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Study of Degree Based Topological Indices of Carbon Nanocones

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ABSTRACT: Let G be a simple and connected graph with n vertices and m edges. The degree d_u of a vertex u ∈V (G) is the number of vertices of G adjacent to u. The nanocones (CNCs) can be considered as the nanoscale conical carbon-based material. In carbon nanocones $CNC_k[n]$, the parameter k defines the length of inner cycle and n defines the number of layers of the graph. In this paper degree based topological indices for carbon nanocones $CNC_3[2]$, $CNC_4[2]$,$CNC_5[2]$,$CNC_6[2]$ and $CNC_7[2]$ and some inequalities are investigated.

KEYWORDS: Topological indices, carbon nanocones, inequality, one pentagonal nanocone, one heptagonal nanocone.

I. INTRODUCTION

A molecular graph is a simple graph such that its vertices correspond to the atoms and the edges to the bonds. 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 disinclination defects in two-dimensional graphenes sheets [3] (fig.1).

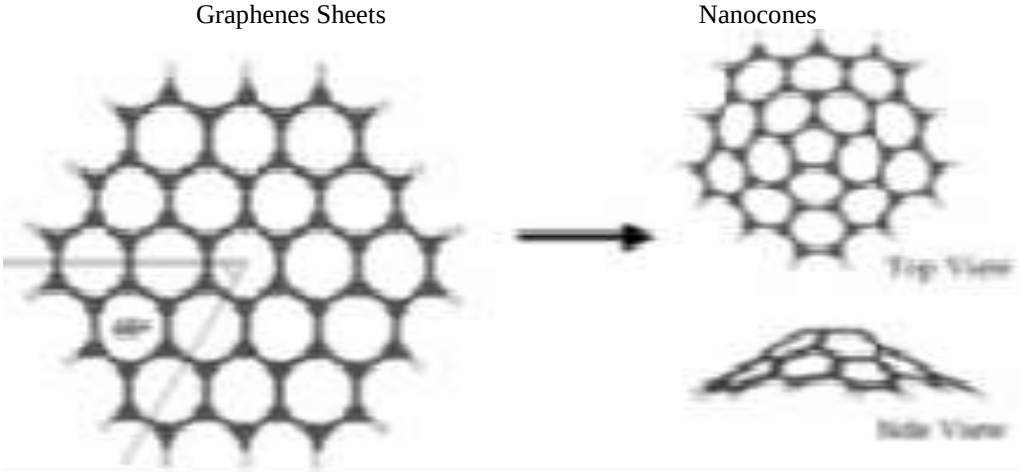

Figure (1): 2-Dimensional sheet of graphene.

Folding graphene sheets have five possible closed distinct CNC structures and the apex angles of a cone can be calculated as

Where θ is the disinclination angle in degrees can be taken as 60^0,120^0,180^0,240^0 and 360^0 [4].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 nanocones $CNC_3[2]$, $CNC_4[2]$,$CNC_5[2]$, consists of triangle ,square and pentagon as its core surrounded by two layers of hexagons respectively fig.(2). The 2-dimensional of graphof $CNC_7[1]$ withheptagon as core is also shown in fig.2. The definitions for degree based topological indices are

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taken from [5-10].In this paper our notations is standard and mainly taken from standard books of graph theory [11-16]. In this paper vertex degree-based topological indices:Randic index R(G), Reciprocal Randics index RR(G), general Randic indices (with = -3,-2,2,3) where is adjustable parameter, Zagreb indices(first $M_1(G)$, second $M_2(G)$ and third $M_3(G)$),modified second Zagreb index$M_2^*(G)$,secondmultiplicative Zagreb index,,modified first Zagreb indexΠ_1^*, reduced second Zagreb index$R(M_2)$, Augmented Zagreb index ABC(G),hyper Zagreb index HM(G),Atom-bond connectivity index ABC(G),Harmonic index H(G),Sum-connectivity index SCI(G),Sum-connectivity indices(with = -3,-2,2,3 where is adjustable parameter),Inverse indeg index IN(G), Geometric-Arithmetic index GA(G) and some inequalities are studied in $CNC_3[2]$, $CNC_4[2]$,$CNC_5[2]$,$CNC_6[2]$ and $CNC_7[2]$ nanocones.

II. RESULTS AND DISCUSSION

Degree-based Topological indices

In carbon nanocones $CNC_k[n]$, the parameter k defines the length of inner cycle and n defines the number of layers of the graph. The 2-dimensional graphs for $CNC_3[2]$,$CNC_4[2]$ and $CNC_5[2]$ and $CNC_7[1]$ are shown in figure (2).

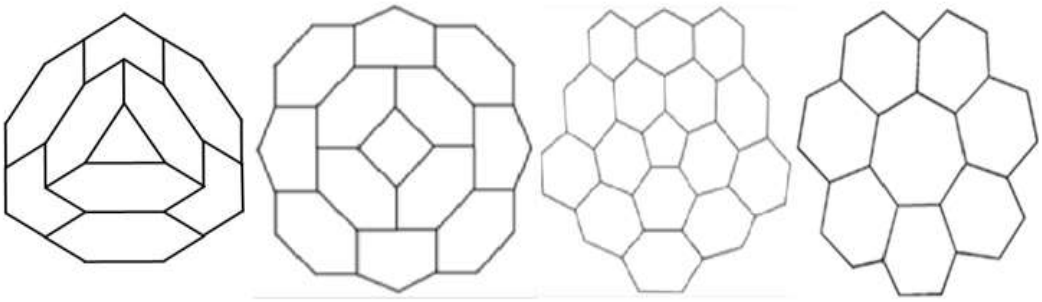

Figure (2): 2-Dimensional graphs of $CNC_3[2]$,$CNC_4[2]$,$CNC_5[2]$ and $CNC_7[1]$ nanocones

From 2-dimensional graphs of These nanocones the edges of degree (3, 3), (2, 2) and (3, 2) are counted and given in table (1).

Table no (1): The number of edges (d_u =3, d_v =3), (d_u =2, d_v = 2) and (d_u =3, d_v =2) for nanocones $CNC_k[2]$.

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)
$CNC_3[2]$	21	3	12
$CNC_4[2]$	29	4	16
$CNC_5[2]$	35	5	20
$CNC_6[2]$	42	6	24
$CNC_7[2]$	49	7	28

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The definitions of degree-based topological indices [5 – 10] :Randic index R(G) ,Reciprocal Randic index RR(G),Randic index (with h = -3,-2,2,3) where h is adjustable parameter, Zagreb indexfirst $M_1(G)$, second $M_2(G)$, third $M_3(G)$,modified Zagreb index $M_2^*(G)$,second multiplicative Zagreb index ∏2,modified first Zagreb indexΠ_1^*, reduced second Zagreb index $R(M_2)$, Augmented Zagreb index ABC(G),hyper Zagreb index HM(G),Atom-bond connectivity index ABC(G),Harmonic index H(G),Sum connectivity index SCI(G),Sum-connectivity indices with h = -3,-2,2,3 where h is adjustable parameter, Inverse indeg index IN(G), Geometric-Arithmetic index GA(G) are used for computing TIsof $CNC_3[2]$, $CNC_4[2]$,$CNC_5[2]$, $CNC_6[2]$ and $CNC_7[2]$ nanocones.

The Randic index

$R(G) = \sum_{u\,v \in E(G)} 1/\sqrt{dudv}$

$= |E_1|/\sqrt{9} + |E_2|/\sqrt{4} + |E_3|/\sqrt{6}$

Nanocone $CNC_3[2]$

$R(G) = \sum_{u\,v \in E(G)} 1/\sqrt{dudv} = |E_1|/\sqrt{9} + \overline{|E_2|}/\sqrt{4} + |E_3|/\sqrt{6} = 21/\sqrt{9} + 3/\sqrt{4} + 12/\sqrt{6}$

$= 13.399$

$CNC_4[2]$

$R(G) = \sum_{u\,v \in E(G)} 1/\sqrt{dudv} = 29/\sqrt{9} + \overline{4/\sqrt{4}} + 16/\sqrt{6} = 18.2$ $CNC_5[2]$

$R(G) = \sum_{u\,v \in E(G)} 1/\sqrt{dudv} = 35/\sqrt{9} + \overline{5/\sqrt{4}} + 20/\sqrt{6} = 22.34$ $CNC_6[2]$

$R(G) = \sum_{u\,v \in E(G)} 1/\sqrt{dudv} = 42/\sqrt{9} + \overline{6/\sqrt{4}} + 24/\sqrt{6} = 26.79$ $CNC_7[2]$

$R(G) = \sum_{u\,v \in E(G)} 1/\sqrt{dudv} = 49/\sqrt{9} + \overline{7/\sqrt{4}} + 28/\sqrt{6} = 31.27$

Using the number of edges of type $(d_u=3,d_v=3)$,$(d_u=2,d_v=2)$,$(d_u=3,d_v=2)$ and the definitions of degree-based indices [5-10],the TIs are computed and tabled in table (2) for $CNC_3[2]$, $CNC_4[2]$,$CNC_5[2]$, $CNC_6[2]$ and $CNC_7[2]$ nanocones.

The general Randic index with h= -3 has least values due the factor × = -3 and second multiplicative Zagreb index has highest values as it is defined in multiplicationform, among the topological indices studied. By knowing number of degrees (d_u,d_v):(3,3),(2,2),(3,2) the first ,second Zagreb and Harmonic polynomials can be computed for $CNC_3[2]$, $CNC_4[2]$,$CNC_5[2]$, $CNC_6[2]$ and $CNC_7[2]$ nanocones[9,19]. The values of TIs increase from $CNC_3[2]$ to $CNC_7[2]$ nanocones due to increase in number ofedges E_1,E_2 and E_3 in $CNC_3[2]$-$CNC_7[2]$.

Inequalities for topological indices

1) H(G)≤GA(G), is obeyed for nanocones with k=3,4,5,6,7 and n=2.
2) H(G)≤X(G), is obeyed (where X(G)-Sum-connectivity index) in $CNC_3[2]$-$CNC_7[2]$.
3) The general inequality for Zagreb first and second indiceswith n vertices and m edges , $M_1(G)/n \leq M_2(G)/m$ is satisfied in $CNC_4[2]$, as is the case for all graphs.

Table number (2): Topological indices of $CNC_3[2]$-$CNC_7[2]$ carbon nanocones

Topological indices	$CNC_3[2]$	$CNC_4[2]$	$CNC_5[2]$	$CNC_6[2]$	$CNC_7[2]$
R(G)	13.399	18.2	22.34	26.79	31.27
RR(G)	98.39	134.18	163.98	196.77	229.57
R(G)λ = -3	0.13123	0.176349	0.21873	0.2625	0.3063
R(G)λ = -2	0.78008	1.052532	1.3005	1.5602	1.8202
R(G)λ = 2	2181	2989	3635	4362	5089
R(G)λ = 3	18093	24853	30155	36186	42217
M_1	198	250	330	396	462
M_2	273	373	455	546	637
M_3	12	16	20	24	28
M_2^*	5.084	6.889	8.473	10.167	11.862
Π_2	163296	400896	756000	1306368	2074464

Π_1^*	1512	2784	4200	6048	8232
$R(M_2)$	111	152	185	222	259
AZI(G)	359.21	490.33	598.69	718.4	834.15
HM(G)	1104	1508	1840	2208	2576
ABC(G)	24.61	34.18626	41.011	49.2132	57.4154
H(G)	13.3	18.07	22.17	26.6	31.34
SCI(G)	15.441	24.9975	30.7365	36.8338	43.0311
SCI(λ = - 3)	0.2401	0.324759	0.4002	0.48019	0.5603
SCI(λ = - 2)	1.25067	1.69562	2.0848	2.50176	2.91872
SCI(λ = 2)	1104	1508	1840	2208	2576
SCI(λ = 3)	6228	8520	10380	12456	14532
IN(G)	48.9	66.7	81.5	85.2	114.1
GA(G)	35.7578	48.6769	59.5962	71.5155	76.4347

III. CONCLUSION

The vertex degree-based topological indices are computed on 2-dimensional graphs of $CNC_3[2]$, $CNC_4[2]$,$CNC_5[2]$, $CNC_6[2]$ and $CNC_7[2]$ nanocones . By knowing number of degrees as (3,3),(2,2) and (3,2) the first ,second Zagreb polynomial and Harmonic polynomial can be computed for $CNC_3[2]$- $CNC_7[2]$ carbon nanocones.The values of vertex degree-based topological indices increase with $CNC_3[2]$-$CNC_7[2]$ carbon nanocones.

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