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Eccentric connectivity indices of titaniananotubes $TiO_2[m;n]$

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The eccentric connectivity index ECI is a chemical structure descriptor that is currently being used for modeling of biological activities of a chemical compound. This index has been proved to provide a high degree of predictability compared to some other well-known indices in case of anticonvulsant, anti-inflammatory, and diuretic activities. The ECI of an infinite class of 1-polyacenic (phenylenic) nanotubes has been recently studied. In this study, we computed Ediz eccentric index and augmented eccentric connectivity index of Titania nanotube $TiO_2[m;n]$.

KEYWORDS

Molecular graph; Eccentricity; Ediz eccentric connectivity index; Augmented eccentric connectivity index; Titania nanotubes $TiO_2[m;n]$.

Introduction

A basic concept of chemistry is that the properties/activities of a molecule depend upon its structural characteristics. Molecular graphs can be used to model the chemical structures of molecules and molecular compounds, by considering atoms as vertices and the chemical bonds between the atoms as edges [1-3]. In the study of quantitative structure-property and structure-activity relationships (QSPR/QSAR), the topological indices are very helpful in detecting the biological activities of a chemical compound [4-7].

A topological index is a numerical graph invariant that is used to correlate the chemical structure of a molecule with its physicochemical properties and biological activities. Generally, topological indices are classified into five generations: first-generation topological indices are integer numbers obtained by simple operations from the local vertex invariants involving only one vertex at a time. Some of the famous topological indices of this class are Wiener index, Hosoya index, and centric indices of Balaban [8]. Second-generation topological indices are real numbers based on integer graph properties. These indices were obtained via the structural operations from integer local vertex invariants, involving more than one vertex at a time. Some examples of this class include molecular connectivity indices, Balaban J index, bond connectivity indices, and kappa shape indices [8]. Third-generation topological indices are real numbers which are based on local properties of the molecular graph. These indices are of recent introduction and have very low degeneracy. These are based on information theory applied to the terms of distance sums or on newly introduced nonsymmetrical matrices. Some examples include information indices [9], the hyper-Wiener index [8], the Kirchhoff index [10], and electrotopological state indices [4]. Recently, fourth- and fifth-generation topological indices are placed as new generations topological indices. Fourth-generation topological indices are of highly discriminating power. Some fourth-generation topological indices are including the eccentric connectivity index [11], superaugmented eccentric connectivity index [12], and superaugmented eccentric connectivity topochemical indices [13]. Detour matrix-based adjacent path eccentric distance sum indices belong to the fifth-generation topological indices [14].

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. The cardinality of vertex set is said to be order of graph G, denoted by |V(G)| and the cardinality of edge set is said to be the size of graph and is 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 ζ(v), is the maximum distance between a vertex to all other vertices i.e.,

$$ecc(v) = \varepsilon(v) = max\{d(u,v) : u \in V(G)\}.$$

The eccentric connectivity index of a graph G was proposed by Sharma, Goswami and Madan in [15], as

$$\zeta^c(G) = \sum_{v \in V(G)} d(v)\varepsilon(v). \qquad (1)$$

Gupta, Singh and Madan in [16] introduced the connective eccentric index for a graph

$$C^{\zeta}(G) = \sum_{v \in V(G)} \frac{d(v)}{\varepsilon(v)}. \qquad (2)$$

Recently, S. Ediz defined Ediz eccentric connectivity index in [17], denoted by ${}^{E}\zeta^c(G)$ and is defined as

$${}^{E}\zeta^c(G) = \sum_{v \in V(G)} \frac{S_v}{\varepsilon(v)}, \qquad (3)$$

where S_v is the sum of degrees of all vertices adjacent to vertex v [18, 19]. A generalization of eccentric connectivity index, known as augmented eccentric connectivity index of a graph G was proposed by Dureja and Madan in [20],

$${}^{A}\zeta^c(G) = \sum_{v \in V(G)} \frac{M_v}{\varepsilon(v)}, \qquad (4)$$

where M_v is the product of degrees of all vertices adjacent to vertex v. For further details about these new connectivity indices see [21- 27].

Discussion and main results

In this work, we discuss the molecular graph of titania nanotubes TiO_2[m;n], where m denotes the number of octagons in a column and n denotes the number of octagons in a row of the titania nanotube. The titanium nanotubular materials, called titania by a generic name, are of high interest metal oxide substances due to their widespread applications in production of catalytic, gas-sensing and corrosion resistance materials [28]. As a well-known semiconductor with numerous technological applications, Titania (TiO_2) nanotubes are comprehensively studied in materials science. The TiO_2 nanotubes were systematically synthesized using different methods and carefully studied as prospective technological materials [29-39].

TiO_2[m;n] is shown in Figure 1. In this section, we computed the Ediz eccentric connectivity index and augmented eccentric connectivity index of TiO_2[m;n].

Consider the molecular graph of Titania nanotube TiO_2[m;n], where m denotes the number of octagons in a row and n denotes the number of octagons in a column of the titania nanotube. This structure consist of *6m(n+1)* vertices. Figure 1 reveals the general representation of Titania nanotube TiO_2[m;n]. To compute the Ediz eccentric index and Augmented eccentric connectivity index of the Titania nanotube, we need vertex partition of the Titania nanotube TiO_2[m;n] based on degree sum and degree multiplication of neighbors vertices, respectively. As seen in Figure 1, there are

2mn+4m vertices of degree 2, 2mn vertices of degree 3, 2m vertices of degree 4 and 2mn vertices of degree 5. We denote the set of vertices of degree two, degree three, degree four and degree five by V_2, V_3, V_4 and V_5, respectively. The graph of titania nanotube has 2n+2 rows and m columns. For each i^{th} row and j^{th} column, we represent the vertices of graph by u_{ij}, v_{ij}, x_{ij} and y_{ij} as illustrated in Figure 2.

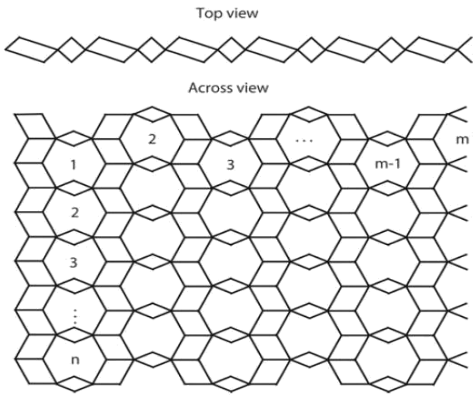

FIGURE 1 The molecular graph of titania nanotube $TiO_2[m;n]$

To compute the sum of degrees of all neighbors of vertices in the Titania nanotube $TiO_2[m;n]$, 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 Titania nanotube $TiO_2[m;n]$,we presented the vertex partitions based on product of degrees, with their cardinalities in Table 2.

Theorem 1. Let $TiO_2[m;n]$ be the graph of titania nanotube, then for $n \le \left\lfloor \frac{m-2}{4} \right\rfloor$ we have

$$^{E}\zeta^{c}(TiO_2[m,n]) = 38n + 24,$$

$$^{A}\zeta^{c}(TiO_2[m,n]) = 258n - 1.$$

TABLE 1 Vertex partition based on degree sum of neighbor vertices

S_v where v∈ V(TiO_2[m;n])	Number of Vertices
8	2m
9	4m
10	2mn
12	2m
13	2mn-2m
14	2m
15	2mn-2m

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

M_v where v∈ V(TiO_2[m;n])	Number of Vertices
16	2m
20	24m
24	2m
72	2m
25	2mn
108	2mn-2m
100	2m
125	2mn-2m

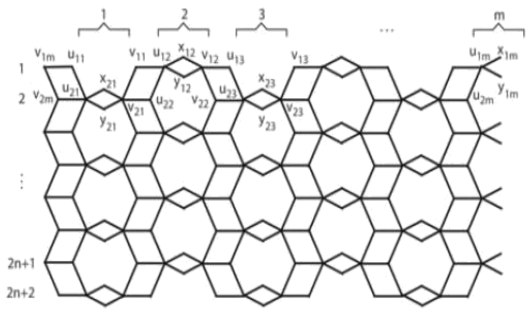

FIGURE 2 Representation of vertices of titania nanotube $TiO_2[m;n]$

Proof: The eccentricity of every vertex in every row is 2m. So, from Table 1 we have

$$^{E}\zeta^{c}(G) = \sum_{v \in V(G)} \frac{S_v}{\varepsilon(v)}$$

$$= \frac{2m(8)}{2m} + \frac{4m(9)}{2m} + \frac{2m(12)}{2m} + \frac{2mn(10)}{2m} + \frac{2m(14)}{2m} + \frac{(2mn-2m)(13)}{2m} + \frac{(2mn-2m)(15)}{2m}$$

$$= 38n + 24.$$

From Table 2, we have

$$^{A}\zeta^{c}(G)=\sum_{v\in V(G)}\frac{M_v}{\varepsilon(v)}=\frac{2m(16)}{2m}+\frac{2m(24)}{2m}+\frac{2m(72)}{2m}+\frac{2mn(25)}{2m}+\frac{2m(100)}{2m}+\frac{2m(20)}{2m}+\frac{(2mn-2m)(108)}{2m}+\frac{(2mn-2m)(125)}{2m}=258n-1.$$ ■

Theorem 2. Let $TiO_2[m;n]$ be the graph of titania nanotube, where m=2p and p=2n then we have

$$^{E}\zeta^{c}(TiO_2[m,n])=\frac{144p}{3p+2n+1}+38n+6,$$

$$^{A}\zeta^{c}(TiO_2[m,n])=\frac{176p}{3p+2n+1}+258n-45.$$

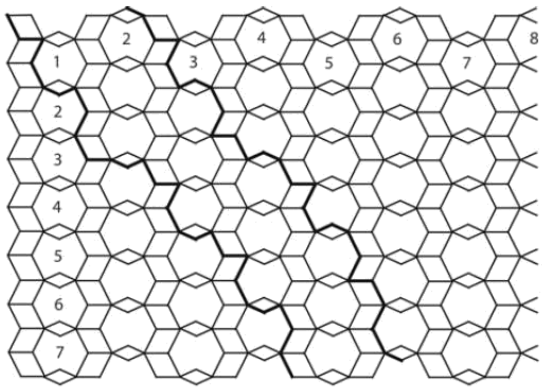

FIGURE 3 Shortest paths with maximal length in $TiO_2[m;n]$

Proof: In this case the eccentricity of the vertices u_{ij}, v_{ij} is 3p+2n+1 where i=1;2n+2. The eccentricity of each vertex in the remaining 2n rows is 4p. Hence from Table 1 we have:

$$^{E}\zeta^{c}(G)=\sum_{v\in V(G)}\frac{S_v}{\varepsilon(v)}=\frac{4(2p)(9)}{3p+2n+1}+\frac{2(2p)14}{4p}+\frac{2(2p)(8)}{4p}+\frac{2(2p)12}{4p}+\frac{2(2p)n(10)}{4p}+\frac{[2(2p)(n)-2(2p)](13)}{4p}+\frac{[2(2p)(n)-2(2p)](15)}{4p}=\frac{144p}{3p+2n+1}+38n+6.$$

From Table 2, we have

$$^{A}\zeta^{c}(G)=\sum_{v\in V(G)}\frac{M_v}{\varepsilon(v)}=\frac{2(2p)(24)}{3p+2n+1}+\frac{2(2p)(20)}{3p+2n+1}+\frac{2(2p)(100)}{4p}+\frac{2(2p)(16)}{4p}+\frac{2(2p)(72)}{4p}+\frac{2(2p)n(25)}{4p}+\frac{[2(2p)(n)-2(2p)](108)}{4p}+\frac{[2(2p)(n)-2(2p)](125)}{4p}=\frac{176p}{3p+2n+1}+258n-45.$$ ■

Theorem 3. Let $TiO_2[m;n]$ be the graph of titania nanotube, where $\frac{p-2}{2}<n<p-1$ and $p\neq 2n$ then we have:

$$^{E}\zeta^{c}(TiO_2[m,n])=\frac{8p(78p+52n+17)}{(3p+2n+1)(3p+2n)}+\frac{224p(2n-p-1)}{4n^2+12np-2n-7p^2-7p}+\frac{160p}{4n^2+12np+4n-7p^2-2p}+2(19p-19n+5),$$

$$^{A}\zeta^{c}(TiO_2[m,n])=\frac{16p(174p+116n+47)}{(3p+2n+1)(3p+2n)}+\frac{1864p(2n-p-1)}{4n^2+12np-2n-7p^2-7p}+\frac{400p}{4n^2+12np+4n-7p^2-2p}+258p-258n+25.$$

Proof: In this case the eccentricity of the vertices u_{ij}, v_{ij} is same as the eccentricity of vertices $u_{(2n+3i)j}$, $v_{(2n+3i)j}$, where i=1;2;...;2n-p+1. The eccentricity of these vertices in i^{th} row is given by

$$\varepsilon(u_{ij})=\varepsilon(v_{ij})=3p+2n+2-i,$$
$$where\, i=1,2,\ldots,2n-p+1.$$

The eccentricity of vertices u_{ij}, v_{ij} in remaining 2p-2n rows is 4p.

Also, the eccentricity of the vertices x_{ij}, y_{ij}, $x_{(i+1)j}$, $y_{(i+1)j}$ is same as the eccentricity of the vertices $x_{(2n+3i)j}$, $y_{(2n+3i)j}$, $x_{(2n+2i)j}$, $y_{(2n+2i)j}$ where $i=1,2,\ldots,\frac{2n-p}{2}$. The eccentricity of these vertices in i^{th} row is given by

$$\varepsilon(x_{ij})=\varepsilon(y_{ij})=3p+2n+2-2i,$$
$$where\, i=1,2,\ldots,\frac{2n-p}{2}.$$

The eccentricity of the vertices x_{ij}, y_{ij} in the remaining (2p-2n+2) rows is 4p. Hence from Table1, we have:

$$
\begin{aligned}
{}^{E}\zeta^{c}(G) &= \sum_{v\in V(G)} \frac{S_v}{\varepsilon(v)} \\
&= \frac{4(2p)(9)}{3p+2n+1} + \frac{2(2p)14}{3p+2n} + \frac{(2p)(4n-2-2p)(15)}{\sum_{i=3}^{2n-p+1}(3p+2n+2-i)} \\
&+ \frac{2p(2p-2n)(15)}{4p} + \frac{2p(4n-2-2p)(13)}{\sum_{i=3}^{2n-p+1}(3p+2n+2-i)} \\
&+ \frac{2p(2p-2n)(13)}{4p} + \frac{2(2p)(8)}{(3p+2n)} + \frac{2(2p)12}{3p+2n} \\
&+ \frac{2(2p)10}{\sum_{i=1}^{\frac{2n-p}{2}}(3p+2n+2-2i)} + \frac{(2p)(2p-2n+2)10}{4p} \\
&= \frac{8p(78p+52n+17)}{(3p+2n+1)(3p+2n)} + \frac{224p(2n-p-1)}{4n^2+12np-2n-7p^2-7p} \\
&+ \frac{160p}{4n^2+12np+4n-7p^2-2p} + 2(19p-19n+5).
\end{aligned}
$$

From Table 2, we have

$$
\begin{aligned}
{}^{A}\zeta^{c}(G) &= \sum_{v\in V(G)} \frac{M_v}{\varepsilon(v)} \\
&= \frac{2(2p)(24)}{3p+2n+1} + \frac{2(2p)(20)}{3p+2n+1} + \frac{2(2p)(100)}{3p+2n} \\
&+ \frac{2p(4n-2-2p)(125)}{\sum_{i=3}^{2n-p+1}(3p+2n+2-i)} + \frac{2p(2p-2n)(125)}{4p} \\
&+ \frac{2p(4n-2-2p)(108)}{\sum_{i=3}^{2n-p+1}(3p+2n+2-i)} + \frac{2p(2p-2n)(108)}{4p} \\
&+ \frac{2(2p)(16)}{3p+2n} + \frac{2(2p)72}{3p+2n} + \frac{2(2p)25}{\sum_{i=1}^{\frac{2n-p}{2}}(3p+2n+2-2i)} \\
&+ \frac{(2p)(2p-2n+2)25}{4p} = \frac{16p(174p+116n+47)}{(3p+2n+1)(3p+2n)} \\
&+ \frac{1864p(2n-p-1)}{4n^2+12np-2n-7p^2-7p} + \frac{400p}{4n^2+12np+4n-7p^2-2p} \\
&+ 258p-258n+25.
\end{aligned}
$$

Theorem 4. Let $TiO_2[m;n]$ be the graph of titania nanotube, where $n\geq p-1$ and n is odd then we have

$$
{}^{E}\zeta^{c}(TiO_2[m,n]) = \frac{4p(104n+156p+34)}{(2n+3p)(2n+3p+1)} + \frac{224p}{3(n+2p)} + \frac{160pn}{(n-1)(3n+6p-1)},
$$

$$
{}^{A}\zeta^{c}(TiO_2[m,n]) = \frac{4p(464n+696p+188)}{(2n+3p)(2n+3p+1)} + \frac{1864p}{3(n+2p)} + \frac{400np}{(n-1)(3n+6p-1)}.
$$

Proof: In this case the eccentricity of vertices u_{ij}, v_{ij} is same as the eccentricity of vertices $u_{(2n+3i)j}$, $v_{(2n+3i)j}$ where *i=1;2;...;n+1.* The eccentricity of these vertices in i^{th} row is given by

$$
\varepsilon(u_{ij}) = \varepsilon(v_{ij}) = 3p+2n+2-i, \quad \text{where } i = 1,2,\ldots,n+1.
$$

Also, the eccentricity of the vertices x_{ij}, y_{ij}, $x_{(i+1)j}$, $y_{(i+1)j}$ is same as the eccentricity of the vertices $x_{(2n+3i)j}, y_{(2n+3i)j}, x_{(2n+2i)j}, y_{(2n+2i)j}$ where $i=1,2,\ldots,\frac{n+1}{2}$. The eccentricity of these vertices in i^{th} row is given by

$$
\varepsilon(x_{ij}) = \varepsilon(y_{ij}) = 3p+2n+2-2i, \quad \text{where } i = 1,2,\ldots,\frac{n+1}{2}.
$$

Hence from Table 1 we have:

$$
\begin{aligned}
{}^{E}\zeta^{c}(G) &= \sum_{v\in V(G)} \frac{S_v}{\varepsilon(v)} \\
&= \frac{4(2p)(9)}{3p+2n+1} + \frac{2(2p)14}{3p+2n} + \frac{2(2p)(n-1)(15)}{\sum_{i=3}^{n+1}(3p+2n+2-i)} \\
&+ \frac{2(2p)(12)}{3p+2n} + \frac{2(2p)(n-1)(13)}{\sum_{i=3}^{n+1}(3p+2n+2-i)} + \frac{2(2p)(8)}{3p+2n} \\
&+ \frac{2(2p)(n)(10)}{\sum_{i=2}^{\frac{n+1}{2}}(3p+2n+2-2i)} \\
&= \frac{4p(104n+156p+34)}{(2n+3p)(2n+3p+1)} + \frac{224p}{3(n+2p)} \\
&+ \frac{160pn}{(n-1)(3n+6p-1)}.
\end{aligned}
$$

The shortest paths with maximal length in $TiO_2[8;7]$ are shown in Figure3. From Table2 we have:

$$
\begin{aligned}
{}^{A}\zeta^{c}(G) &= \sum_{v\in V(G)}\frac{M_v}{\varepsilon(v)} = \frac{2(2p)(24)}{3p+2n+1}+\frac{2(2p)20}{3p+2n+1} \\
&+\frac{2(2p)100}{3p+2n}+\frac{2(2p)(n-1)(125)}{\sum_{i=3}^{n+1}(3p+2n+2-i)}+\frac{2(2p)(72)}{3p+2n} \\
&+\frac{2(2p)(n-1)(108)}{\sum_{i=3}^{n+1}(3p+2n+2-i)}+\frac{2(2p)(16)}{3p+2n}+\frac{2(2p)(n)(25)}{\sum_{i=2}^{\frac{n+1}{2}}(3p+2n+2-2i)} \\
&=\frac{4p(464n+696p+188)}{(2n+3p)(2n+3p+1)}+\frac{1864p}{3(n+2p)}+\frac{400np}{(n-1)(3n+6p-1)}.
\end{aligned}
$$

Theorem 5. Let $TiO_2[m;n]$ be the graph of titania nanotube, where $n \geq p-1$ and n is even then we have

$$
{}^{E}\zeta^{c}(TiO_2[m,n])=\frac{8p(52n+78p+17)}{(2n+3p)(2n+3p+1)}+\frac{32p(12n-19)}{3(n-2)(n+2p)}+10,
$$

$$
{}^{A}\zeta^{c}(TiO_2[m,n])=\frac{4p(464n+696p+188)}{(2n+3p)(2n+3p+1)}+\frac{1864p}{3(n+2p)}+\frac{400(n-1)p}{3(n-2)(n+2p)}.
$$

Proof: In this case the eccentricity of vertices u_{ij}, v_{ij} is same as we discussed in Theorem 4. Also, the eccentricity of the vertices x_{ij}, y_{ij}, $x_{(i+1)j}$, $y_{(i+1)j}$ is same as the eccentricity of the vertices $x_{(2n+3i)j}$, $y_{(2n+3i)j}$, $x_{(2n+2i)j}$, $y_{(2n+2i)j}$ where $i=1,2,\ldots,\frac{n}{2}$. The eccentricity of these vertices in i^{th} row is given by

$$
\varepsilon(x_{ij})=\varepsilon(y_{ij})=3p+2n+2-2i, \text{where } i=1,2,\ldots,\frac{n}{2}.
$$

The eccentricity of the vertices x_{ij}, y_{ij} in the remaining 2 rows is 4p. Hence from Table 1 we have:

$$
\begin{aligned}
{}^{E}\zeta^{c}(G) &= \sum_{v\in V(G)}\frac{S_v}{\varepsilon(v)} \\
&=\frac{4(2p)(9)}{3p+2n+1}+\frac{2(2p)14}{3p+2n}+\frac{2(2p)(n-1)(15)}{\sum_{i=3}^{n+1}(3p+2n+2-i)} \\
&+\frac{2(2p)(12)}{3p+2n}+\frac{2(2p)(n-1)(13)}{\sum_{i=3}^{n+1}(3p+2n+2-i)}+\frac{2(2p)(8)}{3p+2n} \\
&+\frac{2(2p)(n-1)(10)}{\sum_{i=2}^{\frac{n}{2}}(3p+2n+2-2i)}+\frac{2(2p)10}{4p} \\
&=\frac{8p(52n+78p+17)}{(2n+3p)(2n+3p+1)}+\frac{32p(12n-19)}{3(n-2)(n+2p)}+10.
\end{aligned}
$$

From Table 2 we have:

$$
\begin{aligned}
{}^{A}\zeta^{c}(G) &= \sum_{v\in V(G)}\frac{M_v}{\varepsilon(v)} \\
&=\frac{2(2p)(24)}{3p+2n+1}+\frac{2(2p)20}{3p+2n+1}+\frac{2(2p)100}{3p+2n} \\
&+\frac{2(2p)(n-1)(125)}{\sum_{i=3}^{n+1}(3p+2n+2-i)}+\frac{2(2p)(72)}{3p+2n} \\
&+\frac{2(2p)(n-1)(108)}{\sum_{i=3}^{n+1}(3p+2n+2-i)}+\frac{2(2p)(16)}{3p+2n} \\
&+\frac{2(2p)(n-1)(25)}{\sum_{i=2}^{\frac{n}{2}}(3p+2n+2-2i)}+\frac{2(2p)25}{4p} \\
&=\frac{4p(464n+696p+188)}{(2n+3p)(2n+3p+1)}+\frac{1864p}{3(n+2p)} \\
&+\frac{400(n-1)p}{3(n-2)(n+2p)}.
\end{aligned}
$$

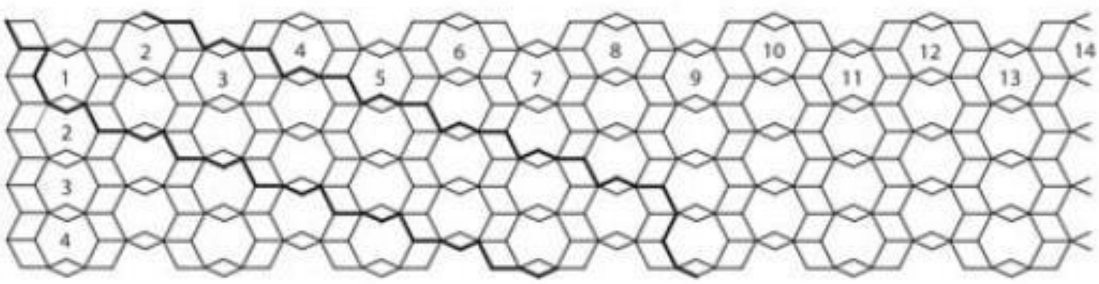

FIGURE 4 Shortest path with maximal length in TiO_2[m;n]

Theorem 6. Let $TiO_2[m;n]$ be the graph of titania nanotube, where m=2p and p=2n-1, then we have

$$^{E}\zeta^{c}(TiO_2[m,n])=\frac{104p(6p+4n+1)}{(3p+2n+1)(3p+2n)}+38n-28,$$

$$^{A}\zeta^{c}(TiO_2[m,n])=\frac{16p(174p+116n+43)}{(3p+2n+1)(3p+2n)}+258n-233.$$

Proof: In this case the eccentricity of the vertices u_{ij}, v_{ij} is same as the eccentricity of vertices $u_{(2n+3i)j}$, $v_{(2n+3i)j}$. where i=1;2. The eccentricity of these vertices in i^{th} row is given by $\varepsilon(u_{ij})=\varepsilon(v_{ij})=3p+2n+2-i, where\, i=1,2.$

The eccentricity of vertices u_{ij}, v_{ij} in remaining 2n-2 rows is 4p. Also, the eccentricity of the vertices x_{1j}, y_{1j} is same as the eccentricity of vertices $x_{(2n+2)j}$, $x_{(2n+2)j}$. The eccentricity of the vertices x_{1j},y_{1j} is given by $\varepsilon(x_{1j})=\varepsilon(v_{1j})=3p+2n+1.$

The eccentricity of the vertices x_{ij}, y_{ij} in the remaining 2n rows is 4p. The shortest path with maximal length in $TiO_2[14;4]$ is shown in Figure 4.

Hence from Table 1, we have

$$^{E}\zeta^{c}(G)=\sum_{v\in V(G)}\frac{S_v}{\varepsilon(v)}$$

$$=\frac{4(2p)(9)}{3p+2n+1}+\frac{2(2p)14}{3p+2n}+\frac{2(2p)(12)}{3p+2n}$$

$$+\frac{2(2p)(n-1)(15)}{4p}+\frac{2(2p)(n-1)(13)}{4p}$$

$$+\frac{2(2p)(8)}{3p+2n+1}+\frac{2(2p)n(10)}{4p}$$

$$=\frac{104p(6p+4n+1)}{(3p+2n+1)(3p+2n)}+38n-28.$$

From Table 2, we have

$$^{A}\zeta^{c}(G)=\sum_{v\in V(G)}\frac{M_v}{\varepsilon(v)}$$

$$=\frac{2(2p)(24)}{3p+2n+1}+\frac{2(2p)(20)}{3p+2n+1}+\frac{2(2p)100}{3p+2n}$$

$$+\frac{2(2p)(72)}{3p+2n}+\frac{2(2p)(n-1)(125)}{4p}$$

$$+\frac{2(2p)(n-1)(108)}{4p}+\frac{2(2p)(16)}{3p+2n+1}+\frac{2(2p)n(25)}{4p}$$

$$=\frac{16p(174p+116n+43)}{(3p+2n+1)(3p+2n)}+258n-233.$$

Theorem 7. Let $TiO_2[m;n]$ be the graph of titania nanotube, where $\frac{p-1}{2}<n<p-1, p\neq 2n-1$ then we have

$$^{E}\zeta^{c}(TiO_2[m,n])=\frac{104p(4n+6p+1)}{(2n+3p)(2n+3p+1)}$$

$$+\frac{224p}{4n^2+12np-2n-7p^2-7p}$$

$$+\frac{320p}{12np-7p^2-8p+4n^2-1}+38p-38n+10,$$

$$^{A}\zeta^{c}(TiO_2[m,n])=\frac{16p(116n+174p+43)}{(2n+3p)(2n+3p+1)}$$

$$+\frac{1864p}{4n^2+12np-2n-7p^2-7p}$$

$$+\frac{800p}{4n^2+12np-7p^2-8p-1}+258p-258n+25.$$

Proof: In this case the eccentricity of the vertices u_{ij}, v_{ij} is same as we discussed in Case2.2 of Theorem 2. The eccentricity of the vertices x_{1j}, y_{1j}, $x_{(2n+2)j}$, $x_{(2n+2)j}$ is same as we discussed in Case 3.1. Also, the eccentricity of the vertices $x_{(i+1)j}$, $y_{(i+1)j}$, $x_{(i+2)j}$, $y_{(i+2)j}$ is same as the eccentricity of the vertices $x_{(2n+2i)j}$, $y_{(2n+2i)j}$, $x_{(2n+1i)j}$, $y_{(2n+1i)j}$ where $i=1,2,\ldots,\frac{2n-p-1}{2}$. The eccentricity of these vertices in $(i+1)^{th}$ row is given by

$$\varepsilon(x_{(i+1)j})=\varepsilon(v_{(i+1)j})=3P+2n+1-2i,$$

$$where\, i=1,2,\ldots,\frac{2n-p-1}{2}.$$

The eccentricity of the vertices x_{ij}, y_{ij} in the remaining (2p-2n+2) rows is 4p. Hence from Table 1 we have:

$$^{E}\zeta^{c}(G)=\sum_{v\in V(G)}\frac{S_v}{\varepsilon(v)}$$

$$=\frac{4(2p)(9)}{3p+2n+1}+\frac{2(2p)14}{3p+2n}+\frac{2(2p)(15)}{\sum_{i=3}^{2n-p+1}3p+2n+2-i}+\frac{2(2p)(12)}{3p+2n}$$

$$+\frac{(2p)(2p-2n)(15)}{4p}+\frac{2(2p)(13)}{\sum_{i=3}^{2n-p+1}(3p+2n+2-i)}+\frac{2p(2p-2n)(13)}{4p}$$

$$+\frac{2(2p)8}{3p+2n+1}+\frac{4(2p)(10)}{\sum_{i=1}^{\frac{2n-p-1}{2}}(3p+2n+1-2i)}+\frac{2p(2p-2n+2)(10)}{4p}$$

$$=\frac{104p(4n+6p+1)}{(2n+3p)(2n+3p+1)}+\frac{224p}{4n^2+12np-2n-7p^2-7p}$$

$$+\frac{320p}{12np-7p^2-8p+4n^2-1}+38p-38n+10.$$

From Table 2 we have:

$$^{A}\zeta^{c}(G)=\sum_{v\in V(G)}\frac{S_v}{\varepsilon(v)}$$

$$=\frac{2(2p)(24)}{3p+2n+1}+\frac{2(2p)(20)}{3p+2n+1}+\frac{2(2p)100}{3p+2n}$$

$$+\frac{2(2p)(125)}{\sum_{i=3}^{2n-p+1}3p+2n+2-i}+\frac{(2p)(2p-2n)(125)}{4p}$$

$$+\frac{2(2p)(72)}{3p+2n}+\frac{2(2p)(108)}{\sum_{i=3}^{2n-p+1}(3p+2n+2-i)}$$

$$+\frac{2p(2p-2n)(108)}{4p}+\frac{2(2p)16}{3p+2n+1}$$

$$+\frac{4(2p)(25)}{\sum_{i=1}^{\frac{2n-p-1}{2}}(3p+2n+1-2i)}+\frac{2p(2p-2n+2)(25)}{4p}$$

$$=\frac{16p(116n+174p+43)}{(2n+3p)(2n+3p+1)}+\frac{1864p}{4n^2+12np-2n-7p^2-7p}$$

$$+\frac{800p}{4n^2+12np-7p^2-8p-1}+258p-258n+25.$$

Theorem 8. Let $TiO_2[m;n]$ be the graph of titania nanotube, where n>p-1 and n is odd, then we have

$$^{E}\zeta^{c}(TiO_2[m,n])=\frac{52p(6p+4n+1)}{(3p+2n+1)(3p+2n)}+\frac{224p}{3(n+2p)}+\frac{160pn}{(n-1)(3n+6p+1)},$$

$$^{A}\zeta^{c}(TiO_2[m,n])=\frac{16p(174p+116n+43)}{(3p+2n+1)(3p+2n)}+\frac{1864p}{3(n+2p)}+\frac{400pn}{(n-1)(3n+6p+1)}.$$

Proof: In this case the eccentricity of the vertices u_{ij}, v_{ij} is same as we discussed in Case2.3. The eccentricity of the vertices x_{1j}, y_{1j}, $x_{(2n+2)j}$, $x_{(2n+2)j}$ is same as we discussed in Case3.1. Also, the eccentricity of the vertices $x_{(i+1)j}$, $y_{(i+1)j}$, $x_{(i+2)j}$, $y_{(i+2)j}$ is same as the eccentricity of the vertices $x_{(2n+2i)j}$, $y_{(2n+2i)j}$, $x_{(2n+1i)j}$, $y_{(2n+1i)j}$ where $i=1,2,\ldots,\frac{n-1}{2}$. The eccentricity of these vertices in (i+1)th row is given by

$$\varepsilon(x_{(i+1)j})=\varepsilon(y_{(i+1)j})=3P+2n+1-2i,$$

$$where\, i=1,2,\ldots,\frac{n-1}{2}.$$

Hence from Table 1, we have

$$^{E}\zeta^{c}(G)=\sum_{v\in V(G)}\frac{S_v}{\varepsilon(v)}$$

$$=\frac{4(2p)(9)}{3p+2n+1}+\frac{2(2p)14}{3p+2n}+\frac{2(2p)(n-1)(15)}{\sum_{i=3}^{n+1}3p+2n+2-i}$$

$$+\frac{2(2p)(12)}{3p+2n}+\frac{2(2p)(n-1)(13)}{\sum_{i=3}^{n+1}3p+2n+2-i}+\frac{2(2p)(8)}{3p+2n+1}$$

$$+\frac{2(2p)n(10)}{\sum_{i=1}^{\frac{n-1}{2}}(3p+2n+1-2i)}$$

$$=\frac{52p(6p+4n+1)}{(3p+2n+1)(3p+2n)}+\frac{224p}{3(n+2p)}+\frac{160pn}{(n-1)(3n+6p+1)}.$$

Hence from Table 2, we have

$$^{A}\zeta^{c}(G)=\sum_{v\in V(G)}\frac{M_v}{\varepsilon(v)}$$

$$=\frac{2(2p)(24)}{3p+2n+1}+\frac{2(2p)(20)}{3p+2n+1}+\frac{2(2p)100}{3p+2n}$$

$$+\frac{2(2p)(n-1)(125)}{\sum_{i=3}^{n+1}3p+2n+2-i}+\frac{2(2p)(72)}{3p+2n}$$

$$+\frac{2(2p)(n-1)(108)}{\sum_{i=3}^{n+1}3p+2n+2-i}+\frac{2(2p)(16)}{3p+2n+1}+\frac{2(2p)n(25)}{\sum_{i=1}^{\frac{n-1}{2}}(3p+2n+1-2i)}$$

$$=\frac{16p(174p+116n+43)}{(3p+2n+1)(3p+2n)}+\frac{1864p}{3(n+2p)}+\frac{400pn}{(n-1)(3n+6p+1)}.$$

Theorem 9. Let $TiO_2[m;n]$ be the graph of titania nanotube, where n≥p-1 and n, then we have

$$^{E}\zeta^{c}(TiO_2[m,n]) = \frac{104p(4n+6p+1)}{(2n+3p)(2n+3p+1)} + \frac{128p}{n+2p},$$
$$^{A}\zeta^{c}(TiO_2[m,n]) = \frac{16p(116n+174p+43)}{(2n+3p)(2n+3p+1)} + \frac{2264p}{3(n+2p)}.$$

Proof: In this case the eccentricity of the vertices $x_{(i+1)j}$, $y_{(i+1)j}$, $x_{(i+2)j}$, $y_{(i+2)j}$ is same as the eccentricity of the vertices $x_{(2n+2-i)j}$,$y_{(2n+2-i)j}$, $x_{(2n+1-i)j}$, $y_{(2n+1-i)j}$ where $i=1,2,\ldots,\frac{n}{2}$. The eccentricity of these vertices in *(i+1)*throw is given by

$$\varepsilon(x_{(i+1)j}) = \varepsilon(y_{(i+1)j}) = 3P+2n+1-2i,$$
$$where\, i=1,2,\ldots,\frac{n}{2}.$$

The eccentricity of the remaining vertices is same as we discussed in case 3. Hence from Table 1 we have

$$^{E}\zeta^{c}(G) = \sum_{v\in V(G)} \frac{S_v}{\varepsilon(v)}$$
$$= \frac{4(2p)(9)}{3p+2n+1} + \frac{2(2p)14}{3p+2n} + \frac{2(2p)(n-1)(15)}{\sum_{i=3}^{n+1} 3p+2n+2-i}$$
$$+\frac{2(2p)(12)}{3p+2n} + \frac{2(2p)(n-1)(13)}{\sum_{i=3}^{n+1} 3p+2n+2-i} + \frac{2(2p)(8)}{3p+2n+1}$$
$$+\frac{2(2p)n(10)}{\sum_{i=1}^{\frac{n}{2}} 3p+2n+1-2i} = \frac{104p(4n+6p+1)}{(2n+3p)(2n+3p+1)} + \frac{128p}{n+2p}.$$

Hence from Table 2, we have

$$^{A}\zeta^{c}(G) = \sum_{v\in V(G)} \frac{M_v}{\varepsilon(v)}$$
$$= \frac{2(2p)(24)}{3p+2n+1} + \frac{2(2p)(20)}{3p+2n+1} + \frac{2(2p)100}{3p+2n}$$
$$+\frac{2(2p)(n-1)(125)}{\sum_{i=3}^{n+1} 3p+2n+2-i} + \frac{2(2p)(72)}{3p+2n} + \frac{2(2p)(16)}{3p+2n+1}$$
$$+\frac{2(2p)(n-1)(108)}{\sum_{i=3}^{n+1} 3p+2n+2-i} + \frac{2(2p)n(25)}{\sum_{i=1}^{\frac{n}{2}} 3p+2n+1-2i}$$
$$= \frac{16p(116n+174p+43)}{(2n+3p)(2n+3p+1)} + \frac{2264p}{3(n+2p)}.$$

Conclusion

In this research study, we studied the Ediz eccentric connectivity index and augmented eccentric connectivity index of the molecular structure Titania nanotube $TiO_2[m;n]$ by taking different variation of number of octagons in rows and columns and investigated the exact formulas of these eccentric connectivity indices of Titania nanotube $TiO_2[m;n]$. Further work on this molecular structure can be performed for other famous distance based topological indices.

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