Original Research Paper

Volume-8 | Issue-3 | March-2018 | PRINT ISSN No 2249-555X

Computer Science

ON THE MULTIPLICATIVE TOPOLOGICAL INDICES OF CARBON NANOCONES

N. K. Raut

Department of Physics, Sunderrao Solanke Mahavidhyalaya Majalgaon, Dist: Beed (M.S.) INDIA.

ABSTRACT Let G be a simple and connected graph with the vertex set V (G) and edge set E (G). The nanocones can be considered as the nanoscale conical carbon-based material. In carbon nanocones CNCk[n], the parameter k defines the length of inner cycle and n defines the number of layers of the graph. In this paper the multiplicative version of SK(G),SK1(G),SK2(G),Reciprocal Randic index, Reduced Reciprocal Randic index, and Root mean square index for nanocones CNC5[n] where n=1 -5,10,12 and 20 are investigated.

KEYWORDS : Topological indices, multiplicative topological indices, carbon nanocones, degree, pentagonal nanocone.

1. Introduction

Let G be a molecular graph .The vertex–set and edge-set of G denoted by V (G) and E (G) respectively. The number of vertices of G, adjacent to a given vertex v, is the degree of this vertex and will be denoted by d_v .A topological index is a number related to a molecular graph invariant automorphism of Graph. The ability of elemental carbon to form extended two dimensional sheet structures with extremely strong bond makes it a stable material to produce isolated objects .The sheets can be resealed notionally to form a cone or horn [1].Nanocones are discovered in 1994 [2].Nanocones are carbon based structures formed by introducing 60^0 inclination defects in two-dimensional graphene sheets. The graph of this molecule consists of one pentagon surrounded by layers of hexagons [3].The nanocone structure of CNC_5[1] is shown in figure (1).The vertex-degree based multiplicative topological indices for molecular graphs are studied by [4-12]. Our notations are standard and mainly taken from books of graph theory [13-14].The partitions of edges (2,2),(2,3) and (3,3) for nanocones CNC_5[n] where n=1-5,10,12 and 20 are taken from [4,15].

In carbon nanocones CNC_k[n] the parameter k defines the length of the inner cycle and n defines the number of layers of the graph. The carbon nanocones CNC_5[2], CNC_5[4] graph consists of pentagon as its core surrounded by two and four layers of hexagons respectively fig (2). The definitions for degree-based topological indices are taken from [16-20]. In this paper the multiplicative version of SK (G), SK_1(G),SK_2(G), Reciprocal Randic index, Reduced Reciprocal Randic index, and Root mean square index are defined and computed for nanocones CNC_5[n] where n=1 -5,10,12 and 20.

2. Materials and Method

A molecular graph is constructed by representing each atom of a molecule by a vertex and bonds between atoms by edges. The number of vertices of G adjacent to a given vertex v, is the degree of this vertex and will be denoted by d_v. The 2-dimensional graph of CNC_5[1] is shown in figure (1).

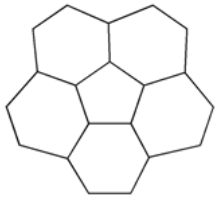

Fig.1. 2-dimensional graph of CNC_5[1].

The vertices of this graph have degree either 2 or 3.The pentagon is surrounded by 5 hexagons. The molecular graph of CNC_5[1] has 25 edges.

If u and v be vertices of any edge then there are 10 edges of degree du = dv = 3,

5 edges of type du = dv = 2, 10 edges of type du =3, dv = 2.

The SK(G),SK_1(G),SK_2(G) are defined in V.Shigehalli [21], Randic index, reciprocal Randic index, reduced reciprocal Randic index are defined in [4-12,16-20] and the root mean square index is defined in [22]. The partitions of edges (2,2),(2,3) and (3,3) for nanocones for CNC_5[n] where n= 1-5,10,12 and 20 are taken from [4,15]. The multiplicative SK (G) index is computed for CNCk[n] from molecular graph of CNC5[1] figure (1). In the molecular graph of pentagonal carbon nanocones edges with endpoints having degrees 2, 2 (E_1) are 5. This may due to pentagon is a shape with five sides and five angles. The edges with endpoints 3, 3 (E_2) and 3, 2 (E_3) are counted on molecular graphs of carbon nanocones. The graphs for CNC5[2] and CNC5[4] are shown in figure (2).The number of edges with du = dv = 2 are 5 in nanocones CNC5[n] with n=1 –5, 10, 12 and 20.

3. Results and discussion

In carbon nanocones CNCk[n] the parameter k defines the length of inner cycle and n defines the number of layers of the graph. The graphs for CNC_5[2] and CNC_5[4] are shown in figure (2).

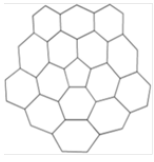

Fig.2. Molecular graphs of CNC5[2] and CNC5[4] nanocones.

From 2-dimensional graphs of these carbon nanocones the edges of degree (3, 3), (2, 2) and (3, 2) are counted [4, 15] and represented in table number (1).

Table 1. The number of edges (d_u =3, d_v =3 E_1), (d_u=2, d_v =2 E_2) and (d_u =3, d_v =2 E_3) for nanocones CNCk[n] where n= 1-5,10,12 and 20.

Carbon Nanocones	The number of edges of type d_u=3,d_v=3 (E_1)	The number of edges of type d_u=2,d_v=2 (E_2)	The number of edges of type d_u=3,d_v=2 (E_3)
CNC5[1]	10	5	10
CNC_5[2]	35	5	20
CNC_5[3]	75	5	30
CNC_5[4]	130	5	40
CNC_5[5]	200	5	50
CNC_5[10]	775	5	100
CNC_5[12]	1110	5	120
CNC_5[20]	3050	5	200

The graph of pentagonal carbon nanocone (fig.1)

CNC5 [1] has 25 edges.

If u and v are vertices of any edge then, there are 10 edges of degree d_u = d_v = 3 (E_1),

5 edges of type d_u = d_v = 2 (E2), 10 edges of type d_u= 3, d_v=2 (E_3).

The SK index of a graph G = (u, v) is defined as [21], SK (G) =

$\sum u,v \in E(G)) \sum_{u,v \in E(G)} \frac{d_u+d_v}{2}$

Where d_u and d_v are the degrees of the vertices u and v.

The multiplicative PSK (G) is defined as,

$$PSK(G) = \prod_{u,v \in E(G)} \frac{d_u + d_v}{2}$$

multiplicative SK_1 (G) index,

$$PSK_1(G) = \prod_{u,v \in E(G)} \frac{d_u \times d_v}{2}$$

multiplicative SK_2 (G) index,

$$PSK_2(G) = \prod_{u,v \in E(G)} \left(\frac{d_u + d_v}{2}\right)^2$$

multiplicative reciprocal Randic index,

$$PRRI(G) = \prod_{u,v \in E(G)} \sqrt{d_u d_v}$$

multiplicative reduced reciprocal Randic index,

$$PRRRI(G) = \prod_{u,v \in E(G)} \sqrt{(d_u - 1)(d_v - 1)}$$

multiplicative root mean square index,

$$PRMSI(G) = \prod_{u,v \in E(G)} \sqrt{(d_u^2 + d_v^2)/2}$$

Almost every topological index can be expressed in the multiplicative version. The multiplicative SK (G) for $CNC_5[1]$ computed from figure (1) as,

$$PSK(G) = \prod_{u,v \in E(G)} \frac{d_u + d_v}{2}$$

$$= \prod_{u,v \in E_1(G)} \frac{d_u + d_v}{2} \times \prod_{u,v \in E_2(G)} \frac{d_u + d_v}{2} \times \prod_{u,v \in E_3(G)} \frac{d_u + d_v}{2}$$

$$= \left(\frac{d_u + d_v}{2}\right)^{E_1} \times \left(\frac{d_u + d_v}{2}\right)^{E_2} \times \left(\frac{d_u + d_v}{2}\right)^{E_3}$$

$$= \left(\frac{3+3}{2}\right)^{10} \left(\frac{2+2}{2}\right)^{5} \left(\frac{3+2}{2}\right)^{10}$$

$$= 7500$$

These definitions of degree-based topological indices [4-12, 16-22] are used for computing the TI's of CNCk[n] where n=1- 5, 10, 12 and 20 and the values of TI's tabled in table 2.

The TI's follows the order PRRRI (G) <PRMSI (G) <PRRI (G) < PSK (G) < PSK_1 (G) < PSK_2(G) for $CNC_5[1]$.

and the order PRRRI(G) <PRMSI(G) <PRRI(G)< PSK(G) <PSK1(G) <PSK2(G) in CNC5[20].

Table 2. The multiplicative topological indices of CNCk[n]where n=1-5, 10, 12 and 20 carbon nanocones.

Topological indices Carbon Nanocones	PSK(G)	PSK_1(G)	PSK_2(G)	PRRI(G)	PRRRI (G)	PRMSI (G)
$CNC_5[1]$	7500	13500	112500	7348.45	1414.2	3354
$CNC_5[2]$	52500	94500	787500	51439.15	9899.4	23478
$CNC_5[3]$	168750	303750	2531250	165340.125	31819.5	75465
$CNC_5[4]$	390000	702000	5850000	382119.4	73538.4	174408
$CNC_5[5]$	750000	1350000	1125000	734845	141420	335400
$CNC_5[10]$	5812a500	10462500	87187500	5695048.75	1096005	2599350
$CNC_5[12]$	9990000	17982000	14985000	*9788135.4*	1883714.4	4467528
$CNC_5[20]$	45750000	82350000	68625000	44825545	8626620	20459400

4. Conclusion

The multiplicative version of SK(G),SK1(G),SK2(G), Reciprocal Randic index, Reduced Reciprocal Randic index and Root mean square index are defined and computed for molecular graphs of CNC5[n] where n=1-5,10,12 and 20 nanocones. The values of multiplicative version of SK(G),SK1(G),SK2(G), Reciprocal Randic index, Reduced Reciprocal Randic index, and Root mean square index increase with n as the layer of hexagons increase with n surrounding the pentagon core in nanocones CNCk[n].The PSK2(G) has highest values for CNC5[1] and CNC5[20] among the CNC_k[n] studied.

REFERENCES

[1] S.Iijima,M.Yudusaka,R.Yamada et al, Nanoagreegates of single-walled graphic carbon nano-horns,Chem.Phys.Lett.1999,309(3-4):165-170.
[2] Krishnan, Ebbesen et al , Nature ,388,(2001)241.
[3] T.Doslic, The hyper-Wiener index of one-pentagonal carbon nanocone, Current Nanoscience, 2013, 9, 557-560.
[4] O.K.Kurucu, E.Asian, Atom bond connectivity index of Carbon nanocones and An Algorithm, Applied Mathematics and Physics, 2015, Vol.3, No.1, 6-9.
[5] M.R.Farahani, M.K.Jamil,M.R.Rajesh Kanna,R.Pradeep Kumar, The multiplicative Zagreb Eccentricity index of Polycyclic Aromatic Hydrocarbon(PAHk),International Journal of Scientific and Engineering Research ,Vol.7,Issue 2,February 2016.
[6] W.Gao, M.R.Farahani, M.R.R.Kanna, The multiplicative Zagreb indices of Nanostructures and Chains, Open Journal of Discrete Mathematics, 2016, 82-88.
[7] N.K.Raut, The Zagreb group indices and polynomials, International Journal of Modern Engineering Research, Vol.6, Issue 10, October-2016, 84-87.
[8] M.Bhanumathi, K. Easu Julia-Rani, On multiplicative Harmonic Index, Multiplicative ISI index and Multiplicative F index of TUC4C8[m, n] and TUC4[m, n] nanotubes, International Journal on Recent Trends in Life Sciences and Mathematics ,Vol.4,Issue 9,Sept 2017, pp.01-08.
[9] V.R.Kulli, A new multiplicative Arithmetic-Geometric index, International Journal of Fuzzy Mathematical Archive, Vol.12, No.2, 2017, 49-53.
[10] V.R.Kulli, Multiplicative connectivity indices of TUC4C8[m, n] and TUC4[m, n] nanotubes, Journal of Computer and Mathematical Sciences, Vol.7(11),599-605,November-2016..
[11] N.K.Raut, G.K.Sanap, V.P.Sangle, On the Topological indices of nanocones, Recent advances in Mathematics, National Conference,21-23 January-2016.
[12] I.Gutman, Degree-based topological indices, Croat. Chem. Acta 86(4) (2013) 351-361.
[13] R.Diestel, Graph theory, Electronic edition, Springer-Verlog, New York, 1997-2000.
[14] D.B.West, Introduction to graph theory, second edition, PHI, Learning Private Ltd. New Delhi, 2009, 67-80.
[15] https://www.google.co.in./search?q=carbon+nanocones.
[16] A.Ali,A.A.Bhatti and Z.Raza,Further inequalities between vertex degree-based, topological indices, arXiv,1401-7511v1(math CO.)29 Jan 2014.
[17] M.J.Nikmeher, N.Soleimani and M.Veylaki, Proceeding of IAM V.3, N.1, 2014, pp.89-97.
[18] I.Gutman and J.Tosovic, Testing the quality of molecular structure descriptors, vertex-degree based topological indices ,J.Serb.Chem.Soc.78(6)805-810(2013).
[19] T.Doslic, Vertex-weighted, Wiener polynomials for composite graphs, ASR Mathematica Contemporanea 1(2008)66-80.
[20] M.R.Farahani, International Journal of Engineering and Technology Research Vol.3, No 1, Feb-2015,pp.01-06.
[21] V.Shigehalli, R.Kanabur, Computing degree-based topological indices of Polyhex nanotubes, Journal of Mathematical Nanosciences 6(1-2)2016, 47-55.
[22] A.Anuradha, V.Kaladevi, A.Abinayaa, International Journal in Physical and Applied Sciences, Vol.4,issue8,August-2017,pp.17-25