New results on eccentric connectivity indices of V-Phenylenic nanotube

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Introduction

Let G=(V;E) be a molecular graph, where V(G) is a non-empty set of vertices and E(G) is a set of edges. Cardinality of the vertex set is said to be order of graph G, denoted by |V(G)| and the cardinality of edge set is the size of graph, denoted by |E(G)|. Number of edges incident with vertex v is called the degree of vertex. The distance from u to v, where u,v∈V(G), is defined as the length of the shortest path from u to v, denoted by d(u;v). The eccentricity of a vertex v∈V(G), denoted by ϵ(v), is the maximum distance between the v vertex to all other vertices i.e.

\[ \epsilon(u) = \max\{d(u,v) \mid \forall \ u \in V(G)\} \]

The topological index which is also referred to molecular descriptor is a real number which describes the properties of a certain chemical compounds. The study of topological indices on different chemical structures has been an attractive area of research for all graph theorist. Actually, it is a bridge between mathematics and chemistry. Simplest topological indices of a graph G are the order, size, degree of vertices v and distance between vertices. Among the molecular descriptors, topological connectivity indices are very important and many of them have found applications as means to model chemical, pharmaceutical and other properties of the molecules. In 1975, oldest topological connectivity index of a connected graph G introduced by M. Randić, who showed this index to reflect the molecular branching [1-3]. Now, we call it Randić connectivity index R(G) is equal to

\[ R(G) = \sum_{u,v \in V(G)} \frac{1}{d(u) d(v)} \]

where d(v) denotes the degree of vertex v of G.

The eccentric connectivity index of a graph G was proposed by Sharma, Goswami and Madan in [4], as \( \zeta_e(G) = \sum_{v \in V(G)} d(v) \epsilon(v) \) The eccentric connectivity index was successfully used for mathematical models of biological activities of diverse nature [45, 46, 47, 48]. The prediction of the physico-chemical,

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pharmacological and toxicological properties of compounds directly from their molecular structure has become an important tool in pharmaceutical drug design. The parameters derived from a graph theoretic model of a chemical structure are being used not only in QSAR studies, but also in the environmental hazard assessment of chemicals. Eccentric connectivity index revealed a high degree of predictability of pharmaceutical properties, providing leads for developing safe and potent anti-HIV compounds [40-44, 49, 50]. Eccentric connectivity index is also proposed as a measure of branching in alkanes [51].

Gupta et al. [5] introduced the connective eccentric index for a graph

$$C^e(G) = \sum_{v \in V(G)} d(v) / \xi(v)$$

Recently, S. Ediz et al. defined Ediz eccentric connectivity index of G, denoted by $$E^e(G)$$ and is defined as

$$E^e(G) = \sum_{v \in V(G)} S_v / \xi(v)$$

where $$S_v$$ is the sum of degrees of all vertices adjacent to vertex v [6, 7]. A generalization of eccentric connectivity index, known as augmented eccentric connectivity index of a graph G was proposed by Dureja and Madan in [8]:

$$A^e(G) = \sum_{v \in V(G)} M_v / \xi(v)$$

where $$M_v$$ is the product of degrees of all vertices adjacent to vertex v. For further details about these new connectivity indices see [9-29].

In this work, we extended the results of [30] and determined the exact formulas for Ediz and Augmented eccentric connectivity indices.

**Result and discussion**

In this study, we deal with the molecular graph of V-Phenylenic nanotube VPHX[p;q], where p denotes the number of hexagons in a column and q denotes the number of hexagons in a row of the V-Phenylenic nanotube.

In this section, we computed the Ediz eccentric connectivity and augmented eccentric connectivity indices of V-Phenylenic nanotube VPHX[p;q]. For further details and more study about the V-Phenylenic nanotube VPHX[p;q] see [31-39]. Rao and Lakshmi calculated some eccentric connectivity index of V-Phenylenic nanotube [52]. In this research study we extend the results found in [52] and calculated above mention eccentric connectivity indices.

Figure 1 demonstrates the representation of V-Phenylenic nanotube VPHX[p;q]. As seen in Figure 1, the number of vertices and edges in G=VPHX[p;q] are equal to 6pq and 9pq-q, respectively. It is clear that there are 2p vertices of degree 2, 6pq-2p vertices of degree 3, We denote the set of vertices of degree two and degree three by V_2 and V_3, respectively. The graph of V-Phenylenic nanotube has 4p rows and q columns.

To compute the Ediz eccentric index and Augmented eccentric connectivity index of the V-Phenylenic nanotube VPHX[p;q], we need vertex partition of the V-Phenylenic nanotube VPHX[p;q] based on degree sum and degree multiplication of neighbors vertices, respectively.

**FIGURE 1** The molecular graph of V-Phenylenic nanotube [30]
TABLE 1 Vertex partition based on degree sum of neighbor vertices

| $S_v$ where $v \in VPHX [p;q]$ | Number of Vertices |
|---------------------------------|-------------------|
| 8                               | 2p                |
| 9                               | 4p                |
| 10                              | 2pq               |
| 12                              | 2p                |
| 13                              | 2pq-2p            |
| 14                              | 2p                |
| 15                              | 2pq-2p            |

TABLE 2 Vertex partition based on product of degree of neighbor vertices

| $M_v$ where $v \in (VPHX [p,q])$ | Number of Vertices |
|-----------------------------------|-------------------|
| 16                                | 2p                |
| 20                                | 24p               |
| 24                                | 2p                |
| 72                                | 2p                |
| 25                                | 2pq               |
| 108                               | 2pq-2p            |
| 100                               | 2p                |
| 125                               | 2pq-2p            |

To compute the sum of degrees of all neighbors of vertices in the V-Phenylenic nanotube $VPHX[p;q]$, we presented the vertex partitions based on degree sum with their cardinalities in Table 1.

To compute the multiplication of degrees of all neighboring vertices in the V-Phenylenic nanotube $VPHX[p;q]$, we presented the vertex partitions based on product of degrees, with their cardinalities in Table 2.

**Theorem 1.** Let $VPHX[p;q]$ be the graph of V-Phenylenic nanotubes, then:

$E \zeta^c (VPHX[p;q]) = \begin{cases} 
100 & \text{when } p = 1 \text{ and } q = 1 \\
66q^2 + 44q & \text{when } p = 1 \text{ and } q \text{ is even} \\
66q^2 + 22q & \text{when } p = 1 \text{ and } q \text{ is odd} \\
198 & \text{when } p = 1 \text{ and } q = 1 \\
135q^2 + 90q & \text{when } p = 1 \text{ and } q \text{ is even} \\
135q^2 + 45q & \text{when } p = 1 \text{ and } q \text{ is odd}
\end{cases}$

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100 & \text{when } p = 1 \text{ and } q = 1 \\
66q^2 + 44q & \text{when } p = 1 \text{ and } q \text{ is even} \\
66q^2 + 22q & \text{when } p = 1 \text{ and } q \text{ is odd} \\
198 & \text{when } p = 1 \text{ and } q = 1 \\
135q^2 + 90q & \text{when } p = 1 \text{ and } q \text{ is even} \\
135q^2 + 45q & \text{when } p = 1 \text{ and } q \text{ is odd}
\end{cases}$

**Proof.** In this case the graph has only 4 rows. The sum of degrees of neighboring vertices in $1^{st}$ and $4^{th}$ rows is 6, whereas the sum of degrees of neighboring vertices in $2^{nd}$ and $3^{rd}$ rows is 8. The product of degrees of neighboring vertices in $1^{st}$ and $4^{th}$ rows is 9, whereas the product of degrees of neighboring vertices in $2^{nd}$ and $3^{rd}$ rows is 18.

**Case 1.** When $p=1$ and $q=1$:

$E \zeta^c (G) = \sum_{v \in V(G)} S_v = 2[6(3) + 2(8)(2)] = 100.$

$A \zeta^c (G) = \sum_{v \in V(G)} M_v = 2[9(3) + 2(18)(2)] = 198.$

**Case 2.** When $p=1$ and $q$ is even:

In this case the eccentricity of every vertex in every row is $\left(\frac{3q + 2}{2}\right)$.

$E \zeta^c (G) = \sum_{v \in V(G)} \frac{S_v}{\varepsilon(v)} = 2[6(q)\left(\frac{3q + 2}{2}\right) + 8(2q)\left(\frac{3q + 2}{2}\right)] = 66q^2 + 44q,$

$A \zeta^c (G) = \sum_{v \in V(G)} \frac{M_v}{\varepsilon(v)} = 2[9(q)\left(\frac{3q + 2}{2}\right) + 18(2q)\left(\frac{3q + 2}{2}\right)] = 135q^2 + 90q.$

**Case 3:** When $p=1$ and $q$ is odd:

In this case the eccentricity of every vertex in every row is $\left(\frac{3q + 1}{2}\right)$, So,

$E \zeta^c (G) = \sum_{v \in V(G)} \frac{S_v}{\varepsilon(v)} = 2[6(q)\left(\frac{3q + 1}{2}\right) + 8(2q)\left(\frac{3q + 1}{2}\right)] = 66q^2 + 22q,$

$A \zeta^c (G) = \sum_{v \in V(G)} \frac{M_v}{\varepsilon(v)} = 2[9(q)\left(\frac{3q + 1}{2}\right) + 18(2q)\left(\frac{3q + 1}{2}\right)] = 135q^2 + 45q.$

**Theorem 2.** Let $VPHX[p;q]$ be the graph of V-Phenylenic nanotubes, when $q \leq p$, $p$ and $q$ are both even, then we have

$E \zeta^c (VPHX[p;q]) = 162p^2q + 27pq^2 - 67pq - 5q^3 + 14q$

$A \zeta^c (VPHX[p;q]) = 486p^2q - 81pq^2 - 369pq - 36q^2 + 108q$

**Proof.** In this case the graph has 4p rows and the eccentricity of a vertex in $i^{th}$ row is same as the eccentricity of a vertex in $(4p+1-i)^{th}$ row.
where \( i = 1,2,\ldots,2p \). Let \( x_i \) be a vertex in \( i^{th} \) row. The eccentricity of \( x_i \) is
\[
\varepsilon(x_i) = \left( \frac{8p + q - i}{2} \right)
\]
where \( i = 1,2,\ldots,2p \). Here the sum of degrees of neighboring vertices in 1st and 4th rows is 6, whereas the sum of degrees of neighboring vertices in 2nd and 3rd rows is 8. The product of degrees of neighboring vertices in 1st and 4th rows is 9, whereas the product of degrees of neighboring vertices in 2nd and 3rd rows is 18. Hence:
\[
\varepsilon^{\varphi^e}(G) = \sum_{v \in V(G)} \frac{S_v}{\varepsilon(v)} = 2[6(q)(\frac{8p + q - 1}{2}) - 1] + 8(2q)((\frac{8p + q - 1}{2}) - 2) + 9(2q)((\frac{8p + q - 1}{2}) - 3)n
\]

\[
+9(q)((\frac{8p + q - 1}{2}) - 4) + 9(q)((\frac{8p + q - 1}{2}) - 5)
\]

\[
+9(q)((\frac{8p + q - 1}{2}) - 6) + 9(q)((\frac{8p + q - 1}{2}) - 7)
\]

\[
+ \ldots + 9(q)((\frac{8p + q - 1}{2}) - 2p)
\]

\[
= 162p^2q^2 + 27pq^2 - 94pq - 5q^2 + 19q
\]

Proof. In this case the graph has 4 rows and the eccentricity of a vertex in \( i^{th} \) row is same as the eccentricity of a vertex in \((4p+1-i)^{th}\) row where \( i = 1,2,\ldots,2p \). Let \( x_i \) be a vertex in \( i^{th} \) row. The eccentricity of \( x_i \) is
\[
\varepsilon(x_i) = \left( \frac{8p + q - i}{2} \right)
\]
where \( i = 1,2,\ldots,2p \). Here the sum of degrees of neighboring vertices in 1st and 4th rows is 6, whereas the sum of degrees of neighboring vertices in 2nd and 3rd rows is 8. The product of degrees of neighboring vertices in 1st and 4th rows is 9, whereas the product of degrees of neighboring vertices in 2nd and 3rd rows is 18. Hence:
\[
\varepsilon^{\varphi^e}(G) = \sum_{v \in V(G)} \frac{S_v}{\varepsilon(v)} = 2[6(q)(\frac{8p + q - 1}{2}) - 1]
\]

\[
+ 8(2q)((\frac{8p + q - 1}{2}) - 2) + 9(2q)((\frac{8p + q - 1}{2}) - 3)n
\]

\[
+ 9(q)((\frac{8p + q - 1}{2}) - 4) + 9(q)((\frac{8p + q - 1}{2}) - 5)
\]

\[
+ 9(q)((\frac{8p + q - 1}{2}) - 6) + 9(q)((\frac{8p + q - 1}{2}) - 7)
\]

\[
+ \ldots + 9(q)((\frac{8p + q - 1}{2}) - 2p)
\]

\[
= 162p^2q^2 + 27pq^2 - 94pq - 5q^2 + 19q
\]
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whereas the product of degrees of neighboring vertices in 2nd and 3rd rows is 18. Hence:

\[ E \varepsilon^{-v}(G) = \sum_{v \in V(G)} S_{v} \varepsilon(v) = 2[6(q)(\frac{8p + q}{2} - 1)] + 8(2q)(\frac{8p + q}{2} - 2) + 9(2q)(\frac{8p + q}{2} - 3) + 9(2q)(\frac{8p + q}{2} - 4) + 9(2q)(\frac{8p + q}{2} - 5) + 9(2q)(\frac{8p + q}{2} - 6) + 9(2q)(\frac{8p + q}{2} - 7) + 9(2q)(\frac{8p + q}{2} - 8) + \ldots + 9(q)(\frac{8p + q}{2} - (4p - 2q))].

\[ + 2[9(3q)(\frac{8p + q}{2} - (4p - 2q + 1)) + 9(3q)(\frac{8p + q}{2} - (4p - 2q + 2)) + \ldots + 9(3q)(\frac{8p + q}{2} - (3p - q))]

= 54q^3 + 189pq^2 - 27pq^2 - 67pq + 4q^2 + 14q

\[ \lambda \varepsilon^{-v}(G) = \sum_{v \in V(G)} S_{v} \varepsilon(v) = 2[6q(q)(\frac{8p + q}{2} - 1)] + 18(2q)(\frac{8p + q}{2} - 2) + 27(2q)(\frac{8p + q}{2} - 3) + 27(q)(\frac{8p + q}{2} - 4) + 27(q)(\frac{8p + q}{2} - 5) + 27(q)(\frac{8p + q}{2} - 6) + 27(q)(\frac{8p + q}{2} - 7) + 27(q)(\frac{8p + q}{2} - 8) + \ldots + 27(q)(\frac{8p + q}{2} - (4p - 2q))]

= 2[27q + 567pq^2 - 81pq^2 - 369pq - 171q^2 + 108q + 12q]

\textbf{Theorem 7.} Let VPHX[p,q] be the graph of V-Phenylenic nanotubes, when p+1 \leq q \leq 2p-1, and q is odd, then we have

\[ E \varepsilon^{-v}(VPHX[p,q]) = 27q^3 + 189pq^2 - 27pq^2 - 94pq - 50q^2 + 28q

\[ \lambda \varepsilon^{-v}(VPHX[p,q]) = 27q^3 + 567pq^2 - 81pq^2 - 486pq - 153q^2 + 171q^2

\textbf{Proof.} In this case the graph has 4 rows and the eccentricity of a vertex in \(i\)th row is same as the eccentricity of a vertex in \((4p+1)i\)th row where \(i = 1, 2, \ldots, 2p\). Let \(x_i\) be a vertex in the \(i\)th row. The eccentricity of \(x_i\) is

\[ \varepsilon(x_i) = \left(\frac{8p + q - 1}{2} - (4p - 2q + i)\right)

\text{where} \ i = 1, 2, \ldots, (q - p).

Here the sum of degrees of neighboring vertices in 1st and 4th rows is 6, whereas the sum of degrees of neighboring vertices in 2nd and 3rd rows is 8. The product of degrees of neighboring vertices in 1st and 4th rows is 9, whereas the product of degrees of neighboring vertices in 2nd and 3rd rows is 18. Hence:

\[ E \varepsilon^{-v}(G) = \sum_{v \in V(G)} S_{v} \varepsilon(v) = 2[6(q)(\frac{8p + q - 1}{2} - 1)] + 8(2q)(\frac{8p + q - 1}{2} - 2) + 9(2q)(\frac{8p + q - 1}{2} - 3) + 9(q)(\frac{8p + q - 1}{2} - 4) + 9(q)(\frac{8p + q - 1}{2} - 5) + 9(q)(\frac{8p + q - 1}{2} - 6) + 9(q)(\frac{8p + q - 1}{2} - 7) + 9(q)(\frac{8p + q - 1}{2} - 8) + \ldots + 9(q)(\frac{8p + q - 1}{2} - (4p - 2q))]

= 27q + 567pq^2 - 81pq^2 - 486pq - 153q^2 + 171q + 12q

\textbf{Theorem 8.} Let VPHX[p,q] be the graph of V-Phenylenic nanotubes, when 2p \leq q and q is even, then we have

\[ E \varepsilon^{-v}(VPHX[p,q]) = 81pq^2 + 81pq^2 - 47pq - 15q^2 + 10q

\[ \lambda \varepsilon^{-v}(VPHX[p,q]) = 243pq^2 + 243pq^2 - 225pq - 162q^2 + 108q

\text{where} \ i = 1, 2, \ldots, (q - p).
**Proof.** In this case the graph has 4 rows and the eccentricity of a vertex in **i**th row is same as the eccentricity of a vertex in (4p+1-1)th row where \( i = 1, 2, \ldots, 2p \). Let \( x \) be a vertex in (2i-1)th or (2i)th row. The eccentricity of \( x_i \) is 
\[ \varepsilon(x_i) = \left(\frac{4p+3q}{2} - i\right) \] where \( i = 1, 2, \ldots, p \). 1st and 4th rows is 6, whereas the sum of degrees of neighboring vertices in 2nd and 3rd rows is 8. The product of degrees of neighboring vertices in 1st and 4th rows is 9, whereas the product of degrees of neighboring vertices in 2nd and 3rd rows is 18. Hence 
\[ E \zeta^c(G) = \sum_{v \in V(G)} \frac{S_v}{\varepsilon(v)} = 2 \sum_{v \in V(G)} \left(\frac{4p+3q}{2} - 1\right) \]
\[ +8(2q)\left(\frac{4p+3q}{2} - 1\right) + 9(3q)\left(\frac{4p+3q}{2} - 2\right) \]
\[ +9(3q)\left(\frac{4p+3q}{2} - 3\right) + \ldots + 9(3q)\left(\frac{4p+3q}{2} - p\right) \]
\[ = 81p^2q^2 + 47pq - 15q^2 + 10q. \]

\[ A \zeta^c(G) = \sum_{v \in V(G)} \frac{M_v}{\varepsilon(v)} = 2 \sum_{v \in V(G)} \left(\frac{4p+3q}{2} - 1\right) \]
\[ +18(2q)\left(\frac{4p+3q}{2} - 1\right) + 27(3q)\left(\frac{4p+3q}{2} - 2\right) \]
\[ +27(3q)\left(\frac{4p+3q}{2} - 3\right) + \ldots + 27(3q)\left(\frac{4p+3q}{2} - p\right) \]
\[ = 243p^2q^2 - 225pq - 162q^2 + 108q. \]

**Theorem 9.** Let VPHX[p;q] be the graph of V-Phenylenic nanotubes, when 2p ≤ q, and q is odd, then we have 
\[ E \zeta^c(VPHX[p;q]) = 81p^2q^2 - 74pq - 15q^2 + 15q \]
\[ A \zeta^c(VPHX[p;q]) = 243p^2q^2 - 306pq - 108q^2 + 108q. \]

**Proof.** In this case the graph has 4 rows and the eccentricity of a vertex in **i**th row is same as the eccentricity of a vertex in (4p+1-1)th row where \( i = 1, 2, \ldots, 2p \). Let \( x_i \) be a vertex in (2i-1)th or (2i)th row. The eccentricity of \( x_i \) is 
\[ \varepsilon(x_i) = \left(\frac{4p+3q}{2} - 1\right) \] where \( i = 1, 2, \ldots, p \). Here the sum of degrees of neighboring vertices in 1st and 4th rows is 6, whereas the sum of degrees of neighboring vertices in 2nd and 3rd rows is 8. The product of degrees of neighboring vertices in 1st and 4th rows is 9, whereas the product of degrees of neighboring vertices in 2nd and 3rd rows is 18. Hence 
\[ E \zeta^c(G) = \sum_{v \in V(G)} \frac{S_v}{\varepsilon(v)} = 2 \sum_{v \in V(G)} \left(\frac{4p+3q}{2} - 1\right) \]
\[ +8(2q)\left(\frac{4p+3q}{2} - 1\right) + 9(3q)\left(\frac{4p+3q}{2} - 2\right) \]
\[ +9(3q)\left(\frac{4p+3q}{2} - 3\right) + \ldots + 9(3q)\left(\frac{4p+3q}{2} - p\right) \]
\[ = 81p^2q^2 + 47pq - 15q^2 + 10q. \]

**Conclusion**

In this work, we extended the eccentric connectivity results for V-Phenylenic nanotube (VPHX[p;q]). We obtained exact values of Ediz eccentric connectivity index and augmented eccentric connectivity index for V-Phenylenic nanotube by taking different variation on rows q and columns p by calculating sum and product of degrees of neighboring vertices using partitions technique. The generalization of eccentric connectivity index, and exact formulas for these eccentric connectivity indices were obtained.

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