic index is the particular case of $R_\alpha(G)$ when $\alpha=-\frac{1}{2}$.

The first and second Zagreb index was introduced by Gutman and Trinajstić [5] in 1972 more than thirty years ago as

$$M_1(G) = \sum_{u,v\in E(G)} [d_u + d_v] \quad (3)$$

$$M_2(G) = \sum_{u,v\in E(G)} [d_u \times d_v] \quad (4)$$

The widely used atom-bond connectivity (ABC) index is introduced by Estrada et al. [6] and is defined as

$$ABC(G) = \sum_{uv\in E(G)} \sqrt{\frac{d_u + d_v - 2}{d_u d_v}} \quad (5)$$

Sum connectivity index(SCI) was introduced by Zhou and Trinajstić [7] as

$$SCI(G) = \sum_{uv\in E(G)} \frac{1}{\sqrt{d_u + d_v}} \quad (6)$$

The Geometric-arithmetic index, GA(G) index of a graph G was introduced by Vukičević and Furtula [8] given by the formula:

$$\mathrm{GA(G)} = \sum_{uv \in E(G)} \frac{2\sqrt{d_u d_v}}{d_u + d_v} \quad (7)$$

Shirdel et al. [9] in 2013 introduced a new degree based Zagreb index named hyper-Zagreb index defined as

$$\mathrm{HM}(G) = \sum_{\mathrm{u,v \in E(G)}} [d_u + d_v]^2 \quad (8)$$

The first and second multiple Zagreb index was introduced by Ghorbani et al. [10] in 2012 as

$$PM_1(G) = \prod_{uv \in E(G)} [d_u + d_v] \quad (9)$$

$$PM_2(G) = \prod_{uv \in E(G)} [d_u \times d_v] \quad (10)$$

In the paper, we computed the degree based topological indices, defined above, for H-Naphtalenic nanotube. Exact formulas for these indices are derived analytically.

2 Methods

The structure of a carbon nanotube is formed by a layer of carbon atoms that are bonded together in a hexagonal mesh. Carbon nanotubes (CNTs) are peri-condensed Benzenoids, which are long thin cylinders of carbon, were discovered in 1991 by Sumio lijima [11]. Nanosheets are two-dimensional lattice of carbon nanotubes whose thickness ranges from 1-100 nm

A H-Naphtalenic Nanosheet is made by alternating hexagons C_6, squares C_4 and octagons C_8 as shown in figure1. The number of vertices in H-Naphtalenic Nanosheet $H[m,n]$ is $10nm$, here m denotes the number of paired hexagons in each alternant row with C_4 cycle and n denotes the number of rows containing C_4.

We can see from definitions of degree based topological indices that the indices depend upon degrees of end vertices of edges. We partition the edges according to the degrees of adjacent vertices. All vertices of H-Naphtalenic nanotube has degrees either 2 or 3. So, we have three different types of edges, we denote the edges whose end vertices have degrees 2,2 by $E_{(2,2)}$. Second types of edges have end vertices of degree 2,3 denoted by $E_{(2,3)}$ and the third type of edges have end vertices of degree 3,3 denoted by $E_{(3,3)}$. Total number of edges of type is $2n$+4, number of edges of type $E_{(2,3)}$ are 4(2m+n-2) and number of edges of type $E_{(3,3)}$ are m(15n-14)-4(n-1). This edge partitioning is summarized in the table given below $E_{(2,2)}$.

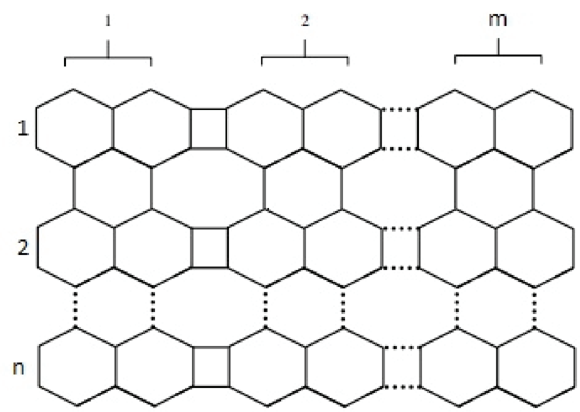

Figure1: Graph of H-Naphtalenic nanosheet H[m,n].

Table 1: Edge partition of nanosheet H[m,n] based on the degree of end vertices of each edges.

Type of edges	$E_{(2,2)}$	$E_{(2,3)}$	$E_{(3,3)}$
(d_u,d_v) $uv \in E(G)$	(2,2)	(2,3)	(3,3)
Number of edge	(2n+4)	4(2m+n-2)	m(15n-14)-4(n-1)

Ethical approval: The conducted research is not related to either human or animal use.

3 Results and Discussion

Theorem 1: Consider the H-Naphtalenic nanotube H[m,n], then its Randic index is given as**:**

$$R_\alpha(H[m,n] = \begin{cases} 45mn+(8\sqrt{6}-42)m+(4\sqrt{6}-8)n-(8\sqrt{6}-12) & for\ \alpha=\frac{1}{2} \\ 5mn+m\left(\frac{24-14\sqrt{6}}{3\sqrt{6}}\right)+n\left(\frac{12-\sqrt{6}}{3\sqrt{6}}\right)+\left(\frac{10\sqrt{6}-12}{3\sqrt{6}}\right) & for\ \alpha=-\frac{1}{2} \end{cases}$$

Proof. Using the edge partition in Table1, we compute the general Randic index of H-Naphtalenic nanotube H[m,n] as defined in equation (2) :

$$R_{\frac{1}{2}}(H[m,n]) = \sum_{uv \in E(G)} \sqrt{d_u d_v}$$

$$= \sum_{uv \in E_{(2,2)}} \sqrt{d_u d_v} + \sum_{uv \in E_{(2,3)}} \sqrt{d_u d_v} + \sum_{uv \in E_{(3,3)}} \sqrt{d_u d_v}$$

Substituting the values from table1, we get:

$$R_{\frac{1}{2}}(H[m,n]) = (2n+4)\sqrt{2 \times 2} + 4(2m+n-2)\sqrt{2 \times 3} + (m(15n-14) - 4(n - 1))\sqrt{3 \times 3}$$

After simplification, we get

$$R_{\frac{1}{2}}(H[m,n]) = 45mn + (8\sqrt{6}-42)m + (4\sqrt{6}-8)n - (8\sqrt{6}-12)$$

Now we find the general Randic index for $\alpha = -\frac{1}{2}$

$$R_{-1/2}(H[m,n]) = \sum_{uv\in E(G)} \frac{1}{\sqrt{d_u d_v}}$$

This implies that

$$R_{-1/2}(H[m,n]) = (2n+4)\frac{1}{\sqrt{2\times 2}} + 4(2m+n-2)\frac{1}{\sqrt{2\times 3}} + \\ + ((15mn-14m)-4(n-1))\frac{1}{\sqrt{3\times 3}}$$

After simplification, we get

$$R_{-\frac{1}{2}}(H[m,n]) = 5mn + m\left(\frac{24-14\sqrt{6}}{3\sqrt{6}}\right) + n\left(\frac{12-\sqrt{6}}{3\sqrt{6}}\right) + \left(\frac{10\sqrt{6}-12}{3\sqrt{6}}\right).$$

Theorem 2: Consider the H-Naphtalenic nanotube H[m,n], then its first Zagreb index is equal to

$$M_1(H[m,n]) = 90mn - 44m + 4n.$$

Proof. We compute the first Zagreb index of H[m,n] as defined in equation (3), by using the edge partition based on the degree of end vertices of each edge in above table.

$$M_1(H[m,n]) = \sum_{uv\in E(G)} [d_u + d_v]$$

$$= \sum_{uv\in E_{(2,2)}}[d_u + d_v] + \sum_{uv\in E_{(2,3)}}[d_u + d_v] + \sum_{uv\in E_{(3,3)}}[d_u + d_v]$$

This implies that

$$M_1(H[m,n]) = (2n+4)(2+2) + 4(2m+n-2)(2+3) + \\ + (15mn-14m-4n+4)(3+3)$$

Simplifying, we get

$$M_1(H[m,n]) = 90mn - 44m + 4n.$$

Theorem 3: Consider the H-Naphtalenic nanotube H[m,n], then its second Zagreb index is equal to:

$$M_2(H[m,n]) = 135mn - 78m - 4n + 4.$$

Proof: We compute the second Zagreb index of H-Naphtalenic nanotube H[m,n] by using equation (4):

$$M_2(H[m,n]) = \sum_{uv\in E(G)} [d_u \times d_v]$$

$$= \sum_{uv\in E_{(2,2)}}[d_u \times d_v] + \sum_{uv\in E_{(2,3)}}[d_u \times d_v] + \sum_{uv\in E_{(3,3)}}[d_u \times d_v]$$

This implies that

$$M_2(H[m,n]) = (2n+4)(2\times 2) + 4(2m+n-2)(2\times 3) + \\ + (15mn-14m-4n+4)(3\times 3)$$

After an easy simplification, we get

$$M_2(H[m,n]) = 135mn - 78m - 4n + 4.$$

Theorem 4: The ABC index of H-Naphtalenic nanotube H[m,n]is given by

$$ABC(H[m,n]) = 10mn + m\left(\frac{12\sqrt{2}-28}{3}\right) + n\left(\frac{9\sqrt{2}-8}{3}\right) + \left(\frac{8-6\sqrt{2}}{3}\right).$$

Proof: We compute the Atom Bond Connectivity index ABC of H-Naphtalenic nanotube H[m,n] using equation (5) as

$$ABC(H[m,n]) = \sum_{uv\in E(G)} \sqrt{\frac{d_u+d_v-2}{d_u d_v}}$$

$$= \sum_{uv\in E_{(2,2)}} \sqrt{\frac{d_u+d_v-2}{d_u d_v}} + \sum_{uv\in E_{(2,3)}} \sqrt{\frac{d_u+d_v-2}{d_u d_v}} + \sum_{uv\in E_{(3,3)}} \sqrt{\frac{d_u+d_v-2}{d_u d_v}}$$

Using table 1 we have

$$ABC(H[m,n]) = (2n+4)\sqrt{\frac{2+2-2}{2\times 2}} + 4(2m+n-2)\sqrt{\frac{2+3-2}{2\times 3}} + \\ + (m(15n-14) - 4(n-1))\sqrt{\frac{3+3-2}{3\times 3}}.$$

After simplification, we get

$$ABC(H[m,n]) = 10mn + m\left(\frac{12\sqrt{2}-28}{3}\right) + n\left(\frac{9\sqrt{2}-8}{3}\right) + \left(\frac{8-6\sqrt{2}}{3}\right).$$

Theorem 5: The sum connectivity index SCI of H-Naphtalenic nanotube H[m,n] is

$$SCI(H[m,n]) = \frac{15}{\sqrt{6}}mn + m\left(\frac{8\sqrt{6}-14\sqrt{5}}{\sqrt{30}}\right) + n\left(\frac{\sqrt{30}+4\sqrt{6}-4\sqrt{5}}{\sqrt{30}}\right) + \\ + \left(\frac{2\sqrt{30}-8\sqrt{6}+4\sqrt{5}}{\sqrt{30}}\right).$$

Proof: We compute the sum connectivity index SCI of H-Naphtalenic nanotube H[m,n] using the definition in equation (6),

$$SCI(H[m,n]) = \sum_{uv\in E(G)} \frac{1}{\sqrt{d_u + d_v}}$$

$$= \sum_{uv\in E_{(2,2)}} \frac{1}{\sqrt{d_u+d_v}} + \sum_{uv\in E_{(2,3)}} \frac{1}{\sqrt{d_u+d_v}} + \sum_{uv\in E_{(3,3)}} \frac{1}{\sqrt{d_u+d_v}}$$

Using table 1, we get

$$SCI(H[m,n] = (2n+4)\frac{1}{\sqrt{2+2}} + 4(2m+n-2)\frac{1}{\sqrt{2+3}} + \\ + ((15mn-14m)-4(n-1))\frac{1}{\sqrt{3+3}},$$

which is simplified to

$$\mathrm{SCI}(H[m,n]) = \frac{15}{\sqrt{6}}mn + m\left(\frac{8\sqrt{6}-14\sqrt{5}}{\sqrt{30}}\right) + n\left(\frac{\sqrt{30}+4\sqrt{6}-4\sqrt{5}}{\sqrt{30}}\right) + + \left(\frac{2\sqrt{30}-8\sqrt{6}+4\sqrt{5}}{\sqrt{30}}\right).$$

Theorem 6: Consider the H-Naphtalenic nanotube H[m,n], then its geometric-arithmetic index is given as

$$\mathrm{GA}(H[m,n]) = 15mn + m\left(\frac{16\sqrt{6}-70}{5}\right) + n\left(\frac{8\sqrt{6}-10}{5}\right) + \left(\frac{40-16\sqrt{6}}{5}\right).$$

Proof: We compute the geometric-arithmetic index of H-Naphtalenic nanotube H[m,n]as follows:

$$\mathrm{GA}(\mathrm{H}[\mathrm{m},\mathrm{n}]) = \sum_{uv\in E(G)} \frac{2\sqrt{d_u d_v}}{d_u + d_v}$$

$$= \sum_{uv\in E_{(2,2)}} \frac{2\sqrt{d_u d_v}}{d_u + d_v} + \sum_{uv\in E_{(3,3)}} \frac{2\sqrt{d_u d_v}}{d_u + d_v} + \sum_{uv\in E_{(3,3)}} \frac{2\sqrt{d_u d_v}}{d_u + d_v}$$

Using the edge partition given in table 1, we get

$$\mathrm{GA}(\mathrm{H}[\mathrm{m},\mathrm{n}]) = (2n+4)\frac{2\sqrt{2\times 2}}{2+2} + 4(2m+n-2)\frac{2\sqrt{2\times 3}}{2+3} + + ((15mn-14m)-4(n-1))\frac{2\sqrt{3\times 3}}{3+3}.$$

After simplification, we get

$$\mathrm{GA}(\mathrm{H}[\mathrm{m},\mathrm{n}]) = 15mn + m\left(\frac{16\sqrt{6}-70}{5}\right) + n\left(\frac{8\sqrt{6}-10}{5}\right) + \left(\frac{40-16\sqrt{6}}{5}\right).$$

Theorem 7: Consider the H-Naphtalenic nanotube H[m,n], then its hyper-Zagreb index is

$$HM(H[m,n]) = 540mn - 304m - 122n - 280.$$

Proof: Using equation (8), hyper-Zagreb index of H-Naphtalenic nanotube H[m,n] is

$$HM(H[m,n]) = \sum_{uv\in E(G)} [d_u + d_v]^2$$

$$= \sum_{uv\in E_{(2,2)}} [d_u + d_v]^2 + \sum_{uv\in E_{(2,3)}} [d_u + d_v]^2 + \sum_{uv\in E_{(3,3)}} [d_u + d_v]^2$$

Table 1 implies

$$HM(H[m,n]) = (2n+4)(2+2)^2 + 4(2m+n-2)(2+ + 3)^2 + (15mn - 14m - 4n + 4)(3+3)^2.$$

Simplifying, we get

$$HM(H[m,n]) = 540mn - 304m - 122n - 280.$$

Theorem 8: Consider the H-Naphtalenic nanotube H[m,n], then its first multiple Zagreb index is equal to:

$$PM_1(H[m,n]) = (4)^{(2n+4)} \times (5)^{4(2m+n-2)} \times \times (6)^{(15mn-14m-4n+4)}.$$

Proof: Using the definition of first multiple Zagreb index of H-Naphtalenic nanotube H[m,n] from equation (9)

$$PM_1(H[m,n]) = \prod_{uv\in E(G)} [d_u + d_v]$$

$$PM_1(H[m,n]) = \prod_{uv\in E_{(2,2)}} [d_u + d_v] \times \prod_{uv\in E_{(2,3)}} [d_u + d_v] \times \prod_{uv\in E_{(3,3)}} [d_u + d_v]$$

This implies that

$$PM_1(H[m,n]) = (2+2)^{(2n+4)} \times (2+3)^{4(2m+n-2)} \times \times (3+3)^{(15mn-14m-4n+4)}$$

After an easy simplification, we get

$$PM_1(H[m,n]) = (4)^{(2n+4)} \times (5)^{4(2m+n-2)} \times \times (6)^{(15mn-14m-4n+4)}.$$

Theorem 9: Consider the H-Naphtalenic nanotube H[m,n], then its second multiple Zagreb index is equal to:

$$PM_2(H[m,n]) = (4)^{(2n+4)} \times (6)^{4(2m+n-2)} \times \times (9)^{(15mn-14m-4n+4)}.$$

Proof: We compute the second multiple Zagreb index of H-Naphtalenic nanotube H[m,n] defined in equation (10) as:

$$PM_2(H[m,n]) = \prod_{uv\in E(G)} [d_u \times d_v]$$

Which can be split as

$$PM_2(H[m,n]) = \prod_{uv\in E_{(2,2)}} [d_u \times d_v] \times \prod_{uv\in E_{(2,3)}} [d_u \times d_v] \times \times \prod_{uv\in E_{(3,3)})} [d_u \times d_v]$$

This implies that

$$PM_2(H[m,n]) = (2\times 2)^{(2n+4)} \times (2\times 3)^{4(2m+n-2)} \times \times (3\times 3)^{(15mn-14m-4n+4)}$$

After an easy simplification, we get

$$PM_2(H[m,n]) = (4)^{(2n+4)} \times (6)^{4(2m+n-2)} \times \times (9)^{(15mn-14m-4n+4)}.$$

Topological indices provide a way to quantify the information from chemical graphs. These indices encode numerical form of basic properties of molecules and these can be used in QSAR modeling of the nanotube, as the indices are correlated to physio-chemical properties of the nanotube like boiling point, heat capacity, melting point, chemical reactivity, stability, enthalpy of formation, chirality, molar refraction, and many others.

4 Conclusion

In this paper, we derived analytically the well-known degree depending topological descriptors of H-Naphtalenic nanosheet like Randic index, different variants of Zagreb indices, atom bond connectivity index, Geometric Arithmetic index, sum connectivity index and gave closed formulae for these descriptors. It can help a lot to find a deep insight in the topological structure of nanotubes and can predict their reactivity with other compounds.

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