International Journal of Mathematical Archive-13(1), 2022, 1-7
Available online through www.ijma.info ISSN 2229 – 5046

CONTRAHARMONIC QUADRATIC INDEX OF CERTAIN NANOSTAR DENDRIMERS

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(Received On: 10-01-22 & Accepted On: 22-01-22)

ABSTRACT

Chemical Graph Theory is a branch of Mathematical Chemistry which has an important effect on the development of the Chemical Sciences. We introduce the contaharmonic-quadratic index of a molecular graph. In this paper, we determine the contraharmonic-quadratic index of some standard classes of graphs. We also compute the contraharmonic-quadratic index of certain important nanostar dendrimers.

Mathematics Subject Classification: *05C05, 05C12, 05C35.*

Keywords: *contraharmonic-quadratic index, dendrimer.*

1. INTRODUCTION

Let G be a finite, simple, connected graph with vertex set $V(G)$ and edge set $E(G)$. The degree $d_G(v)$ of a vertex v is the number of vertices adjacent to v. The edge connecting the vertices u and v will be denoted by uv. We refer to [1] for undefined term and notation.

A molecular graph is a simple graph related to the structure of a chemical compound. Each vertex of this graph represents an atom of the molecule and its edges to the bonds between atoms. Numerous topological indices are useful for establishing correlations between the structure of a molecular compound and its physico-chemical properties, see [2].

The quadratic-contraharmonic index [3] of a graph G was defined as

$$QC(G)=\sum_{uv\in E(G)}\frac{d_G(u)+d_G(u)}{\sqrt{2(d_G(u)^2+d_G(v)^2)}}.$$

We introduce the contraharmonic-quadratic index of a graph G and defined it as

$$CQ(G)=\sum_{uv\in E(G)}\frac{(d_G(u)^2+d_G(v)^2)/(d_G(u)+d_G(u))}{\sqrt{(d_G(u)^2+d_G(v)^2)/2}}=\sum_{uv\in E(G)}\frac{\sqrt{2(d_G(u)^2+d_G(v)^2)}}{d_G(u)+d_G(u)}.$$

This equation consists from contraharmonic mean of end vertex degrees of an edge uv, $(d_G(u)^2+d_G(v)^2)/(d_G(u)+d_G(u))$ as numerator and quadratic mean of end vertex degrees of the edge uv, $\sqrt{(d_G(u)^2+d_G(v)^2)/2}$ as denominator.

The geometric-arithmetic index and arithmetic-geometric index were studied, for example, in [4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14,15, 16, 17].

In this paper, we compute the contraharmonic-quadratic index of certain nanostar dendrimers. For more information about nanostar dendrimers, see [18, 19].

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2. RESULTS FOR SOME STANDARD GRAPHS

Proposition 1: Let $K_{r,s}$ be a complete bipartite graph with $1 \leq r \leq s$, and $s \geq 2$ vertices. Then

$$CQ(G) = \frac{rs\sqrt{2\left(r^2+s^2\right)}}{r+s}.$$

Proof: Let $G = K_{r,s}$ be a complete bipartite graph with $r+s$ vertices and rs edges such that $|V_1|= r$, $|V_2|= s$, $V(K_{r,s}) = V_1 \cup V_2$ for $1 \leq r \leq s$; $s \geq 2$. Every vertex of V_1 is incident with s edges and every vertex of V_2 is incident with r edges.

$$CQ(G) = \frac{rs\sqrt{2\left(r^2+s^2\right)}}{r+s}.$$

Corollary 1.1: Let $K_{r,r}$ be a complete bipartite graph with $r \geq 2$. Then

$$CQ\left(K_{r,r}\right) = r^2.$$

Corollary 1.2: Let $K_{1,r-1}$ be a star with $r \geq 2$. Then

$$CQ\left(K_{1,r-1}\right) = \frac{(r-1)\sqrt{2\left(r^2-2r+2\right)}}{r}.$$

Proposition 2: If G is an r-regular graph with n vertices and $r \geq 2$, then

$$CQ(G) = \frac{nr}{2}.$$

Proof: Let G be an r-regular graph with n vertices, $r \geq 2$ and $\frac{nr}{2}$ edges.

$$CQ(G) = \frac{nr}{2}\left(\frac{\sqrt{2\left(r^2+r^2\right)}}{r+r}\right) = \frac{nr}{2}.$$

Corollary 2.1: Let C_n be a cycle with $n \geq 3$ vertices. Then $CQ(C_n) = n$.

Corollary 2.2: Let K_n be a complete graph with $n \geq 3$ vertices. Then $CQ\left(K_n\right) = \frac{n(n-1)}{2}$.

Proposition 3: If P_n is a path with n vertices and $n \geq 3$, then $CQ\left(P_n\right) = n - 3 + \frac{2\sqrt{10}}{3}$.

3. RESULTS FOR DENDRIMER NANOSTARS $D_1[n]$

In this section, we consider a family of dendrimer nanostars with n growth stages, denoted by $D_1[n]$. The graph of $D_1[n]$ with 4 growth stages is depicted in Figure 1.

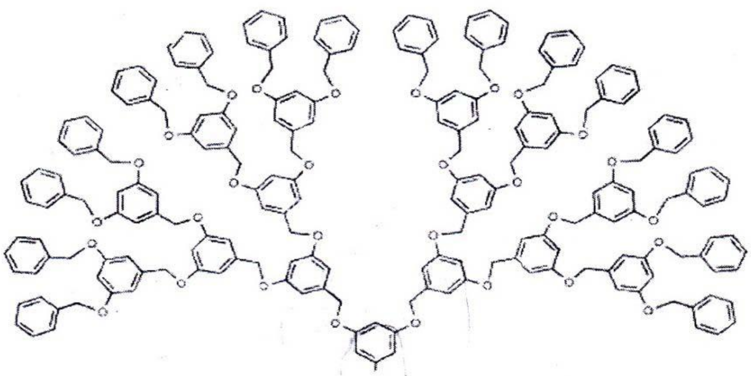

Figure-1: The molecular graph of $D_1[4]$

Let G be the graph of a dendrimer nanostar $D_1[n]$. By calculation, we obtain that G has $18 \times 2^n - 11$ edges. Also by calculation, we obtain that the edge set $E(D_1[n])$ can be divided into three partitions based on the degree of end vertices of each edge as follows:

$E_{13} = \{uv \in E(G) \mid d_G(u) = 1, d_G(v) = 3\}$, $|E_{13}| = 1$.
$E_{22} = \{uv \in E(G) \mid d_G(u) = d_G(v) = 2\}$, $|E_{22}| = 6 \times 2^n - 2$.
$E_{23} = \{uv \in E(G) \mid d_G(u) = 2, d_G(v) = 3\}$, $|E_{23}| = 12 \times 2^n - 10$.

In the following theorem, we compute the contraharmonic-quadratic index of $D_1[n]$.

Theorem 1: Let G be the graph of a dendrimer $D_1[n]$. Then

$$CQ(D_1[n]) = 6 \times 2^n + \frac{\sqrt{26}}{5} \times 12 \times 2^n + \frac{\sqrt{5}}{2} - 2 + 2\sqrt{26}.$$

Proof: From definition and by cardinalities of the edge partitions of $D_1[n]$, we have

$$CQ(D_1[n]) = \sum_{uv \in E(G)} \frac{\sqrt{2(d_G(u)^2 + d_G(v)^2)}}{d_G(u) + d_G(u)}$$

$$= \frac{\sqrt{2(1^2+3^2)}}{1+3} + \frac{(6 \times 2^n - 2)\sqrt{2(2^2+2^2)}}{2+2} + \frac{(12 \times 2^n - 10)\sqrt{2(2^2+3^2)}}{2+3}$$

gives the desired result after simplification.

4. RESULTS FOR DENDRIMER NANOSTARS $D_3[n]$

We consider the dendrimer nanostar with n growth stages, denoted by $D_3[n]$, where $n \geq 0$, see Figure 2. Let G be the dendrimer nanostar $D_3[n]$. From Figure 2, it is easy to see that the vertices of $D_3[n]$ are either of degree 1, 2 or 3. By calculation, we obtain that $D_3[n]$ has $24 \times 2^n - 20$ vertices and $24(2^{n+1} - 1)$ edges.

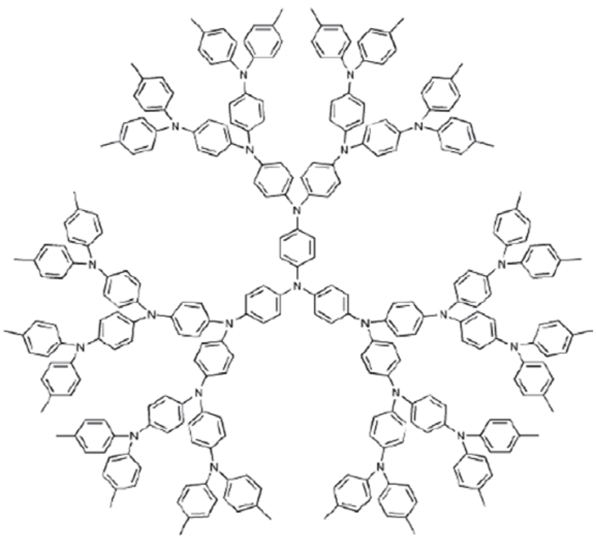

Figure-2: Dendrimer nanostar with 3-growth $D_3[n]$

Also by algebraic method, we partition $E(G)$ into four sets based on the sum of degrees of the end vertices of each edge.

$E_{13} = \{uv \in E(G) \mid d_G(u) = 1, d_G(v) = 3\}$, $|E_{13}| = 3 \times 2^n$.
$E_{22} = \{uv \in E(G) \mid d_G(u) = d_G(v) = 2\}$, $|E_{22}| = 12 \times 2^n - 6$.
$E_{23} = \{uv \in E(G) \mid d_G(u) = 2, d_G(v) = 3\}$, $|E_{23}| = 24 \times 2^n - 12$.
$E_{33} = \{uv \in E(G) \mid d_G(u) = d_G(v) = 3\}$, $|E_{33}| = 9 \times 2^n - 6$.

In the following theorem, we compute the contraharmonic-quadratic index of $D_3[n]$.

Theorem 2: Let G be the graph of a dendrimer $D_3[n]$. Then

$$CQ(D_3[n]) = \left(\frac{3\sqrt{5}}{2} + \frac{24\sqrt{26}}{5} + 21\right)2^n - \frac{12\sqrt{26}}{5} - 12.$$

Proof: From definition and by cardinalities of the edge partitions of $D_3[n]$, we have

$$CQ(D_3[n]) = \sum_{uv\in E(G)} \frac{\sqrt{2(d_G(u)^2 + d_G(v)^2)}}{d_G(u)+d_G(u)}$$

$$= \frac{(3\times 2^n)\sqrt{2(1^2+3^2)}}{1+3} + \frac{(12\times 2^n - 6)\sqrt{2(2^2+2^2)}}{2+2} + \frac{(24\times 2^n - 12)\sqrt{2(2^2+3^2)}}{2+3}$$

$$+ \frac{(9\times 2^n - 6)\sqrt{2(3^2+3^2)}}{3+3}.$$

After simplification, we obtain the desired result.

5. RESULTS FOR $NS_1[n]$ DENDRIMER NANOSTARS

In this section, we focus on the polypropylenimine octaamine dendrimer, denoted by $NS_1[n]$, where n is the steps of growth in this type of dendrimer. The graph of $NS_1[n]$ nanostar dendrimer is presented in Figure 3.

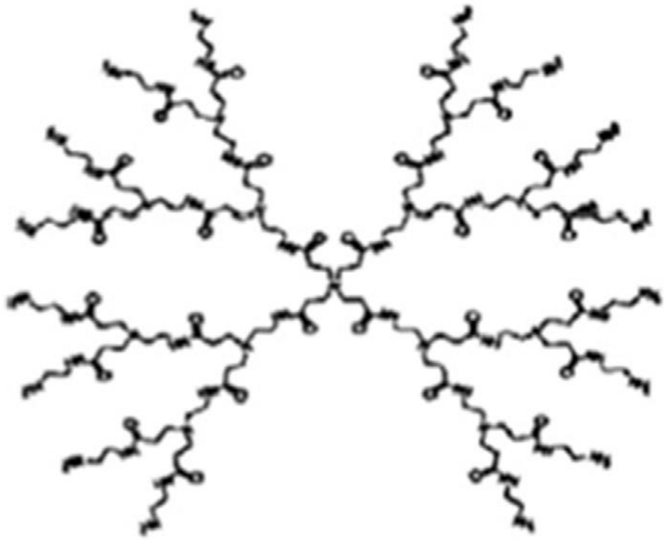

Figure-3: The molecular graph of $NS_1[n]$

Let G be the graph of polypropylenimine octaamine dendrimer $NS_1[n]$. By calculation, we obtain that G has $32 \times 2^n - 29$ edges. From Figure 3, it is easy to see that the vertices of NS_1[n] are either of degree 1, 2 or 3. Also by calculation, we obtain that the edge set $E(NS_1[n])$ can be divided into four partitions based on the degree of end vertices of each edge as follows:

$E_{12} = \{uv \in E(G) \mid d_G(u) = 1, d_G(v) = 2\}$, $|E_{12}| = 2 \times 2^n$.
$E_{13} = \{uv \in E(G) \mid d_G(u) = 1, d_G(v) = 3\}$, $|E_{13}| = 4 \times 2^n - 4$.
$E_{22} = \{uv \in E(G) \mid d_G(u) = d_G(v) = 2\}$, $|E_{22}| = 12 \times 2^n - 11$.
$E_{23} = \{uv \in E(G) \mid d_G(u) = 2, d_G(v) = 3\}$, $|E_{23}| = 14 \times 2^n - 14$.

In the following theorem, we compute the contraharmonic-quadratic index of $NS_1[n]$.

Theorem 3: Let G be the graph of a dendrimer $NS_1[n]$. Then

$$CQ\left(NS_1[n]\right)=\left(\frac{2\sqrt{10}}{3}+2\sqrt{5}+12+\frac{14\sqrt{26}}{5}\right)2^n-2\sqrt{5}-11-\frac{14\sqrt{26}}{5}.$$

Proof: From definition and by cardinalities of the edge partitions of $NS_1[n]$, we have

$$\begin{aligned}CQ\left(NS_1[n]\right)&=\sum_{uv\in E(G)}\frac{\sqrt{2(d_G(u)^2+d_G(v)^2)}}{d_G(u)+d_G(u)}\\&=\frac{(2\times 2^n)\sqrt{2\left(1^2+2^2\right)}}{1+2}+\frac{(4\times 2^n-4)\sqrt{2\left(1^2+3^2\right)}}{1+3}+\frac{(12\times 2^n-11)\sqrt{2\left(2^2+2^2\right)}}{2+2}\\&+\frac{(14\times 2^n-14)\sqrt{2\left(2^2+3^2\right)}}{2+3}.\end{aligned}$$

After simplification, we obtain the desired result.

6. RESULTS FOR DENDRIMERS NANOSTARS $NS_2[n]$

In this section, we focus on the polypropylenimine octaamine dendrimer, denoted by $NS_2[n]$, where n is the steps of growth in this type of dendrimer. The graph of $NS_2[n]$ dendrimer nanostar is presented in Figure 4.

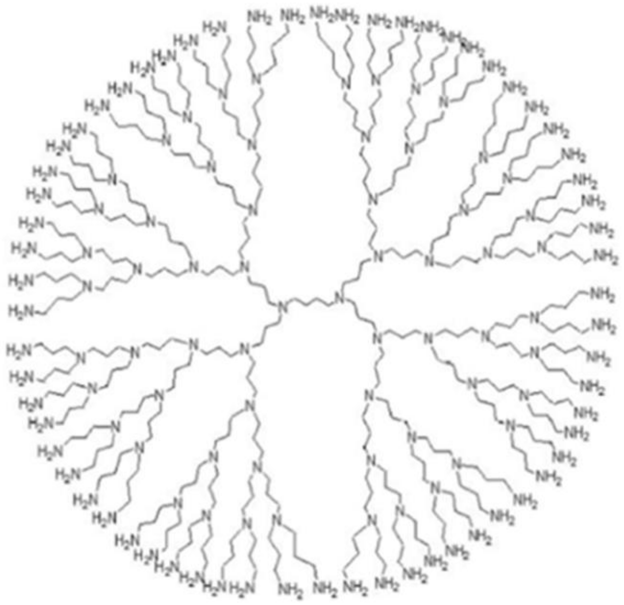

Figure-4: The structure of $NS_2[n]$

Let G be the graph of polypropylenimine octaamine dendrimer $NS_2[n]$. By calculation, we obtain that G has $16 \times 2^n - 11$ edges. From Figure 4, it is easy to see that the vertices of $NS_2[n]$ are either of degree 1, 2 or 3. Also by calculation, we obtain that the edge set $E(NS_2[n])$ can be divided into three partitions based on the degree of end vertices of each edge as follows:

$E_{12} = \{uv \in E(G) \mid d_G(u) = 1, d_G(v) = 2\}$, $|E_{12}| = 2 \times 2^n$.

$E_{22} = \{uv \in E(G) \mid d_G(u) = d_G(v) = 2\}$, $|E_{22}| = 8 \times 2^n - 5$.

$E_{23} = \{uv \in E(G) \mid d_G(u) = 2, d_G(v) = 3\}$, $|E_{23}| = 6 \times 2^n - 6$.

In the following theorem, we compute the contraharmonic-quadratic index of $NS_2[n]$.

Theorem 4: Let *G* be the graph of a dendrimer $NS_2[n]$. Then

$$CQ\left(NS_2[n]\right) = \left(\frac{2\sqrt{10}}{3} + 8 + \frac{6\sqrt{26}}{5}\right)2^n - 5 - \frac{6\sqrt{26}}{5}.$$

Proof: From definition and by cardinalities of the edge partitions of $NS_2[n]$, we have

$$CQ\left(NS_2[n]\right) = \sum_{uv\in E(G)} \frac{\sqrt{2(d_G(u)^2 + d_G(v)^2)}}{d_G(u) + d_G(u)}$$

$$= \frac{(2\times 2^n)\sqrt{2\left(1^2+2^2\right)}}{1+2} + \frac{(8\times 2^n - 5)\sqrt{2\left(2^2+2^2\right)}}{2+2} + \frac{(6\times 2^n - 6)\sqrt{2\left(2^2+3^2\right)}}{2+3}.$$

After simplification, we obtain the desired result.

7. RESULTS FOR *NS*$_3$[*n*] DENDRIMER NANOSTARS

In this section, we focus on the molecular graph structure of the first class of dendrimer nanostars. This family of dendrimer nanostars is denoted by $NS_3[n]$, where *n* is the steps of growth in this type of dendrimer nanostars. The molecular graph structure of $NS_3[3]$ dendrimer nanostar is presented in Figure 5.

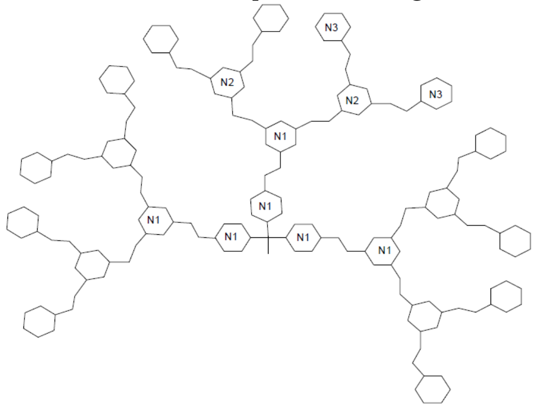

Figure-5: The structure of $NS_3[3]$

Let G be the molecular graph of a dendrimer nanostar $NS_3[n]$. By calculation, we obtain that *G* has $27 \times 2^n - 5$ edges. From Figure 5, it is easy to see that the vertices of $NS_3[n]$ are either of degree 1, 2, 3 or 4. Also by calculation, we obtain that the edge set $E(NS_3[n])$ can be divided into three partitions based on the degree of end vertices of each edge as follows:

$E_{14} = \{uv \in E(G) \mid d_G(u) = 1, d_G(v) = 4\}$, $|E_{14}| = 1$
$E_{22} = \{uv \in E(G) \mid d_G(u) = d_G(v) = 2\}$, $|E_{22}| = 9 \times 2^n + 3$.
$E_{23} = \{uv \in E(G) \mid d_G(u) = 2, d_G(v) = 3\}$, $|E_{23}| = 18 \times 2^n - 12$.
$E_{34} = \{uv \in E(G) \mid d_G(u) = 3, d_G(v) = 4\}$, $|E_{34}| = 3$.

In the following theorem, we compute the contraharmonic-quadratic index of $NS_3[n]$.

Theorem 5: Let *G* be the graph of a dendrimer $NS_3[n]$. Then

$$CQ\left(NS_3[n]\right) = \left(9 + \frac{18\sqrt{26}}{5}\right)2^n + \frac{\sqrt{34}}{5} + 3 - \frac{12\sqrt{26}}{5} + \frac{15\sqrt{2}}{7}.$$

Proof: From definition and by cardinalities of the edge partitions of $NS_3[n]$, we have

$$CQ\left(NS_3[n]\right) = \sum_{uv\in E(G)} \frac{\sqrt{2(d_G(u)^2 + d_G(v)^2)}}{d_G(u) + d_G(u)}$$

$$= \frac{\sqrt{2\left(1^2+4^2\right)}}{1+4} + \frac{(9\times 2^n + 3)\sqrt{2\left(2^2+2^2\right)}}{2+2} + \frac{(18\times 2^n - 12)\sqrt{2\left(2^2+3^2\right)}}{2+3} + \frac{3\sqrt{2\left(3^2+4^2\right)}}{3+4}.$$

After simplification, we obtain the desired result.

8. CONCLUSION

In this study, we have introduced the contraharmonic-quadratic (CQ) index of a graph. We have computed the CQ index for some standard graphs. Also we have determined the CQ index for some important chemical structures such as nanostar dendrimers. Many questions are suggested by this research, among them are the following:

1. Find the extremal values and extremal graphs of the CQ index.
2. Characterize the CQ index in terms of other degree based topological indices.

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Source of support: Nil, Conflict of interest: None Declared.