

Computation of E-Banhatti Nirmala Indices of Tetrameric 1,3-Adamantane

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Abstract. In this paper, we introduce the E-Banhatti Nirmala index and the modified E-Banhatti Nirmala index and their corresponding exponentials of a graph. Furthermore, we determine these newly defined E-Banhatti Nirmala indices and their corresponding exponentials for some standard graphs and tetrameric 1,3-Adamantane.

Keywords: E-Banhatti Nirmala index, modified E-Banhatti Nirmala index, tetrameric 1,3-adamantane.

AMS Mathematics Subject Classification): 05C05, 05C07, 05C09, 05C92

1. Introduction

Throughout this paper, we consider simple graphs which are finite, connected, undirected graphs without loops and multiple edges. Let G be such a graph with vertex set $V(G)$ and edge set $E(G)$. The degree $d_G(u)$ of a vertex u is the number of vertices adjacent to u . For term and concept not given here, we refer the book [1].

A molecular graph is a simple graph, representing the carbon atom skeleton of an organic molecule of the hydrocarbon. Therefore the vertices of a molecular graph represent the carbon atoms and its edges the carbon-carbon bonds. Chemical Graph Theory is a branch of Mathematical Chemistry which has an important effect on the development of Chemical Sciences. Several graph indices [2] have found some applications in Chemistry, especially in QSPR/QSAR research [3].

In [4], Kulli defined the Bhanhatti degree of a vertex u of a graph G as

$$B(u) = \frac{d_G(e)}{n - d_G(u)},$$

where n is the number of vertices of G and the vertex u and edge e are incident in G .

The first and second E-Banhatti indices were introduced by Kulli in [4] and they are defined as

$$EB_1(G) = \sum_{uv \in E(G)} [B(u) + B(v)],$$
$$EB_2(G) = \sum_{uv \in E(G)} B(u)B(v).$$

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We propose the E-Banhatti Nirmala index of a graph G and defined it as

$$EBN(G) = \sum_{uv \in E(G)} \sqrt{B(u) + B(v)}.$$

We introduce the modified E-Banhatti Nirmala index of a graph G and defined it as

$${}^m EBN(G) = \sum_{uv \in E(G)} \frac{1}{\sqrt{B(u) + B(v)}}.$$

Considering the E-Banhatti Nirmala and modified E-Banhatti Nirmala indices, we define their corresponding exponentials of a graph G as

$$EBN(G, x) = \sum_{uv \in E(G)} x^{\sqrt{B(u) + B(v)}},$$

$${}^m EBN(G, x) = \sum_{uv \in E(G)} x^{\frac{1}{\sqrt{B(u) + B(v)}}}.$$

In Chemical Graph Theory, several graph indices were introduced and studied such as the Wiener index [6, 7], the Zagreb indices [8, 9], the Revan indices [10, 11], the Gourava indices [12, 13], the reverse indices [14, 15] and the Bhanthi indices [16, 17].

In this paper, we compute the E-Banhatti Nirmala index and the modified E-Banhatti Nirmala index for some standard graphs and tetrameric 1,3-adamanane.

2. Results for some standard graphs

Proposition 1. If G is an r -regular graph with n vertices and $r \geq 2$, then

$$EBN(G) = nr \sqrt{\frac{r-1}{n-r}}.$$

Proof: Let G be an r -regular graph with n vertices and $r \geq 2$. Then G has $\frac{nr}{2}$ edges. For any edge $uv=e$ in G , $d_G(e) = d_G(u) + d_G(v) - 2 = 2r - 2$.

From definition we have

$$\begin{aligned} EBN(G) &= \sum_{uv \in E(G)} \sqrt{B(u) + B(v)} \\ &= \frac{nr}{2} \sqrt{\left(\frac{2r-2}{n-r}\right) + \left(\frac{2r-2}{n-r}\right)} = nr \sqrt{\frac{r-1}{n-r}}. \end{aligned}$$

Corollary 1.1. Let C_n be a cycle with $n \geq 3$ vertices. Then

$$EBN(C_n) = 2n \sqrt{\frac{1}{n-2}}.$$

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Corollary 1.2. Let K_n be a complete graph with $n \geq 3$ vertices. Then

$$EBN(K_n) = n(n-1)\sqrt{n-2}.$$

Proposition 2. Let P_n be a path with $n \geq 3$ vertices. Then

$$\begin{aligned} EBN(P_n) &= 2 \left[\left(\frac{1}{n-1} \right) + \left(\frac{2}{n-2} \right) \right]^{\frac{1}{2}} + (n-3) \left[\left(\frac{2}{n-2} \right) + \left(\frac{2}{n-2} \right) \right]^{\frac{1}{2}} \\ &= n \sqrt{\frac{3n-4}{(n-1)(n-2)}} + 2(n-3) \sqrt{\frac{1}{n-2}}. \end{aligned}$$

Proposition 3. Let $K_{m,n}$ be a complete bipartite graph with $1 \leq m \leq n$ and $n \geq 2$. Then

$$EBN(K_{m,n}) = \sqrt{mn} \sqrt{(m+n)(m+n-2)}.$$

Proof: Let $K_{m,n}$ be a complete bipartite m n graph with $m+n$ vertices and mn edges such that $|V_1| = m$, $|V_2| = n$, $V(K_{r,s}) = V_1 \cup V_2$ for $1 \leq m \leq n$, and $n \geq 2$. Every vertex of V_1 is incident with n edges and every vertex of V_2 is incident with m edges. Then $d_G(e) = d_G(u) + d_G(v) - 2 = m + n - 2$.

$$\begin{aligned} EBN(K_{m,n}) &= \sum_{uv \in E(G)} \sqrt{B(u) + B(v)} \\ &= mn \left[\left(\frac{m+n-2}{m+n-n} \right) + \left(\frac{m+n-2}{m+n-m} \right) \right]^{\frac{1}{2}} \\ &= \sqrt{mn} \sqrt{(m+n)(m+n-2)}. \end{aligned}$$

Corollary 3.1. Let $K_{n,n}$ be a complete bipartite graph with $n \geq 2$. Then

$$EBN(K_{n,n}) = 2n\sqrt{n(n-1)}.$$

Corollary 3.2. Let $K_{1,n}$ be a star with $n \geq 2$. Then

$$EBN(K_{1,n}) = \sqrt{n} \sqrt{(n+1)(n-1)}.$$

3. Results for Tetrameric 1,3-Adamantane

In Chemistry, diamondoids are variants of the carbon cage known as a adamantane (C_{10} , H_{16}), the smallest unit cage structure of the diamond crystal lattice. We focus on the molecular graph structure of the family of tetrameric 1,3-adamantane, denoted by $TA[n]$. Let G be the graph of a tetrameric 1,3-adamantane $TA[n]$. The graph of a tetrameric 1,3-adamantane $TA[4]$ is presented in Figure 1.

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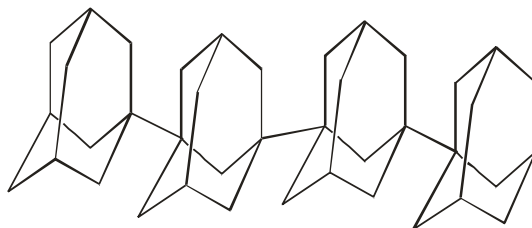


Figure 1

By calculation, G has $10n$ vertices and $13n - 1$ edges. Also by calculation, we obtain three edge partitions of G based on the degrees of the end vertices of each edge as follows:

$$\begin{aligned} E_1 &= \{uv \in E(G) \mid d_G(u)=2, d_G(v)=3\}, & |E_1| &= 6n + 6. \\ E_2 &= \{uv \in E(G) \mid d_G(u)=2, d_G(v)=4\}, & |E_2| &= 6n - 6. \\ E_3 &= \{uv \in E(G) \mid d_G(u)=d_G(v) = 4\}, & |E_3| &= n - 1. \end{aligned}$$

Therefore, in $TA[n]$, there are three types of edges based on the Banhatti degree of end vertices of each edge as follow:

$$\begin{aligned} BE_1 &= \{uv \in E(G) \mid B(u) = \frac{3}{10n-2}, B(v) = \frac{3}{10n-3}\}, & |BE_1| &= 6n+6. \\ BE_2 &= \{uv \in E(G) \mid B(u) = \frac{4}{10n-2}, B(v) = \frac{4}{10n-4}\}, & |BE_2| &= 6n-6. \\ BE_3 &= \{uv \in E(G) \mid B(u) = \frac{6}{10n-4}, B(v) = \frac{6}{10n-4}\}, & |BE_3| &= n-1. \end{aligned}$$

We determine the E-Banhatti Nirmala index of $TA[n]$.

Theorem 1. Let G be the graph of a tetrameric 1,3-adamantane $TA[n]$ with $10n$ vertices and $13n-1$ edges. Then

$$EBN(TA[n]) = (6n+6)\sqrt{\frac{60n-15}{(10n-2)(10n-3)}} + (6n-6)\sqrt{\frac{20n-6}{(5n-1)(5n-2)}} + (n-1)\sqrt{\frac{6}{5n-2}}.$$

Proof: From definition and by cardinalities of the Banhatti edge partition of $TA[n]$, we obtain

$$\begin{aligned} EBN(TA[n]) &= \sum_{uv \in E(TA[n])} \sqrt{B(u) + B(v)} \\ &= (6n+6)\sqrt{\left(\frac{3}{10n-2}\right) + \left(\frac{3}{10n-3}\right)} + (6n-6)\sqrt{\left(\frac{4}{10n-2}\right) + \left(\frac{4}{10n-4}\right)} \end{aligned}$$

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$$+(n-1)\sqrt{\left(\frac{6}{10n-4}\right)+\left(\frac{6}{10n-4}\right)}.$$

After simplification, we get the desired result.

We compute the modified E-Banhatti Nirmala index of $TA[n]$.

Theorem 2. Let G be the graph of a tetrameric 1,3-adamantane $TA[n]$ with $10n$ vertices and $13n-1$ edges. Then

$${}^m EBN(TA[n]) = (6n+6)\sqrt{\frac{(10n-2)(10n-3)}{60n-15}} + (6n-6)\sqrt{\frac{(5n-1)(5n-2)}{20n-6}} + (n-1)\sqrt{\frac{5n-2}{6}}.$$

Proof: From definition and by cardinalities of the Banhatti edge partition of $TA[n]$, we have

$$\begin{aligned} {}^m EBN(TA[n]) &= \sum_{uv \in E(TA[n])} [B(u) + B(v)]^{-\frac{1}{2}} \\ &= (6n+6)\left[\left(\frac{3}{10n-2}\right) + \left(\frac{3}{10n-3}\right)\right]^{-\frac{1}{2}} + (6n-6)\left[\left(\frac{4}{10n-2}\right) + \left(\frac{4}{10n-4}\right)\right]^{-\frac{1}{2}} \\ &\quad + (n-1)\left[\left(\frac{6}{10n-4}\right) + \left(\frac{6}{10n-4}\right)\right]^{-\frac{1}{2}} \end{aligned}$$

gives the desired result after simplification.

By using definitions and by cardinalities of the Banhatti edge partition of $TA[n]$, we obtain the E-Banhatti Nirmala and modified E-Banhatti Nirmala exponentials of $TA[n]$.

Theorem 3. The E-Banhatti Nirmala exponential of $TA[n]$ is given by

$$EBN(TA[n], x) = (6n+6)x^{\sqrt{\frac{60n-15}{(10n-2)(10n-3)}}} + (6n-6)x^{\sqrt{\frac{20n-6}{(5n-1)(5n-2)}}} + (n-1)x^{\sqrt{\frac{6}{5n-2}}}.$$

Theorem 4. The modified E-Banhatti Nirmala exponential of $TA[n]$ is given by

$${}^m EBN(TA[n], x) = (6n+6)x^{\sqrt{\frac{(10n-2)(10n-3)}{60n-15}}} + (6n-6)x^{\sqrt{\frac{(5n-1)(5n-2)}{20n-6}}} + (n-1)x^{\sqrt{\frac{5n-2}{6}}}.$$

4. Conclusion

In this study, we have introduced the E-Banhatti Nirmala index and the modified E-Banhatti Nirmala index and their corresponding exponentials of a graph. These newly defined E-Banhatti Nirmala indices and their corresponding exponentials for some standard graphs and tetrameric 1,3-adamantane have been determined. This study is a new direction in Graph Indices.

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Authors' Contributions. All the authors contributed equally to this work.

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