Quest Journals
Journal of Research in Environmental and Earth Sciences
Volume 7 ~ Issue 10 (2021) pp: 53-59
ISSN(Online) :2348-2532
www.questjournals.org

Research Paper

On topological indices of carbon nanocone and fullerene

N.K.Raut
Ex.Head, Department of Physics,
Sunderrao Solanke Mahavidyalaya Majalgaon, Dist. Beed (M.S.) INDIA.

ABSTRACT
New degree based topological indices are introduced and studied continuously in chemical graph theory. In this paper second R-index $R^2(G)$,third R-index $R^3(G)$,R-degree Nirmala index $N(G)_R$ are studied by M-polynomials for carbon nanocone $C_4[2]$ and also third R-index $R^3(G)$, F-Revan polynomial and F-Revan index for fullerene with 38 vertices and 16 cycles are computed.
***KEYWORDS**: Carbon nanocone, F-Revan polynomial, fullerene, M-polynomial, Nirmala index, R-polynomial, topological index.*

Received 27 September, 2021; Revised: 08 October, 2021; Accepted 10 October, 2021

I. INTRODUCTION

A graph G consists of a set of vertices V(G) and set of edges E(G). In chemical graph theory each vertex represents an atom of the molecule and covalent bonds between atoms are represented by the edges between the corresponding vertices. A topological index is a numerical parameter mathematically derived from the graph structure. It is a graph invariant thus it does not depend on the labelling or pictorial representation of a graph. Carbon nanocones have been used to cap ultrafine gold needles.Such needles are widely used in scanning probe microscopy owing their high chemical stability and electrical conductivity. The first and second Revan indices are similar to third and second R-indices except their defining nature.

Nowadays topological indices are extensively used in QSPR/QSAR/QATR [1]. Closed formulas for some new degree based topolgical descriptors using M-polynomial and Boron triangular nanotube is investigated by D.Y.Shin et al. [2].Computational aspects of line graph of nanocones are studied by Z.Hussain [3] in which they computed the degree based topological indices of carbon nanocones. Collective eccentric index of fullerenes are studied by M.Ghorbani [4].Some topological indices of family of C_{12n+4} fullerenes are studied by H.Darabi et al. [5]. F-indices and F-polynomials for carbon nanocones $CNC_k[n]$ is studied by N.K.Raut [6]. Degree and distance based topological indices of molecular graph is studied by S.Hayat et al. [7]. Atom bond connectivity and geometric indices of nanocones are studied by A.Khaskar et al. [8]. Carbon nanostructures have attached considerable attention due to their potential use in many applications including energy storage, gas sensors, biosensors, nanoelectronic device and chemical probes [9]. Nanocones are carbon based structures formed by introducing 60^0 inclination in two-dimensional graphene sheets.The multiplicative topological indices of nanocones are studied by N.K.Raut [10].The fourth atom bond connectivity index of carbon nanocones $C_4[2]$ is computed by E.Aslan [11]. In [12] Furtula and Gutman studied F-index and defined it as

$$F(G) = \sum_{uv\in E(G)} (d_u^2 + d_v^2).$$

Revan polynomials of Chloroquine, Hydroxychloroquine, and Remdesivir: Research for treatment of COVID-19 is investigated by V.R.Kulli [13].The Sombor index is defined by Gutman in [14].Degree based Nirmala index is introduced by V.R.Kulli [15].The R-index of some molecular graphs is studied by G.Indulal [16]. Ediz in [17] introduced the concept of R-degree of a vertex and defined some R-indices.Let G be a graph and v∈V(G) then the R-degree of a vertex v is defined as $r(v) = S_v + M_v$,where S_v is sum degree of v and M_v is the multiplication degree of v.The second R-index of a simple connected graph G is defined as

$$R^2 (G) = \sum_{uv\in E(G)} r(u)\, r(v).$$

The third R-index of a simple graph G is defined as

$$R^3 (G) = \sum_{uv\in E(G)} [r(u) + r(v)].$$

The new R-index of path graph, star graph, wheel graph, gear graph and helm graph are studied by A.Sumathi [18].R-index of some bridge graphs are studied by A.Sumathi in [19].
Degree based Nirmala index is introduced by V.R.Kulli [15]. We introduce the R-degree Nirmala index and denote it by $N(G)_R$ .The Nirmala index of a molecular graph G is defined as

$$N(G) = \sum_{uv \in E(G)} \sqrt{d_{(G)}(u) + d_{(G)}(v)}\,.$$

Considering the Nirmala index, we define the R-degree Nirmala index by

$$N(G)_R = \sum_{uv \in E(G)} \sqrt{r(u) + r(v)}\ ,$$

and formula for $N(G)_R$ in M-polynomial as

$$(D_x)^{1/2}\, J\,(M(G;x,y))|_{x=y=1}.$$

Revan indices of oxide and honeycomb networks are studied by V.R.Kulli [20] in which Revan vertex degree of a vertex v in G is defined as

$$r_G(v) = \Delta(G) + \delta(G) - d_G(v).$$

F-Revan polynomial of a molecular graph G is

$$FR(G,x) = \sum_{uv \in E(G)} x^{((rG(u)^2 + (rG(v)^2)}$$

and F-Revan index is

$$FR(G) == \sum_{uv \in E(G)} (r_G(u)^2 + r_G(v)^2).$$

Revan indices and Revan polynomials of silicon carbide graphs are studied by R.Ashraf [21]. In [22] N.K.Raut et al.studied vertex degree of fullerene with vertices 38 and 16 cycles.The 2-D graph of fullerene with vertices 38 and cycles 16 has common vertices of degree 3 for each vertex.
The forgotten index can be studied by three approaches for graph G(V,E) as

$$F(G) = \sum_{uv \in E(G)} d_u^{\,3} = \sum_{uv \in E(G)} (d_u^{\,2} + d_v^{\,2}),$$

by forgotten polynomial of graph,

$$F(G,x) = \sum_{uv \in E(G)} x^{(d_u^{\,2} + d_v^{\,2})}$$

and by M-polynomial as

$$F(G) = (D_x^{\,2} + D_y^{\,2})\, M(G;x,y)|_{x=y=1}.$$

Here we compute forgotten index in Revan degree by M-polynomial as

$$D_x\,(F(G,x))|_{x=1}.$$

The M-polynomial of graph G is defined as

$$M(G;x,y) = \sum_{\delta \le i \le j \le \Delta} m_{ij}(G)\, x^i y^j,$$

where $\delta = \min\{d_v | v \in V(G)\}$, $\Delta = \max\{d_v | v \in V(G)\}$, and $m_{ij}(G)$ is the edge $vu \in E(G)$ such that $i \le j$, with $D_x = x\,\frac{\partial f(x,y)}{\partial x}$, $D_y = y\,\frac{\partial f(x,y)}{\partial y}$, $S_x = \int_0^x \frac{f(t,y)}{t}\,dt$, $S_y = \int_0^y \frac{f(x,t)}{t}\,dt$, $J(f(x,y)) = f(x,x)$, $Q_\alpha(f(x,y)) = x^\alpha f(x,y)$.

The notations used in this paper are standard and mainly taken from books of chemical graph theory [23-26]. In this paper second R-index $R^2(G)$, third R-index $R^3(G)$, R-degree Nirmala index $N(G)_R$ are studied by M-polynomials for carbon nanocone $C_4[2]$ and third R-index, F-Revan polynomial and F-Revan index for fullerene with 38 vertices,16 cycles are computed.

II. MATERIALS AND METHODS

A molecular graph is a simple and connected graph.The molecular graph of carbon nanocones $CNC_k[n]$ have conical structures with a cycle of length k at its core and n layers of hexagons placed at the conical surface around its centre.Carbon nanocones are conical structures which are made predominantly from carbon and which have at least one dimension of the order of one micrometer or smaller.The molecular graph of carbon nanocone $C_4[2]$ is shown in figure 1.It has vertices |V| = 36 and edges |E| = 48.The M-polynolmial of molecular graph of carbon nanocone $C_4[2]$ is written from edge set of molecular graph.The edge set of $C_4[2]$ are $|E_{(5,7)}|$, $|E_{(7,9)}|$, $|E_{(5,5)}|$, $|E_{(6,7)}|$, $|E_{(9,9)}|$ in sum degree of vertices and $|E_{(6,12)}|$, $|E_{(12,27)}|$, $|E_{(6,6)}|$, $|E_{(9,12)}|$,$|E_{(27,27)}|$ in multiplication degree of vertices with degree of vertices as $d_u = d_v = 3$, $d_u = d_v = 2$ and $d_u = 2$, $d_v = 3$.To compute Revan indices and Revan polynomials for fullerene, the Revan degree is observed from degree of vertices of molecular graph of fullerene (figure 2).Let G(V,E) be a graph with vertex set V and edge set E.The degree of a vertex $v \in E(G)$ is denoted by d_v and is the number of verices that are adjacent to v.The Revan degree of a vertex v in G is defined as

$$r_G(v) = \Delta(G) + \delta(G) - d_G(v).$$

The Revan edge connecting the Revan vertices u and v will be denoted by uv.The molecular graph of fullerene with vertices 38 and cycles 16 is shown in figure 2.It has vertices |V| = 36 and edges |E| = 57.The formulas used in terms of R-indices from M-polynomials are represented in table 3.

III. RESULTS AND DISCUSSION

3.1 R-indices of Carbon nanocone $C_4[2]$

The 2-D graph of carbon nanocone $C_4[2]$ has 48 edges and 36 vertices with degrees $d_u = d_v = 3$, $d_u = d_v = 2$ and $d_u = 2$, $d_v = 3$. It is observed from figure 1 that there are $S_{u/v}$ the sum degree of u/v as (5,7) = 8, (7,9) = 8, (5,5) = 4, (6,7) = 8 and (9,9) = 20 edges.The multiplication degree of u/v denoted by $M_{u/v}$ are (6,12) = 8,(12,27) = 8, (6,6) = 4, (9,12) = 8 and (27,27) = 20 edges.

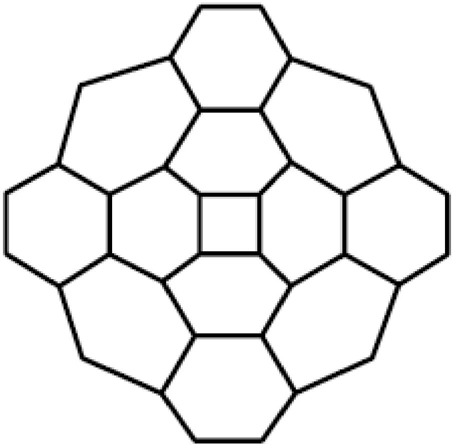

Figure 1. 2-D graph of carbon nanocone $C_4[2]$.

(S_u, S_v)	(5,7)	(7,9)	(5,5)	(6,7)	(9,9)
(M_u, M_v)	(6,12)	(12,27)	(6,6)	(9,12)	(27,27)
Number of edges	8	8	4	8	20

Table 1.The degree sum of vertices and mulitiplication degree of vertices to compute the R-degree of vertices of carbon nanocone $C_4[2]$.

Theorem 1. The second R-index $R^2(G)$ of carbon nanocone $C_4[2]$ is 35828.

Proof. Consider a molecular graph of carbon nanocone $C_4[2]$ as shown in figure 1.By using the formula of second R-index $R^2(G)$ and table 1 we get

$R^2(G) = \sum_{uv\in E(G)} r(u)\, r(v)$

$= \sum_{uv\in E(G)} (S_u + M_u)\,(S_v + M_v)$

=8((5+6)*(7+12))+8((7+12)*(9+27))+4((5+6)*(5+6))+8((6+9)*(7+12))+ 20((9+27)*(9+27)) = 35828.

The M-polynomial of $C_4[2]$

$M(G;x,y) = \sum_{\delta\le i\le j\le\Delta} m_{ij}(G)\, x^i y^j$

$=\sum_{11\le 19} m_{1119}(G)\, x^{11}y^{19} + \sum_{19\le 36} m_{1936}(G)\, x^{19}y^{36} + \sum_{11\le 11} m_{1111}(G)\, x^{11}y^{11} + \sum_{15\le 19} m_{1519}(G)\, x^{15}y^{19} + \sum_{36\le 36} m_{3636}(G)\, x^{36}y^{36}$.

$=|E_{(5,7)}|\, x^{11}y^{19}+|E_{(7,9)}|\, x^{19}y^{36}+|E_{(5,5)}|\, x^{11}y^{11}+|E_{(7,6)}|\, x^{15}y^{19}+|E_{(9,9)}|\, x^{36}y^{36}$.

$=8\, x^{11}y^{19}+8\, x^{19}y^{36}+4\, x^{11}y^{11}+8\, x^{15}y^{19}+20\, x^{36}y^{36}$.

In order to find second R-index $R^2(G)$ we need the following,

$M(G;x,y) = 8\, x^{11}y^{19}+8\, x^{19}y^{36}+4\, x^{11}y^{11}+8\, x^{15}y^{19}+20\, x^{36}y^{36}$.

$D_yM(G;x,y) = 152\, x^{11}y^{19}+288\, x^{19}y^{36}+44\, x^{11}y^{11}+152\, x^{15}y^{19}+720\, x^{36}y^{36}$.

$D_xD_yM(G;x,y) = 1672\, x^{11}y^{19}+5472\, x^{19}y^{36}+484\, x^{11}y^{11}+2280\, x^{15}y^{19}+25920\, x^{36}y^{36}$.

$R^2(G) = D_xD_yM(G;x,y)|_{x=y=1} = 35828$.

Theorem 2. The third R-index $R^3(G)$ of carbon nanocone $C_4[2]$ is 2480.

Proof. Consider a molecular graph of carbon nanocone $C_4[2]$ figure 1. By using the formula of third R-index $R^3(G)$ and table 1 we get

$R^3(G) = \sum_{uv\in E(G)} (r(u) + r(v))$

$= \sum_{uv\in E(G)} (S_u + M_u) + (S_v + M_v)$

=8((5+6)+(7+12))+8((7+12)+(9+27))+4((5+6)+(5+6))+8((6+9)+(7+12))+ 20((9+27)+(9+27)) =2480
.
The M-polynomial of $C_4[2]$
M(G;x,y) = $\sum_{\delta \le i \le j \le \Delta} m_{ij}(G)\, x^i y^j$
=$\sum_{11 \le 19} m_{1119}(G)\, x^{11}y^{19} + \sum_{19 \le 36} m_{1936}(G)\, x^{19}y^{36} + \sum_{11 \le 11} m_{1111}(G)\, x^{11}y^{11} + \sum_{15 \le 19} m_{1519}(G)\, x^{15}y^{19} + \sum_{36 \le 36} m_{3636}(G)\, x^{36}y^{36}$.
=$|E_{(5,7)}|\, x^{11}y^{19}+|E_{(7,9)}|\, x^{19}y^{36}+|E_{(5,5)}|\, x^{11}y^{11}+|E_{(7,6)}|\, x^{15}y^{19}+|E_{(9,9)}|\, x^{36}y^{36}$.
=$8\, x^{11}y^{19}+8\, x^{19}y^{36}+4\, x^{11}y^{11}+8\, x^{15}y^{19}+20\, x^{36}y^{36}$.
In order to find third R-index $R^3(G)$ by M-polynomial we need the following,
M(G;x,y) = $8\, x^{11}y^{19}+8\, x^{19}y^{36}+4\, x^{11}y^{11}+8\, x^{15}y^{19}+20\, x^{36}y^{36}$.

D_xM(G;x,y) = $88\, x^{11}y^{19}+152\, x^{19}y^{36}+44\, x^{11}y^{11}+120\, x^{15}y^{19}+720\, x^{36}y^{36}$.

D_yM(G;x,y) = $152\, x^{11}y^{19}+288\, x^{19}y^{36}+44\, x^{11}y^{11}+152\, x^{15}y^{19}+720\, x^{36}y^{36}$.

(D_x+D_y)M(G;x,y) =$240\, x^{11}y^{19} + 440\, x^{19}y^{36} + 88\, x^{11}y^{11} + 272\, x^{15}y^{19} + 1440\, x^{36}y^{36}$.
$R^3(G) = (D_x+D_y)M(G;x,y)|_{x=y=1}$ = 2480.

Theorem 3. The R-degree Nirmala index of carbon nanocone $C_4[2]$ is 338.3.

Proof. Consider a molecular graph of carbon nanocone $C_4[2]$ figure 1.By using the formula of R-degree Nirmala index and table 1 we get
R-degree Nirmala index $N(G)_R = \sum_{uv \in E(G)} \sqrt{\, r(u) + r(v)}$
$= \sum_{uv \in E(G)} \sqrt{(S_u + M_u) + (S_v + M_v)}$
$=8((5+6)+(7+12))^{1/2}+8((7+12)+(9+27))^{1/2}+4((5+6)+(5+6))^{1/2}+8((6+9)+(7+12))^{1/2}+ 20((9+27)+(9+27))^{1/2}$
=338.3.
The M-polynomial of $C_4[2]$
M(G;x,y) = $\sum_{\delta \le i \le j \le \Delta} m_{ij}(G)\, x^i y^j$
=$8\, x^{11}y^{19}+8\, x^{19}y^{36}+4\, x^{11}y^{11}+8\, x^{15}y^{19}+20\, x^{36}y^{36}$.
In order to find R-degree Nirmala index we need the following,
M(G;x,y) = $8\, x^{11}y^{19}+8\, x^{19}y^{36}+4\, x^{11}y^{11}+8\, x^{15}y^{19}+20\, x^{36}y^{36}$.
J M(G;x,y) = $8\, x^{30}+8\, x^{55}+4\, x^{22}+8\, x^{34}+20\, x^{72}$.

$(D_x)^{1/2}$ J M(G;x,y) = $8*30^{1/2}\, x^{30}+8*55^{1/2}\, x^{55}+4*22^{1/2}\, x^{22}+8*34^{1/2}\, x^{34}+20*72^{1/2}\, x^{72}$.

R-degree Nirmala index $N(G)_R = (D_x)^{1/2}$ J $M(G;x,y)|_{x=1}$ = 338.3.

3.2 Topological indices of Fullerene

The 2-D molecular graph of fullerene with vertices 38 and 16 cycles is shown in figure 2.It is observed from figure 2, all the vertices has equal degree $d_u = d_v = 3$.The R-degree of a vertex v is defined as $r(v) = S_v + M_v$,where S_v is sum degree of v and M_v is the multiplication degree of v. Revan vertex degree of a vertex v in G is defined as $r_G(v) = \Delta(G) + \delta(G) - d_G(v)$. S_v, M_v and number of edges are given in table 2.In this section we study third R-index $R^3(G)$, F-Revan polynomial and F-Revan index of fullerene with vertices 38 and 16 cycles.

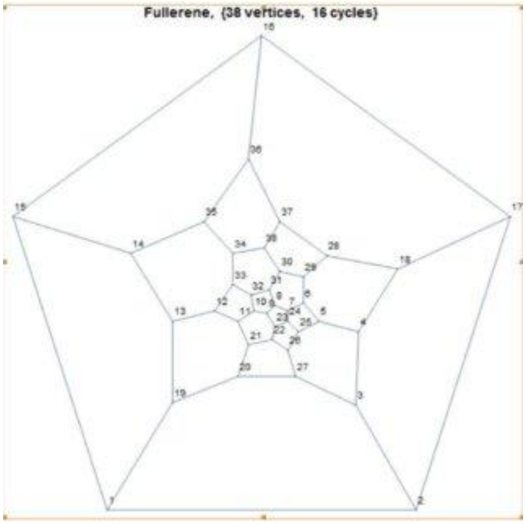

Figure 2. 2-D graph of fullerene with vertices 38 and 16 cycles.

d_u,d_v	(S_u,S_v)	(M_u,M_v)	Revan degree $(r_G(u), r_G(v))$	Number of edges
(3,3)	(9,9)	(27,27)	(3,3)	57

Table 2.The degree sum of vertices and mulitiplication degree of vertices of R-degree and Revan degree of fullerene with vertices 38 and 16 cycles.

Theorem 4. The third R-index $R^3(G)$ of fullerene with vertices 38 and 16 cycles is 4104.

Proof. Consider a molecular graph of fullerene with vertices 38 and 16 cycles figure 2.By using the formula of third R-index $R^3(G)$ and table 3 we get

$R^3(G) = \sum_{uv\in E(G)}(r(u)+r(v))$

$= \sum_{uv\in E(G)}(S_u+M_u)+(S_v+M_v)$

$=57((9+27) + (9+27)) = 4104.$

The M-polynomial of fullerene with vertices 38 and 16 cycles is

$M(G;x,y) = \sum_{\delta\le i\le j\le\Delta} m_{ij}(G)\,x^i y^j$

$=\sum_{9\le 27} m_{927}(G)\,x^9y^{27} + \sum_{9\le 27} m_{927}(G)\,x^9y^{27}.$

$=|E(_{9,27})|\,x^9y^{27}+|E(_{9,27})|\,x^9y^{27}.$

$=57(\,x^9y^{27}+x^9y^{27}).$

In order to find third R-index $R^3(G)$ we need the following,

$M(G;x,y) = 57(\,x^9y^{27}+x^9y^{27}).$

$D_xM(G;x,y) = 57(\,9x^9y^{27}+9\,x^9y^{27}).$

$D_yM(G;x,y) = 57(\,27x^9y^{27}+27y^{27}).$

$(D_x+D_y)M(G;x,y) = 57((\,9x^9y^{27}+9\,x^9y^{27})+(\,27x^9y^{27}+27\,x^9y^{27})).$

$R^3(G) = (D_x+D_y)M(G;x,y)|_{x=y=1} = 4104.$

Theorem 5. The F-Revan polynomial of fullerene with vertices 38 and 16 cycles is $57x^{((3)^2+(3)^2)}$.

Proof. Consider a molecular graph of fullerene with vertices 38 and 16 cycles figure 2.By using the formula of F-Revan polynomial of a molecular graph G

$FR(G,x) = \sum_{uv\in E(G)} x^{(r_G(u)^2+r_G(v)^2)}.$

$=|E(_{3,3})|\sum_{uv\in E(G)} x^{((3)^2+(3)^2)}.$

$= 57 \sum_{uv\in E(G)} x^{((3)^2+(3)^2)}.$

$= 57x^{((3)^2+(3)^2)}.$

Theorem 6. The F-Revan index of fullerene with vertices 38 and 16 cycles is 1026.

Proof. Consider a molecular graph of fullerene with vertices 38 and 16 cycles as shown in figure 2.By using the formula of F-Revan index of a molecular graph G and table 2.

$FR(G) = \sum_{uv\in E(G)}(r_G(u)^2 + r_G(v)^2).$

$=|E_{(3,3)}|\sum_{uv\in E(G)}((3)^2 + (3)^2).$

= 57 $((3)^2 + (3)^2)$.
= 1026.
F-Revan index of fullerene with vertices 38 and 16 cycles by M-F-polynomial is1026.
Consider a molecular graph of fullerene with vertices 38 and 16 cycles figure 2 and table 3.By using the formula $D_x(F(G,x))|_{x=1}$.
The F-Revan polynomial of a molecular graph G
FR(G,x) = $\sum_{uv\in E(G)} x^{(r_G(u)^2 + r_G(v)^2)}$.
= 57 $\sum_{uv\in E(G)} x^{((3)^2 + (3)^2)}$.
= $57x^{((3)^2+(3)^2)}$.
The F-Revan index $D_x(F(G,x))|_{x=1}$,
FR(G,x) = 57 $x^{((3)^2+(3)^2\}}$.
D_x FR(G,x) = 57 * 18 $x^{((3)^2+(3)^2\}}$
$D_x(F(G,x))|_{x=1}$ = (57 * 18 $x^{((3)^2+(3)^2)}|_{x=1}$ = 1026.

Topological index	Derivation from M(G;x,y)
Second R-index $R^2(G)$	$(D_x * D_y)(M(G;x,y))|_{x=1}$
Third R-index $R^3(G)$	$(D_x + D_y)(M(G;x,y))|_{x=y=1}$
F-Revan index F R(G)	$D_x(F(G;x))|_{x=1}$
R-degree Nirmala index $N(G)_R$	$(D_x)^{1/2}$ J $(M(G;x,y))|_{x=y=1}$

Table 3.Derivational formulas for topological indices by M-polynomial.

IV. CONCLUSION

Based on the standard degree-topological indices the new topological indices are introduced and studied in chemical graph theory continuously for the new chemical compounds.In this paper we computed second R-index $R^2(G)$ index, third R-index $R^3(G)$ index and R-degree Nirmala index $N(G)_R$ for carbon nanocone $C_4[2]$ and third R-index $R^3(G)$, F-Revan polynomial and F-Revan index for fullerene with 38 vertices and 16 cycles by using degree based formulas.

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