Annals of R.S.C.B., ISSN:1583-6258, Vol. 25, Issue 6, 2021, Pages. 3036 - 3044
Received 25 April 2021; Accepted 08 May 2021.

Computation of Entire Zagreb Index Based on Several Nanotubes

N. Parvathi [1], S.RajeswariSaminathan[2]

[1,2] Department of Mathematics, College of Engineering and Technology,

SRMIST, Kattankulathur, Chennai – 603203, India.

Corresponding author: parvathn@srmist.edu.in

Abstract:

A topological index is a molecular descriptor. From this index, it is possible to search mathematical values and further investigate from physicochemical properties of a molecule. There are different types of these indices like based on degrees, distance and counting related topological indices. Carbon nanotubes (CNTs) are types of nanostructures having a cylindrical shape. We also compute First Zagreb index and Second Zagreb index of nanotubes.We determine Hyper Zagreb index, First and Second Zagreb polynomial, and Sum-Connectivity index of carbon nanotubes.

Keywords:

Topological index, carbon nanotubes, Zagreb index, Hyper Zagreb index, Augmented Zagreb index, Zagreb polynomial, Sum-Connectivity index.

Introduction:

A topological index, also known as a connectivity index, is a type of molecular descriptor calculated based on the molecular graph of a chemical compound in the fields of chemical graph theory, molecular, topology, and mathematical chemistry. Topological indices are graph invariants that are used to establish Quantitative Structure-Activity Relationships (QSAR)[13]. In this situation, thevertices and edges of a chemical graph correspond to the atoms and bonds, respectively[2]. These indices can be thought of as molecular structure descriptors because they represent the degree of branching of the molecular carbon-atom skeleton.

The use of matter on an atomic, molecular, and supra-molecular scale for industrial purposes is known as "nanotechnology". Nanotechnology is the analysis of nanostructures with sizes ranging from 1 to 100 nanometers[15]. Richard Feynman, a physicist, is known as the "Father of Nanotechnology." Many new materials and devices with a broad range of applications in medicine, electronics, and computing are being developed with the aid of nanotechnology.

Carbon Nanotubes (CNTs) are a form of nanostructure that is made up of carbon allotropes and has a cylindrical shape. SumioIijima was the first to implement it in 1991[15]. Fullerence materials, such as carbon nanotubes (CNTs), have applications in electronics, optics, materials science, and architecture. CNT is made up of a layer of carbon atoms that are bound together in a hexagonal (honeycomb) pattern.Graphene is a one-atom thick film of carbon that is wrapped around a cylinder and bonded together to form a CNT. Single walled carbon nanotubes (SWCNT) and multi walled carbon nanotubes (MWCNT) are two types of carbon nanotubes. The diameter (SWCNT) are 0.8 to 2nm and (MWCNT) are 5nm to 20 nm respectively, form a rope like structure. In addition to the two different possible structures there are three different possible types of (CNTs). These three types of CNTs are Armchair, Zig-Zag and Chiral.

A Lattice is a periodic sequence of points in which each point is indistinguishable from every other point and has the same surroundings. The two dimensional lattice graph also known as grid graph is the cartesian product of path graph of m and n vertices named as 2-D lattice

"ID(G) = $\sum_{i=1}^{n} \frac{1}{d_i}$ is the inverse degree of a graph G with no isolated vertices.

Annals of R.S.C.B., ISSN:1583-6258, Vol. 25, Issue 6, 2021, Pages. 3036 - 3044
Received 25 April 2021; Accepted 08 May 2021.

Where d_i is the vertex's degree $v_i \in V(G)$. The inverse degree first drew attention thanks to conjectures made by the Graffiti computer programme [8]. In the 1980s, Narumi and Katayama considered the product

$$N K = N K(G) = \prod_{i=1}^{n} d_i$$

And it named as "simple topological index"[9]. In more recent works on this graph invariant [7] the name "Narumi- Katayama index" has been used. Some properties of the Narumi-Katayama index wereestablished in [10]".

An important topological index introduced more 30 years ago by I. Gutman and N. Trinajistic is the first and second Zagreb indices($M_1(G)$ and $M_2(G)$)[3].

The Hyper Zagreb index ($HM(G)$) being introduced by Shirdel et al. It is a distance based Zagreb index in 1913.[5] .

The Augmented Zagreb index (AZI (G)) was introduced by Furtula et al.[5].

The first and second Zagreb polynomial($Z_{g_1}(G,x)$ and $Z_{g_2}(G,x)$) was introduced by Gutman et al.[3]

The Sum Connectivity Index ($SCI(G)$)being introduced by Zhou and Trinajstic[7]

Let G = (V, E) be a simple graph with n vertices and m edges and a vertex set V (G) = $v_1, v_2, \ldots v_n$The number of edges in the shortest path connecting a and b, denoted by d (a, b), is defined as the distance between two vertices, say a and b of G. [1, 2].

PRELIMINARIES:

Definition1:

"Let G be a graph. The First and Second Zagreb index of G is defined as

$$M_1(G) = \sum_{e=ab\in E(G)} (d_a + d_b)$$

$$M_2(G) = \sum_{e=ab\in E(G)} (d_a \,.\, d_b)$$

Definition 2:

Let G be a graph. The Hyper-zagreb index is defined as

$$HM(G) = \sum_{e=ab\in E(G)} (d_a + d_b)^2$$

Definition 3:

For a graph G the augmented Zagreb index is defined as

$$AZI(G) = \sum_{e=ab\in E(G)} \left(\frac{d_a . d_b}{d_a + d_b - 2}\right)^3$$

Definition 4:

Let G be a graph. The first and second Zagreb polynomial is defined as

$$Zg_1(G, x) = \sum_{e=ab\in E(G)} x^{(d_a + d_b)}$$

$$Zg_2(G, x) = \sum_{e=ab\in E(G)} x^{(d_a . d_b)}$$

Definition 5:

Let G be a graph. The sum-connectivity index is defined as"

Annals of R.S.C.B., ISSN:1583-6258, Vol. 25, Issue 6, 2021, Pages. 3036 - 3044
Received 25 April 2021; Accepted 08 May 2021.

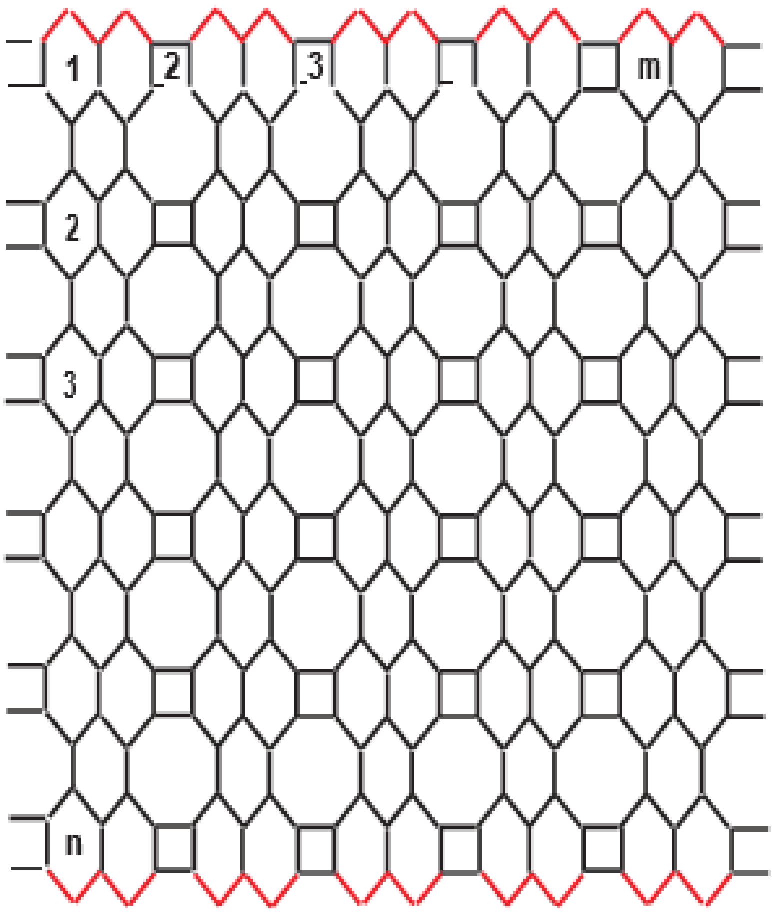
$$\text{SCI(G)} = \sum_{e=ab\in E(G)} \frac{1}{\sqrt{d_a+d_b}}$$

2.MAIN RESULTS:

The First and Second Zagreb index, Hyper-zagreb index, Augmented Zagreb index, First and Second Zagreb polynomials, and Sum-Connectivity index of H-Naphthalenic nanotubes and TUC_4(p, q) nanotubes are all investigated in this paper. These topological indices for H-Naphthalenic nanotubes and TUC_4 (p, q) nanotubes are computed in the following section.

2.1 H- Naphthalenic Nanotubes Results:

The entire lattice in this section is a plane tiling of C_4, C_6, and C_8, which can be used to cover a cylinder or a torus. As shown in figure 1, the H- Naphthalenic nanotube is denoted by NPHX [p, q], where p denotes the number of pairs of hexagons in a row and q denotes the number of hexagons in a column.



In fig.1. A 2D-lattice of H-Naphtalenic nanotube.

The edges ab with d_a= 2 and d_b = 3 are shown in red, while the edges ab with $d_a = d_b = 3$ are shown in black.

Lemma 1:

Let NPHX [p, q] represent the graph of H- Naphthalenic nanotubes with (p,q> 1). Then V (NPHX [p, q]) = 10pq is its vertex set.

Annals of R.S.C.B., ISSN:1583-6258, Vol. 25, Issue 6, 2021, Pages. 3036 - 3044
Received 25 April 2021; Accepted 08 May 2021.

Lemma 2:

Consider the graph of H- Naphthalenic nanotubes (p, q > 1) then its edge set is

E (NPHX [p, q]) = 15pq – 2p

Now we can see that the two partitions of the edges in 2D- lattice from this nanotube.

i.e., $E_{2,3} = \{e = ab \in E(G) / d_a = 2, d_b = 3\}$

$E_{3,3} = \{e = ab \in E(G) / d_a = 3, d_b = 3\}$

The number of edges of the given sets are given as below

$E_{2,3}$ = 8pand $E_{3,3}$ = 15pq – 10p

Theorem 1:

Let's take a look at the graph of H-Naphtalenic nanotubes. The First and Second Zagreb indexes are then equivalent

$M_1(G)$ = 90pq – 20p

$M_2(G)$ = 135pq – 42p

Proof:

Let NPHX[p, q] be a graph. By using the edge partition of number of edges. Using lemma 2, then we compute First and Second Zagreb index

$M_1(G) = \sum_{e=ab\in E(G)}(d_a + d_b)$

This implies that

$M_1(G) = \sum_{ab\in E_{2,3}}(d_a + d_b) + \sum_{ab\in E_{3,3}}(d_a + d_b)$

= (8p) (2 + 3) + (15pq – 10p) (3 + 3)

= 40p + 90pq – 60p

$M_1(G)$ = 90pq – 20p

Also $M_2(G) = \sum_{e=ab\in E(G)}(d_a . d_b)$

$= \sum_{ab\in E_{2,3}}(d_a . d_b) + \sum_{ab\in E_{3,3}}(d_a . d_b)$

= (8p) (2.3) + (15pq – 10p) (3.3)

= 48p + 135pq – 90p

$M_2(G)$ = 135pq – 42p.

Annals of R.S.C.B., ISSN:1583-6258, Vol. 25, Issue 6, 2021, Pages. 3036 - 3044
Received 25 April 2021; Accepted 08 May 2021.

Theorem 2:

Consider the NPHX [p, q] nanotube graph. And there's the Hyper-zagreb index.

HM(G) = 540pq – 160p

Proof:

Let the graph of NPHX[p, q]. Then we calculate the Hyper-Zagreb index is

HM(G) = $\sum_{e=ab\in E(G)}(d_a + d_b)^2$

This implies that

HM(G) = $\sum_{ab\in\in E_{2,3}}(d_a + d_b)^2 + \sum_{ab\in\in E_{3,3}}(d_a + d_b)^2$

= (8p) $(2 + 3)^2$ + (15pq – 10p) $(3 + 3)^2$

= (8p) (25) + (15pq -10p) (36)

= 200p + 540pq – 360p

HM(G) = 540pq – 160p

This completes the proof.

Theorem 3:

Assume that the graph of NPHX[p, q] nanotube. Then its Augmented Zagreb index is

AZI(G) = 21, 357.3pq – 14, 174.2p

Proof:

Let the graph of NPHX[p, q]. Then we compute the Augmented Zagreb index is

AZI(G) = $\sum_{e=ab\in E(G)}\left(\frac{d_a.d_b}{d_a+d_b-2}\right)^3$

= $\sum_{ab\in E_{2,3}}\left(\frac{d_a.d_b}{d_a+d_{b-2}}\right)^3 + \sum_{ab\in E_{3,3}}\left(\frac{d_a.d_b}{d_a+d_{b-2}}\right)^3$

= (8p) $\left(\frac{2.3}{2+3-2}\right)^3$ + (15pq – 10p) $\left(\frac{3.3}{3+3-2}\right)^3$

= (8p) $(2)^3$ + (15pq – 10p) $(11.25)^3$

= (8p) (8) + (15pq – 10p) (1423.82)

AZI(G) = 21, 357.3pq – 14,174.2p.

Hence the proof.

2.2 Nanotubes Covered by C_4:

Annals of R.S.C.B., ISSN:1583-6258, Vol. 25, Issue 6, 2021, Pages. 3036 - 3044
Received 25 April 2021; Accepted 08 May 2021.

The 2D lattice of this family of nanotubes is a plane tiling of C_4 in this section. $TUC_4[p, q]$, where p is the number of squares in a row and q is the number ofsquares in a column, denotes this family of nanotubes.

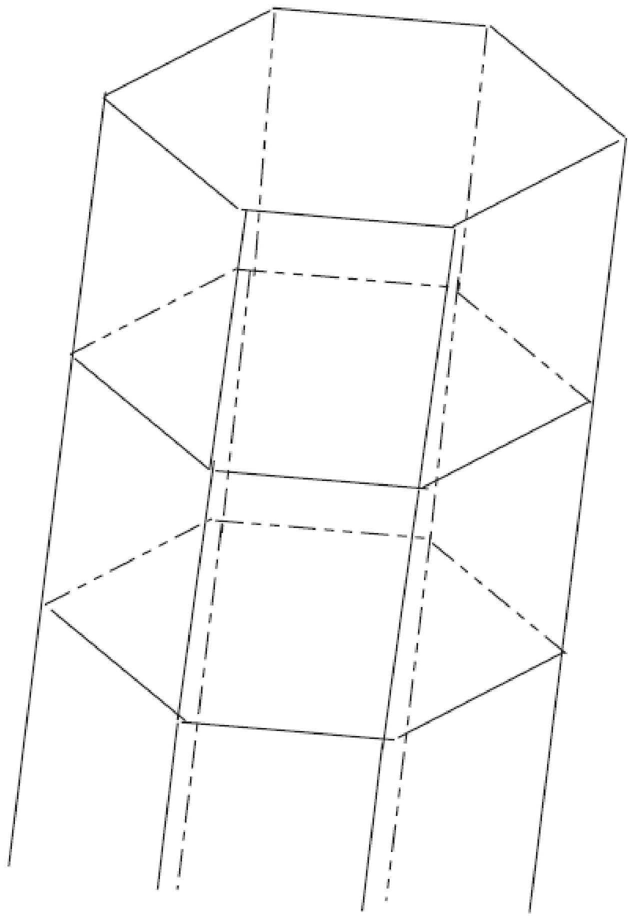


Figure 2: A C_4-coated $TUC_4[p, q]$ nanotube.

Lemma 3:

If TUC_4 [p, q] is the graph of nanotubes protected by C_4, then V (TUC_4 [p, q]) = (q + 1) (p + 1) is the number of vertices.

Lemma 4:

Consider the graph of TUC_4 [p, q] nanotubes; the edge set of this graph is E(TUC_4 [p, q]) = (2q + 1)(p + 1)

Now we can see that the partitions of the

i.e., $E_{3,3} = \{e = ab \in E(G) / d_a = 3, d_b = 3\}$

$E_{3,4} = \{e = ab \in E(G) / d_a = 3, d_b = 4\}$

$E_{4,4} = \{e = ab \in E(G) / d_a = 4, d_b = 4\}$

The number of edges of the given sets are given as follows.

$E_{3,3} = 2p + 2$

Annals of R.S.C.B., ISSN:1583-6258, Vol. 25, Issue 6, 2021, Pages. 3036 - 3044
Received 25 April 2021; Accepted 08 May 2021.

$E_{3,4} = 2P + 2$

$E_{4,4} = (p + 1)(2q – 3)$

Theorem 4:

Consider the graph of $TUC_4[p,q]$ nanotubes covered by C_4, then its First and Second Zagreb polynomial is

$$Zg_1(TUC_4[p, q], x) = (p+1)2x^6 + (p+1)2x^7 + (2pq – 3p + 2q – 3)x^8$$

$$Zg_2(TUC_4[p, q], x) = (p+1)2x^9 + (p+1)2x^{12} + (2pq – 3p + 2q - 3)x^{16}$$

Proof:

The First Zagreb polynomial is defined as

$$Zg_1(G, x) = \sum_{e=ab\in E(G)} x^{(d_a+d_b)}$$

This implies that

$$Zg_1(TUC_4[p, q], x) = \sum_{ab\in E_{3,3}} x^{(d_a+d_b)} + \sum_{ab\in E_{3,4}} x^{(d_a+d_b)} + \sum_{ab\in E_{3,4}} x^{(d_a+d_b)}$$

$$= (2p + 2)x^{3+3} + (2p + 2)x^{3+4} + (p + 1)(2q – 3)x^{4+4}$$

$$= (2p + 2)x^6 + (2p + 2)x^7 + (2pq – 3p + 2q – 3)x^8$$

The Second Zagreb polynomial is defined as

$$Zg_2(G, x) = \sum_{e=ab\in E(G)} x^{(d_a.d_b)}$$

$$Zg_2(TUC_4[p, q], x) = \sum_{ab\in E(G)} x^{(d_a.d_b)}$$

$$= \sum_{ab\in E_{3,3}} x^{(d_a.d_b)} + \sum_{ab\in E_{3,4}} x^{(d_a.d_b)} + \sum_{ab\in E_{3,4}} x^{(d_a.d_b)}$$

$$= (2p + 2)x^{3.3} + (2p + 2)x^{3.4} + (p + 1)(2q – 3)x^{4.4}$$

$$= (2p + 2)x^9 + (2p + 2)x^{12} + (p + 1)(2q – 3)x^{16}$$

$$= (2p + 2)x^9 + (2p + 2)x^{12} + (2pq – 3p + 2q – 3)x^{16}.$$

Hence the proof.

Theorem 5:

Let the graph of $TUC_4[p, q]$ nanotubes then its Sum-Connectivity index is

$$SCI(G) = \frac{2(p+1)}{3} + \frac{(p+1)}{\sqrt{3}} + \frac{(p+1)(2q-3)}{4}$$

Annals of R.S.C.B., ISSN:1583-6258, Vol. 25, Issue 6, 2021, Pages. 3036 - 3044
Received 25 April 2021; Accepted 08 May 2021.

Proof:

By the definition of Sum-Connectivity index is

$$SCI(G) = \sum_{e=ab\in E(G)} \frac{1}{\sqrt{d_a+d_b}}$$

This implies that

$$SCI(G) = \sum_{e=ab\in E(G)} \frac{1}{\sqrt{d_a+d_b}}$$

$$= \sum_{ab\in E_{3,3}} \frac{1}{\sqrt{d_a+d_b}} + \sum_{ab\in E_{3,4}} \frac{1}{\sqrt{d_a+d_b}} + + \sum_{ab\in E_{4,4}} \frac{1}{\sqrt{d_a+d_b}}$$

$$= (2p + 2)\frac{1}{\sqrt{3.3}} + (2p + 2)\frac{1}{\sqrt{3.4}} + (p + 1)(2q - 3)\frac{1}{\sqrt{4.4}}$$

$$= (2p + 2)\frac{1}{\sqrt{9}} + (2p + 2)\frac{1}{\sqrt{12}} + (p + 1)(2q - 3)\frac{1}{\sqrt{16}}$$

$$= \frac{2(p+1)}{3} + \frac{(p+1)}{\sqrt{3}} + \frac{(p+1)(2q-3)}{4}$$

Hence the proof.

Conclusion:

Certain degree-based topological indices, such as the First and Second Zagreb index, the Hyper-Zagreb index, and the Augmented Zagreb index for nanotubes protected by C_4, C_6, and C_8, are discussed in this paper. We also looked at the Sum-Connectivity index and the First and Second Zagreb polynomials. For NPHX[p,q] and TUC_4[p, q] nanotubes, we found closed formulae for these topological indices.

References:

1. J.A. Bondy, U.S.R. Murthy, Graph Theory with Applications, Macmillan Press, New York. 1976.
2. R. Todeschini, V.Consonni, Handbook of Molecular Descriptors, Wiley-VCH, Weinheim, 2000.3.
3. I. Gutman, N. Trinajstic, Graph Theory and molecular orbitals. Total π-electron energy of alternant hydrocarbons, Chem. Phys. Lett.17(1972) 535-538.
4. N. Trinajstic, Chemical graph theory, CRC Press, Boca Raton, FL(1992).
5. B. Zhou, Zagreb indices, MATCH Commun.Math.Comput. Chem.52(2004) 113-118.
6. B. Zhou, I. Gutman, Further properties of Zagreb indices, MATCH Commun. Math. Comput. Chem. 54 (2005) 233 – 239.
7. . Zhou, B.;Trinajstic,N. On general sum-connectivity index.J.Math.Chem.2010,47,210-218.Zhou, B.Trinajstic,N. On general sum-connectivity index.J.Math.Chem.2010,47,210-218.
8. Fajtlowicz S. On conjectures of graffiti II. CongrNumer, 1987, 60:189-197.
9. Narumi H, Katayama M. Simple topological index. A newly divisedinde characterizing the topological nature of structural isomers of saturated hydrocarbons. Mem FacEngin Hokkaido Univ, 1984,16: 209-214.
10. Gutman I, Ghorbani M. Some properties of the Narumi-Katyama index. Applied Math Lett, 2012, 25: 1435-1438.
11. M.V. Diudea, I. Gutman and J. Lorentz, Molecular Topology, Nova, Huntington (2001).
12. A.T. Balaban, I.Motoc, D.Bonchev, O.Mekenyan, Topological indices for structure-activity corrections, Topics Cur. Chem 114(1983) 21-55.

13. Lucic B, Nikolic S, Trinajstic N, Zhou B, Turk S I. Sum-connecctivity index. In: Gutman I, Furtula B, edg. Novel Molecluar Structure descriptors-Theory and Applications I. University of Kragujevac, Kragujevac, 2010,101-136.11.
14. B. Zhou, I. Gutman, Further properties of Zagreb indices, MATCH Commun. Math. Comput. Chem. 54 (2005) 233 – 239.
15. A. Bahramia and J. Yazdani, Digest journal of Nanomaterials and Biostructures, 3. 265 (2008).

s