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On Nirmala indices of carbon nanocone $C_4[2]$

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Abstract
Nirmala index of a graph is recently introduced degree based topological indexwhich is defined as N(G) = $\sum_{uv\in E(G)}\sqrt{(d_{(G)}(u)+d_{(G)}(v)}$, where G is finite,simple, connected graph with vertex set V(G) and edge set E(G) and d_v is the degree of vertex v∈V(G).In this paper different versions of Nirmala index of carbon nanocone $C_4[2]$ are investigated.

***Keywords**: Carbon nanocone $C_4[2]$, degree,multiplication degree, Nirmala index, reduced inverse Nirmala index,sum connectivity index. vertex degree sum.*

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I. Introduction

Let G be a finite,simple,connected graph with vertex set V(G) and edge set E(G).The degree of vertex v∈V(G),d_v is the number of edges incident with v.A topological index is a numerical parameter mathematically derived from the graph structure.The function

F(x,y) = $(x+y)^{\lambda}$ for the general sum connectivity index where λ is an adjustable parameter were discussed by I.Gutman and J.Tosovic for testing quality of topological indices [1].The topological indices of Vitamin D_3 are computed by M.R.R.Kanna et al. in [2].

The molecular graph of carbon nanocones CNCk[n] have conical structures with a cycle of length k at its center and n layers of hexagons placed at the conical surface around its center [3].Carbon nanocones are one of the forms of carbon nanostructures and these have been proposed as possible molecular gas storagedevices [4].V.R. Kulli introduced Nirmala index,first and second inverse Nirmala indicesof a graph G[5-6] as

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

first inverse Nirmala index $IN_1(G)= \sum_{uv\in E(G)}(\frac{1}{d_u}+\frac{1}{d_v})^{\frac{1}{2}}$,

andsecond inverse Nirmala index $IN_2(G) =\sum_{uv\in E(G)}(\frac{1}{d_u}+\frac{1}{d_v})^{-\frac{1}{2}}$.

We introduce reduced first andsecond inverse, δ-first and δ-second inverse and average Nirmala indices of a graph G as

reduced first inverse Nirmala index $RIN_1(G) = \sum_{uv\in E(G)}(\frac{1}{d_u-1}+\frac{1}{d_v-1})^{\frac{1}{2}}$,

reduced second inverse Nirmala index $RIN_2(G) = \sum_{uv\in E(G)}(\frac{1}{d_u-1}+\frac{1}{d_v-1})^{-\frac{1}{2}}$,

δ-first inverse Nirmala index $\delta IN_1(G) = \sum_{uv\in E(G)}(\frac{1}{d_u-\delta(G)+1}+\frac{1}{d_v-\delta(G)+1})^{\frac{1}{2}}$,

and δ-second inverse Nirmala index $\delta IN_2(G) = \sum_{uv\in E(G)}(\frac{1}{d_u-\delta(G)+1}+\frac{1}{d_v-\delta(G)+1})^{-\frac{1}{2}}$,

where δ(G) ≥ 2,δ(G) is the minimum degree among the vertices of G.
Recently introduced degree based and mostly studied topological index is Sombor index
$SO(G) = \sum_{uv\in E(G)}\sqrt{(d_u^2+d_v^2)}$,where d_v is degree of vertex v in graph G [7].

The average Sombor index is introduced and studied for graphs in [8-9] as

$SO_{avg}(G) =\sum_{uv\in E(G)}[\,(d_u-\frac{2m}{n})^2+(d_v-\frac{2m}{n})^2]^{\frac{1}{2}}$,where |V(G)| = n and |E(G)| = m.

Like average Sombor index we propose average Nirmala index as

$N_{avg}(G) =\sum_{uv\in E(G)}[\,(d_u-\frac{2m}{n})+(d_v-\frac{2m}{n})]^{\frac{1}{2}}$,where |V(G)| = n and |E(G)| = m.

Different versions of Nirmala index of certain chemical structures were studied by V.R. Kulli in [10]. Inverse degree,Randic indexand Harmonic index of graphs were discussed by K.C. Daset al. [11].In [12] different versions of Harmonic indices of certain nanotubes are discussed by authors wherein six types of Harmonic indices were defined and computed. Sixth version of Harmonic index is Q_u type Harmonic index.Harmonic index in terms of Q_u parameter is

$$H_{gen}(G) = \sum_{uv\in E(G)} \frac{2}{Q_u+Q_v},$$

where Q_u is the unique parameter which is acquired from the vertex u $\in V(G)$,we call it Q_u type Harmonic index for multiplication degree of vertices [13]which is

$$H_{Q_u}(G) = \sum_{uv\in E(G)} \frac{2}{M_u+M_v} \text{ ,where } M_v = \prod_{u\in N(v)} \deg(u).$$

We introduce Q_u type Nirmala index as

$$N_{Q_u}(G) = \sum_{uv\in E(G)} (M_u + M_v)^{\frac{1}{2}}, \text{where } M_v= \prod_{u\in N(v)} \deg(u).$$

R-degree Nirmala index by M-polynomials for carbonnanocone $C_4[2]$ wasstudied by N.K. Raut in[14].The sum connectivity index was studied by [15-18] which is defined as

$$\square = \sum_{uv\in E(G)} (d_u + d_v)^{-\frac{1}{2}} .$$

Multiplicative sum connectivity index wasinvestigated by Y.C. Kwun et al. in [19].Thereduced sum connectivity index and reduced product connectivity indices of $TUC_4C_8[S]$ was computed by N.K.Raut [20]. The reduced reciprocal Randic indexis defined by M.K.Jamil in [21] as

$$RRR(G) = \sum_{uv\in E(G)} \sqrt{(d_u-1) \quad + (d_v-1)} \quad .$$

Like reduced Banhatti-Sombor index or reduced Sombor index, increased Sombor index was introduced by W. Ning[22-23]as

$$SO^1(G) = \sum_{uv\in E(G)} \sqrt{(d_u + 1)^2 + (d_v + 1)^2}.$$

We propose first and second increased inverse Nirmala indices as [24]

$IN_1^1(G) = \sum_{uv\in E(G)} (\frac{1}{d_u+1} + \frac{1}{d_v+1})^{\frac{1}{2}}$ and $IN_2^1(G) = \sum_{uv\in E(G)} (\frac{1}{d_u+1} + \frac{1}{d_v+1})^{-\frac{1}{2}}$ respectively.

By using the first derivative of the Schultz, modified Schultz polynomials of Jahangir graph $J_{3,m}$(evaluated at x = 1) one can compute the Schultz, modified Schultz indices [25] as

$$Sc(J_{3,m}) = \frac{\partial Sc(J_{3,m},x,y)}{\partial x}\Big|_{x=1} .$$

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

$$N_R(G) = \sum_{uv\in E(G)} \sqrt{r(u) \quad + r(v)} \text{ ,where } M_v= \prod_{u\in N(v)} \deg(u) \text{ and}$$
$$S_v = \sum_{u\in N(v)} \deg(u) \text{ and } r(v) = M_v + S_v.$$

The terms and notations used in this paper are standard and mainly taken from books of graph theory [26-28].

In this paper reduced first and secondinverse Nirmala indices ($RIN_1(G)$and$RIN_2(G)$),δ-first and δ-second inverse Nirmala indices($\delta IN_1(G)$and $\delta IN_2(G)$),average Nirmala index ($N_{avg}(G)$),Q_u type Nirmala index($N_{Q_u}(G)$),R-degree Nirmala index ($N_R(G)$), first and secondincreased inverse Nirmala indices ($IN_1^1(G)$ and $IN_2^1(G)$) are investigated for carbon nanocone$C_4[2]$.

II. Materials and Methods

A molecular graph is a simple and connected graph.The 2-dimensional graph of carbon nanocone $C_4[2]$ is shown in figure 1.Let the graph ofcarbon nanocone $C_4[2]$ be denoted by G.There are three edges in G given by E_1= 4,E_2 =16,E_3 = 28 as $E_1 = \{uv\in E(G)|d_u=d_v=2\}$,$E_2 = \{uv\in E(G)|d_u= 2 \text{ and } d_v= 3\}$and $E_3 = \{uv\in E(G)|d_u=d_v= 3\}$.It is observed from figure that the vertex set = 36 and edge set = 48. Edge set of $C_4[2]$ are $|E_{(5,7)}|$,$|E_{(7,9)}|$,$|E_{(5,5)}|$,$|E_{(6,7)}|$ and $|E_{(9,9)}|$ in sum degree of vertices and $|E_{(6,12)}|$,$|E_{(12,27)}|$,$|E_{(6,6)}|$,$|E_{(9,12)}|$and $|E_{(27,27)}|$ in multiplication degree of vertices.To compute Q_u type and R-degree Nirmala indices,multiplication degree of vertices and sum-multiplication degree of vertices are used respectively.The edge partition of carbon nanocone $C_4[2]$ is used tostudy $RIN_1(G)$,$RIN_2(G)$,δ-first and δ-second inverse,$N_{avg}(G)$,first and second increased inverse Nirmala indices and for Q_u type Nirmala index,R-degree Nirmala index, multiplication degree and sum-multiplication degree. In this study$RIN_1(G)$,$RIN_2(G)$,$\delta IN_1(G)$,$\delta IN_2(G)$, $N_{avg}(G)$,$N_{Q_u}(G)$,$N_R(G)$,$IN_1^1(G)$ and $IN_2^1(G)$ are computed.

III. Results and Discussion

3.1 Reduced first,second,δ-first,δ-secondinverse Nirmala indices and average Nirmala indexof carbon nanocone $C_4[2]$

The molecular graph of carbon nanocone $C_4[2]$ is shown in figure 1.Let the graph ofcarbon nanocone $C_4[2]$ be denoted by G.

The 2-D graph of carbon nanocone $C_4[2]$ has 48 edges and 36vertices and degree of vertices 2 and 3.The edge partition of carbon nanocone $C_4[2]$is given in table1and sum degree and multiplication degree of vertices in table 2.

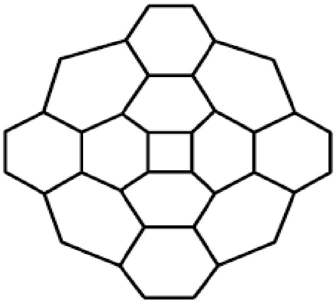

Figure 1. 2-D graph of carbon nanocone $C_4[2]$.

(d_u, d_v)	(2,2)	(2,3)	(3,3)
Number of edges	4	16	28

Table 1. Edge partition 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 2. The sum degree and multiplication degree of vertices of carbon nanocone $C_4[2]$.

Theorem 1. The first reduced inverse Nirmala index of carbon nanocone $C_4[2]$ is 53.

Proof. Consider a molecular graph of carbon nanocone $C_4[2]$as shown in figure 1.Let $E_{(u,v)}$ denote the edge connecting the vertices of u and v.The graph contains $E_{(2,2)}$,$E_{(2,3)}$ and $E_{(3,3)}$ edges.Using edge partition from table 1 we get first reduced inverse Nirmala index.

$RIN_1(G) = \sum_{uv\in E(G)}(\frac{1}{d_u-1}+\frac{1}{d_v-1})^{\frac{1}{2}}$

$= |E_{(2.2)}|\,(\frac{1}{2-1}+\frac{1}{2-1})^{\frac{1}{2}} + |E_{(2.3)}|(\frac{1}{2-1}+\frac{1}{3-1})^{\frac{1}{2}} + |E_{(3.3)}|\,(\frac{1}{3-1}+\frac{1}{3-1})^{\frac{1}{2}}$

$= 4\,(2)^{\frac{1}{2}} + 16(1.5)^{\frac{1}{2}} + 28\,(1)^{\frac{1}{2}}$.

= 53.

Theorem 2. The second reduced inverse Nirmala index of carbon nanocone $C_4[2]$ is 44.

Proof. Consider a molecular graph of carbon nanocone $C_4[2]$ as shown in figure 1. Let $E_{(u,v)}$ denote the edge connecting the vertices of u and v.The graph contains $E_{(2,2)}$, $E_{(2,3)}$ and $E_{(3,3)}$ edges. Using edge partitionfrom table 1 we get second reduced inverse Nirmala index.

$RIN_2(G) = \sum_{uv\in E(G)}(\frac{1}{d_u-1}+\frac{1}{d_v-1})^{-\frac{1}{2}}$

$= |E_{(2.2)}|\,(\frac{1}{2-1}+\frac{1}{2-1})^{-\frac{1}{2}} + |E_{(2.3)}|(\frac{1}{2-1}+\frac{1}{3-1})^{-\frac{1}{2}} + |E_{(3.3)}|\,(\frac{1}{3-1}+\frac{1}{3-1})^{-\frac{1}{2}}$

$= 4\,(2)^{-\frac{1}{2}} + 16(1.5)^{-\frac{1}{2}} + 28\,(1)^{-\frac{1}{2}}$.

= 44.

Theorem 3. The δ-first inverse Nirmala index of carbon nanocone $C_4[2]$ is 53.

Proof. Using edge partition from table 1 we get δ-first inverse Nirmala index.

Here $\delta(G)\geq 2$,where δ(G) is the minimum degree amongvertices. In graphGdegree of vertices are 2 and 3,so$\delta(G) = 2$.

The δ-first inverse Nirmala index $\delta IN_1(G) = \sum_{uv\in E(G)}(\frac{1}{d_u-\delta(G)+1}+\frac{1}{d_v-\delta(G)+1})^{\frac{1}{2}}$

$= |E_{(2.2)}|\,(\frac{1}{2-2+1}+\frac{1}{2-2+1})^{\frac{1}{2}} + |E_{(2.3)}|(\frac{1}{2-2+1}+\frac{1}{3-2+1})^{\frac{1}{2}} + |E_{(3.3)}|\,(\frac{1}{3-2+1}+\frac{1}{3-2+1})^{\frac{1}{2}}$

$= 4\,(2)^{\frac{1}{2}} + 16(1.5)^{\frac{1}{2}} + 28\,(1)^{\frac{1}{2}}$.

= 53.

Theorem 4. The δ-second inverse Nirmala index of carbon nanocone $C_4[2]$ is 44.

Proof. Using edge partition from table 1 we get δ-second inverse Nirmala index.

Here $\delta(G) \geq 2$,where δ(G) is the minimum degree among vertices.In graph G degree of vertices are 2 and 3,so $\delta(G) = 2$.

The δ-second inverse Nirmala index $\delta IN_2(G) = \sum_{uv\in E(G)}(\frac{1}{d_u-\delta(G)+1}+\frac{1}{d_v-\delta(G)+1})^{-\frac{1}{2}}$

$= |E_{(2.2)}| \left(\frac{1}{2-2+1} + \frac{1}{2-2+1}\right)^{-\frac{1}{2}} + |E_{(2.3)}|\left(\frac{1}{2-2+1} + \frac{1}{3-2+1}\right)^{-\frac{1}{2}} + |E_{(3.3)}| \left(\frac{1}{3-2+1} + \frac{1}{3-2+1}\right)^{-\frac{1}{2}}$
$= 4\,(2)^{-\frac{1}{2}} + 16(1.5)^{-\frac{1}{2}} + 28\,(1)^{-\frac{1}{2}}$
$= 44.$

Theorem 5. The average Nirmala index of carbon nanocone $C_4[2]$ is $4\sqrt{-1.332} + 16\sqrt{-0.332} + 28\sqrt{0.668}$.

Proof. Using edge partition from table 1 we get average Nirmala index.
Here $|V(G)| = n = 36$ and $|E(G)| = m = 48$, hence $\frac{2m}{n} = \frac{2*48}{36} = 2.666$.
$N_{avg}(G) = \sum_{uv\in E(G)} \left[\left(d_u - \frac{2m}{n}\right) + \left(d_v - \frac{2m}{n}\right)\right]^{\frac{1}{2}}$
$= |E_{(2.2)}|\,[(2-2.666) + (2-2.666)]^{\frac{1}{2}} + |E_{(2.3)}|[(2-2.666) + (3-2.666)]^{\frac{1}{2}} + |E_{(3,3)}|[(3-2.666) + (3-2.666)]^{\frac{1}{2}}$

$= 4\sqrt{-1.332} + 16\sqrt{-0.332} + 28\sqrt{0.668}$.

3.2 Q_u type, R-degree, first and second increased inverse Nirmala indicesof carbon nanocone $C_4[2]$
In the following section Q_u type, R-degree,first and second increased inverse Nirmala indices are computed.

Theorem 6. TheQ_u type Nirmala index of carbon nanocone $C_4[2]$ is 281.3.

Proof. Consider a molecular graph of carbon nanocone $C_4[2]$ as shown in figure 1. Let $M_{u/v}$ denote the multiplication degree of vertices u and v in G. The graph contains $M_{(6,12)}$,$M_{(12,27)}$,$M_{(6,6)}$,$M_{(9,12)}$ and $M_{(27,27)}$edges. Using edge partition from table 2,we get Q_u type of Nirmala index.

$$N_{Q_u}(G) = \sum_{uv\in E(G)} (M_u + M_v)^{\frac{1}{2}}, \text{where } M_v = \prod_{u\in N(v)} \deg(u)$$

$= |E_{(6,12)}|(M_u + M_v)^{\frac{1}{2}} + |E_{(12,27)}|(M_u + M_v)^{\frac{1}{2}} + |E_{(6,6)}|(M_u + M_v)^{\frac{1}{2}} + E_{(9,12)}|(M_u + M_v)^{\frac{1}{2}} + |E_{(27,27)}|(M_u + M_v)^{\frac{1}{2}}$
$= 8(6+12)^{\frac{1}{2}} + 8(12+27)^{\frac{1}{2}} + 4(6+6)^{\frac{1}{2}} + 8(9+12)^{\frac{1}{2}} + 20(27+27)^{\frac{1}{2}}$
$= 281.3.$

Theorem 7. The R-degree Nirmala index of carbon nanocone C4[2] is 338.9.

Proof. Consider a molecular graph of carbon nanocone $C_4[2]$ as shown in figure 1. Let $M_{u/v}$ denote the multiplication degree and $S_{u/v}$ denote sum degree of vertices of u and v in G.

The R-degree Nirmala index $N_R(G) = \sum_{uv\in E(G)} \sqrt{r(u) + r(v)}$,
where $M_v = \prod_{u\in N(v)} \deg(u)$, $S_v = \sum_{u\in N(v)} \deg(u)$ and $r(v) = M_v + S_v$.

The R-degree Nirmala exponential is $N_R(G,x) = \sum_{uv\epsilon E(G)} x^{\sqrt{r(u) + r(v)}}$
$= 8x^{\sqrt{11+19}} + 8x^{\sqrt{19+36}} + 4x^{\sqrt{11+11}} + 8x^{\sqrt{15+19}} + 20x^{\sqrt{36+36}}$.
R-degree Nirmala index $N_R(G) = \frac{\partial(G,x)}{\partial x}\Big|_{x=1}$
$= 8\sqrt{30} + 8\sqrt{55} + 4\sqrt{22} + 8\sqrt{34} + 20\sqrt{72}$
$= 338.9.$

Theorem 8. The firstincreased inverse Nirmala index of carbon nanocone $C_4[2]$ is 35.
Proof. Consider a molecular graph of carbon nanocone $C_4[2]$ as shown in figure 1. Let $E_{(u,v)}$ denote the edge connecting the vertices of u and v in G.The graph contains E_1,$E_2$and E_3edges. Using edge partitionfrom table 1 we get firstincreased inverse Nirmala index.
$IN_1^1(G) = \sum_{uv\in E(G)} \left(\frac{1}{d_u+1} + \frac{1}{d_v+1}\right)^{\frac{1}{2}}$
$= |E_{(2.2)}| \left(\frac{1}{2+1} + \frac{1}{2+1}\right)^{\frac{1}{2}} + |E_{(2.3)}|\left(\frac{1}{2+1} + \frac{1}{3+1}\right)^{\frac{1}{2}} + |E_{(3.3)}| \left(\frac{1}{3+1} + \frac{1}{3+1}\right)^{\frac{1}{2}}$
$= 4\left(\frac{1}{3} + \frac{1}{3}\right)^{\frac{1}{2}} + 16\left(\frac{1}{3} + \frac{1}{4}\right)^{\frac{1}{2}} + 28\left(\frac{1}{4} + \frac{1}{4}\right)^{\frac{1}{2}}$
$= 35.$

Theorem 9. The secondincreased inverse Nirmala index of carbon nanocone $C_4[2]$ is 65.

Proof. Using edge partition from table 1 we get secondincreased inverse Nirmala index.

$IN_2^1(G) = \sum_{uv\in E(G)}(\frac{1}{d_u+1}+\frac{1}{d_v+1})^{-\frac{1}{2}}$

$= |E_{(2.2)}|\ (\frac{1}{2+1}+\frac{1}{2+1})^{-\frac{1}{2}} + |E_{(2.3)}|(\frac{1}{2+1}+\frac{1}{3+1})^{-\frac{1}{2}} + |E_{(3.3)}|\ (\frac{1}{3+1}+\frac{1}{3+1})^{-\frac{1}{2}}$

$= 4\ (\frac{1}{3}+\frac{1}{3})^{-\frac{1}{2}} + 16(\frac{1}{3}+\frac{1}{4})^{-\frac{1}{2}} + 28\ (\frac{1}{4}+\frac{1}{4})^{-\frac{1}{2}}$

$= 65.$

IV. Conclusion

We have introduced and computed some Nirmala indices. The reduced first inverse Nirmala index andδ-first inverse Nirmala index is equal to 53 and the second inverse Nirmala index and δ-second inverse Nirmala index is equal to 44 for carbon nanocone $C_4[2]$.Average Nirmala index, Q_u type Nirmala index,R-degree Nirmala index,first and second increased inverse Nirmala indicesare investigated for carbon nanocone $C_4[2]$.

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