Connective Eccentric Index of Circumcoronene Homologous Series of Benzenoid $H_k$

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ABSTRACT

Let $G$ be a molecular graph, a topological index is a numeric quantity related to $G$ which is invariant under graph automorphisms. The eccentric connectivity index $\xi(G)$ is defined as $\xi(G) = \sum_{v \in V(G)} d_v \times \varepsilon(v)$ where $d_v$, $\varepsilon(v)$ denote the degree of vertex $v$ in $G$ and the largest distance between $v$ and any other vertex $u$ of $G$. The connective eccentric index of graph $G$ is defined as $C\xi(G) = \sum_{v \in V(G)} \frac{d_v}{\varepsilon(v)}$. In the present paper we compute the connective eccentric index of Circumcoronene Homologous Series of Benzenoid $H_k$ ($k \geq 1$).

Keywords: Molecular graphs; Benzenoid; Connective eccentric index; Eccentric connectivity index

1. INTRODUCTION

In theoretical chemistry molecular structure descriptor or topological indices, are used to compute properties of chemical compounds. Throughout this paper, graph means simple connected graph [1-3]. Let $G$ be a molecular graph, the vertex and edge sets of a graph $G$ are denoted by $V(G)$ and $E(G)$, respectively. If $x,y \in V(G)$ then the distance $d(x,y)$ between $x$ and $y$ is defined as the length of a minimum path connecting $x$ and $y$.

In 1997, the Eccentric Connectivity index $\xi(G)$ of the molecular graph $G$ was proposed by Sharma, Goswami and Madan and is defined as [4]:

$$\xi(G) = \sum_{v \in V(G)} d_v \times \varepsilon(v)$$

where $d_v$ denotes the degree of the vertex $v$ in $G$ and $\varepsilon(v)$ denote the largest distance between $v$ and any other vertex $u$ of $G$. In other words, $\varepsilon(v) = \text{Max}\{d(v,u) | \forall v \in V(G)\}$.

In 2000, the Connective Eccentric index $C\xi(G)$ was defined by Gupta, Singh and Madan [5,6] as follows:

$$C\xi(G) = \sum_{v \in V(G)} \frac{d_v}{\varepsilon(v)}$$
where \( d_v, \varepsilon(v) \) denote the degree and eccentric of vertex \( v \) in \( G \). See [7-26] for more details and other versions of \textit{Eccentric indices} and \textit{Eccentric polynomials}.

The goal in this paper is computing the Connective eccentric index of \textit{Circumcoronene Homologous Series of Benzenoid} \( H_k \) \((k \geq 1)\).

2. RESULTS AND DISCUSSION

In this section, we compute the Connective eccentric index \( C^\varepsilon(G) \) of \textit{Circumcoronene Homologous Series of Benzenoid}. Three first members of this Benzenoid family \((H_1 = benzene, H_2 = coronene and H_3 = circumcoronene)\) are shown in Figure 1. \textit{Circumcoronene Homologous Series of Benzenoid} is generated from famous molecule \textit{Benzene} or cycle \( C_6 \). We encourage reader to references [18-38] to study some properties of this Benzenoid family.

![Figure 1](image-url)

\( H_1 = C_6 \)  
\( H_2 = C_a(C_6) \)  
\( H_3 = \text{circumcoronene} \)

\( \forall k \in \mathbb{N} \) \textit{Circumcoronene Homologous Series of Benzenoid} \( H_k \) has \( 6k^2 \) atoms/vertices and \( 9k^2 - 6k \) bonds/edges (see Figure 2). For further study and more detail of this Benzenoid family, see the paper series [27-35]. Now, we have following theorem for this benzenoid graphs.

**Theorem 1.** Let \( G \) be the \textit{Circumcoronene Homologous Series of Benzenoid} \( H_k \) \((\forall k \geq 1)\). Then the Connective Eccentric index \( C^\varepsilon(G) \) of \( H_k \) is equal to

\[
C^\varepsilon(H_k) = \sum_{i=1}^{k-1} \left( \frac{9i(4k+4i-1)}{2i^2+(4k^2i+2k^2-k)} \right) + \frac{12k}{4k-1}
\]

Before prove the Theorem 1, we denote all vertices and edges of \textit{Circumcoronene Homologous Series of Benzenoid} \( H_k \) as follow adn is shown in Figure 2, \((Z_i, \text{ is the cycle finite group}):\)

\[
V(H_k) = \{ \gamma^i_{z,j}, \beta^i_{z,l} \mid i = 1, \ldots, k; j \in Z_i, l \in Z_{i-1}, z \in Z_6 \}
\]
and \( E(H_k) = \{ \beta_{z,j}^i \gamma_{z,j}^i, \beta_{z,j}^i \gamma_{z,j+1}^i, \beta_{z,j}^i \gamma_{z,j+1}^{i+1}, \beta_{z,j}^i \gamma_{z,j+1}^{i-1} \mid i \in Z_k, j \in Z_i, z \in Z_6 \} \)

**Proof.** By considering Circumcoronene Homologous Series of Benzenoid \( G = H_k (\forall k \geq 1) \) as shown in Figure 2 and refer to [18-26] and using the Ring-cut Method for circumcoronene homologous series of Benzenoid, we can compute its connective eccentric index. The Ring-cut Method is a modify version of the thoroughbred Cut Method. The general form of this method is introduced in [18-26] For more study and detail information of the Cut Method see [28,31,32].

![Figure 2. The general representation of Circumcoronene Homologous Series of Benzenoid \( H_k (k \geq 1) \) [18-26]. To compute the connective eccentric index of \( H_k \), we see that

\[ \forall i = 2, \ldots, k; j \in Z_{i-1} \& z \in Z_6: \varepsilon(\beta_{z,j}^i) = 2k+2i-2 \]

\[ \forall i = 1, \ldots, k; j \in Z_i \& z \in Z_6: \varepsilon(\gamma_{z,j}^i) = 2k+2i-1 \]
Also, by according to Figure 2, one can see that the vertices in general representation of molecular graph Circumcoronene Homologous Series of Benzenoid $H_k$ have degree two or three, such that

$$V_2(H_k) = \{ v \in V(H_k) \mid d_v = 2 \} = \{ \gamma^k_{z,1} \mid \forall i \in Z_i \& z \in Z_6 \}$$

and alternatively

$$V_3(H_k) = V(H_k) - V_2(H_k).$$

$$C^\xi(H_k) = \sum_{v \in V(G)} \frac{d_v}{\epsilon(v)}$$

$$= \sum_{\gamma^k_{z,j} \in V_2(H_k)} \frac{2}{4k-1} + \sum_{\gamma^k_{z,j} \in V_3(H_k)} \frac{3}{2k+2i-1} + \sum_{\beta^i_{z,j} \in V_3(H_k)} \frac{3}{2k+2i-2}$$

$$= \sum_{i=1}^{k-1} \sum_{j=1}^{i-1} \left( \frac{2}{4k-1} \right) + \sum_{i=1}^{k-1} \sum_{j=1}^{k-i} \left( \frac{3}{2k+2i-1} \right) + \sum_{i=1}^{k-1} \sum_{j=1}^{k-i} \left( \frac{3}{2k+2i-2} \right)$$

$$= 2 \times 6k \left( \frac{2}{4k-1} \right) + \sum_{i=1}^{k-1} \left( \frac{3 \times 6i}{2k+2i-1} \right) + \sum_{j=1}^{k-1} \left( \frac{3 \times 6j}{2k+2j} \right)$$

$$= \frac{18i}{2(k+i)(2k+2i-1)} + \frac{12k}{4k-1}$$

Thus $\forall k \geq 1$, the connective eccentric index of $H_k$ is equal to

$$C^\xi(H_k) = \sum_{i=1}^{k-1} \left( \frac{9i(4k+4i-1)}{2i^2 + (4k-1)i + 2k^2 - k} \right) + \frac{12k}{4k-1}$$

and this completed the proof of Theorem 1.
3. CONCLUSION

The eccentric connectivity index $\xi(G)$ is defined as $\xi(G)=\sum_{v \in V(G)} d_v \times \epsilon(v)$ where $d_v$, $\epsilon(v)$ denote the degree of vertex $v$ in $G$ and the largest distance between $v$ and any other vertex $u$ of $G$. In this paper, we counting the connective eccentric index $C^\xi(G)=\sum_{v \in V(G)} d_v/\epsilon(v)$ of Circumcoronene Homologous Series of Benzenoid $H_k (k \geq 1)$.

References


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