Eccentricity-Based Topological Descriptors of First Type of Hex-Derived Network

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1. Introduction

Graph theory is a vital organ of scientific tools to study the mechanism of different molecular structures and networks without going into the labor of laboratory work. It provides valid reasons to adopt the techniques of topological indices to cater for the difficult molecular structures which might not be studied by any other technique. It has several applications in social sciences, computer science, neural network, genomics, molecular biology, and chemistry. Chemical graph theory is a hot topic among researchers and allows us to estimate some physicochemical features of chemical substances just by looking at their visual representations [1, 2]. A molecular frame can be described by covalent bonds which connects the atoms. In case of graph theory, atoms are vertices and these covalent bonds are edges between atoms.
impact on chemical science advancement. 

d(i, j) is distance between i and j and can be defined as the length of shortest path in G if i, j ∈ V(G). Eccentricity is distance between vertex i and the farthest vertex in the graph.

In a numerical format, 

\[ \mathcal{E}(i) = \max \{d(i, j) | i \in V(G)\}. \]  

(1)

Farooq and Malik [5] proposed the total eccentricity index as 

\[ \zeta(G) = \sum_{s \in V(G)} \mathcal{E}(s), \]  

(2)

where \( \mathcal{E}(s) \) is the eccentricity of the vertex s. Average eccentricity of a graph \( \text{avec}(\mathcal{E}) \) is 

\[ \text{avec}(G) = \frac{1}{n} \sum_{s \in V(G)} \mathcal{E}(s). \]  

(3)

Many researchers like Hinz, Ilic, Dankelmann, and Tang have worked on average eccentricity index, demonstrated by few references [6–9].

Ghorbani and Khaki [10] proposed the geometric-arithmetic index based on eccentricity, as 

\[ \text{GA}_4(G) = \sum_{r \in E(G)} \frac{2 \sqrt{\mathcal{E}(r). \mathcal{E}(s)}}{\mathcal{E}(r) + \mathcal{E}(s)}. \]  

(4)

Additional details on the average eccentricity and eccentricity-based geometric-arithmetic indices can be seen in [11]. Farahani [12] proposed the eccentricity version of the ABC index, expressed as 

\[ \text{ABC}_5(G) = \sum_{r \in E(G)} \sqrt{\mathcal{E}(r) + \mathcal{E}(s) - 2 \mathcal{E}(r) \mathcal{E}(s)}. \]  

(5)

Imran et al. computed \( \text{ABC}_5 \) and \( \text{GA}_4 \) indices of copper oxide in [13], and Gao et al. [14] shows the results of linear polycene parallelogram benzenoid.

Some modified eccentric versions of Zagreb indices mentioned in [15, 16] are 

\[ M_1^e(G) = \sum_{r \in E(G)} [\mathcal{E}(r) + \mathcal{E}(s)]. \]  

(6)

Second and third eccentric versions of Zagreb indices are as follows, respectively:

\[ M_2^e(G) = \sum_{r \in E(G)} \mathcal{E}(s)^2, \]  

(7)

\[ M_3^e(G) = \sum_{r \in E(G)} \mathcal{E}(r) \mathcal{E}(s). \]  

(8)

2. Applications and Motivation

Because degree-based TI’s are beneficial for analyzing the chemical properties of various molecule structures. As a result of this inspiration, we concentrate on eccentricity-based TI’s. Topological index based on eccentricity is a useful method to predict physicochemical and toxicological properties of a substance [17–19]. Recent activity on hex-derived networks can be studied in [20–22].

Zobair et al. studied TI’s of carbon nanocones as well as TI’s of different families of David-derived networks in [23,
that hexagonal structures. Figure 1(a) shows a hex-derived net-

strength. Hex-derived networks are under consideration in the materials to get minimum weight and maximum scales, and the materials used to allow the minimization of research direction is to comprehend the unique characteris-

and recently bioinformatics. The greatest challenge in this di-

Hexagonal structures had observed a lot of applications in

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[29

prediction potential than the Randic connectivity index

of hydrocarbons. [25

24

One index, known as the ABC index, has extremely

analytic methods, degree counting, and the sum of degrees

vertex and edge partitioning technique, tools for graphs,

Sets

| $\mathcal{E}(r)$ | Number of vertices | Range of $\beta$ and $n$ |
|-----------------|--------------------|---------------------------|
| $V_1$           | $n-1$              | $\beta = 1, n \geq 2$    |
| $V_2$           | $n + \beta - 2$    | $2 \leq \beta \leq n, n \geq 2$ |

Table 2: Eccentricity-based edge partition of HDN$_1(n)$.

Sets | $\mathcal{E}(r)$, $\mathcal{E}(s)$ | Edge frequency | $\beta$ value range | Range of $m$ and $n$ |
|-----|---------------------------------|----------------|---------------------|---------------------|
| $E_1$ | $(n + \beta - 3, n + \beta - 2)$ | $30m - 18$ | $2 \leq \beta \leq n$ | $1 \leq m \leq n - 1$ |
| $E_2$ | $n + \beta - 2, n + \beta - 2$ | $24m - 6$  | $2 \leq \beta \leq n$ | $1 \leq m \leq n - 1$ |

24]. One index, known as the ABC index, has extremely
good results for determining the stability and strain energy
of hydrocarbons. [25–28]. The GA index has much stronger
prediction potential than the Randic connectivity index
[29–31]. Within specified approximate formulas, the Zagreb
indices used for computation of total $\Pi$-electron energy of
the molecules [32].

3. Hex-Derived Network

Hexagonal structures had observed a lot of applications in
different fields including chemical engineering, transporta-
tion, mechanical engineering, architecture, nanofabrication,
and recently bioinformatics. The greatest challenge in this
research direction is to comprehend the unique characteris-
tics of hex-derived structures, relying on their structures,
scales, and the materials used to allow the minimization of
the materials to get minimum weight and maximum strength.
Hex-derived networks are under consideration in the
present research article which are further extracted from
hexagonal structures. Figure 1(a) shows a hex-derived
network for two dimension, Figure 1(c) demonstrates
that $HX(2)$ has faces, and Figure 2 shows an example of HD
$N_1(3)$ [33].

We adopt the combinatorial computing approach, the
vertex and edge partitioning technique, tools for graphs,
analytic methods, degree counting, and the sum of degrees
of neighbours techniques to compute our results [34, 35].
Furthermore, for numerical calculations and verifications,
we use MATLAB software. We also plot mathematical con-
clusions using the Maple software.

(i) For major findings, based on eccentricity, we divide
the vertices of the HDN$_1(n)$ into two sets. The ecen-
tricity of the set $V_1$ is $\mathcal{E}(r) = n - 1$, and the number of
vertices in the set is $1, \beta = 1$, and $n \geq 2$. The set
$V_2$ contains the vertices with the eccentricity $\mathcal{E}(s) = n + \beta - 2$, and the number of vertices in the set
$V_2$ is $6(3\beta - 4), 2 \leq \beta \leq n, n \geq 2$. In addition, the variable $\beta$ denotes the distance between two vertices,
which assists in the creation of this vertex division. Additionally, $\beta$ denotes the range of the total number of
vertices having that eccentricity. Table 1 shows the

vertex division of a HDN$_1$ depending on the eccentricity of each vertex.

(ii) Now, we divide the edges of the HDN$_1(n)$ based on
the eccentricity into two sets of the end vertices. The set $E_1$ contains edges with eccentricities $(\mathcal{E}(r), \mathcal{E}(s) ) = (n + \beta - 3, n + \beta - 2), 2 \leq \beta \leq n, n \geq 2$, and $E_1$ set
is $(30m - 18), 1 \leq m \leq n - 1$. The set $E_2$ contains
the edges with eccentricities $(\mathcal{E}(r), \mathcal{E}(s) ) = (n + \beta - 2, n + \beta - 2), 2 \leq \beta \leq n, n \geq 2$, and $E_2$ set is $(24m - 6)$
, $1 \leq m \leq n - 1$. In addition, $\beta$ denotes the total
number of pairing with that eccentricities. Table 2 shows the
edge division of a HDN$_1(n)$ Â depending

on the eccentricity of end vertices.

3.1. Main Results for HDN$_1(n)$. The close approximations
of some TT’s for this network were calculated in this section.
We have found here the closed results for total eccentricity,
average eccentricity, eccentricity version of Zagreb, eccentric
ABC, and GA indices for hex-derived networks of first type.

Theorem 3.1.1. Consider HDN$_1(n), \forall n \in N, n \geq 2$, be the
graph of first type of hex-derived network, then $\zeta$ index of
HDN$_1(n)$ is

$$\zeta(HDN_1(n)) = 15n^3 - 36n^2 + 28n - 7. \quad (9)$$

Proof. Consider HDN$_1(n)$, $\forall n \in N, n \geq 2$, be the first type
Hex-derived network.

We calculated the total eccentricity index as follows,
using the vertices partitioned from Table 1 and Equation (2):

$$\zeta(G) = \sum_{s \in V(G)} \mathcal{E}(s) \zeta(HDN_1(n)) = \sum_{s \in V_1(G)} \mathcal{E}(s) + \sum_{s \in V_2(G)} \mathcal{E}(s),$$

$$= \sum_{\beta=1}^{(n-1)} (n-1) + \sum_{\beta=2}^{n} 6(3\beta - 4)(n + \beta - 2), (n-1)$$

$$+ 6 \sum_{\beta=2}^{n} (3\beta - 4)(n + \beta - 2). \quad (10)$$

After calculations, we have

$$\Rightarrow \zeta(HDN_1(n)) = 15n^3 - 36n^2 + 28n - 7. \quad (11)$$

Theorem 3.1.2. Consider HDN$_1(n), \forall n \in N, n \geq 2$, be the
graph of first type of hex-derived network, then the avec index
of HDN$_1(n)$ is

$$avec(HDN_1(n)) = \frac{1}{9n^2 - 15n + 7} (15n^3 - 36n^2 + 28n - 7). \quad (12)$$

Proof. Consider HDN$_1(n), \forall n \in N$ and $n \geq 2$ containing 9
$n^2 - 15n + 7$ vertices and $27n^2 - 51n + 24$ edges.
Figure 3: The graphical representation of $\zeta$ and avec indices, respectively.

Figure 4: The graphical representation of $M^*_1$ and $M^{* *}_1$ indices, respectively.
We calculated the average eccentricity index as follows, using the vertices partitioned from Table 1 and Equation (3):

\[
avec(G) = \frac{1}{n} \sum_{s \in V(G)} \mathcal{E}(s) = \frac{1}{n} \sum_{s \in V(G)} \mathcal{E}(s) \\
+ \frac{1}{n} \sum_{s \in V_2(G)} \mathcal{E}(s) = \frac{1}{9n^2 - 15n + 7} \left( \sum_{\beta=1}^{n-1} (1)(n-1) \\
+ \sum_{\beta=2}^{n} (3\beta - 4)(n + \beta - 2) \right).
\]

(13)

After calculations, we have

\[
\Rightarrow avec(HDN_1(n)) = \frac{1}{9n^2 - 15n + 7} \left( 15n^3 - 36n^2 + 28n - 7 \right).
\]

(14)

**Theorem 3.1.3.** Consider HDN_1(n), \(\forall n \in \mathbb{N}, \ n \geq 2\), be the graph of first type of hex-derived network, then \(M_1^*\) of HD N_1(n) is

\[
M_1^*(HDN_1(n)) = 3(n-1)^2 (27n^2 - 47n + 22).
\]

(15)

**Proof.** Consider HDN_1(n), \(\forall n \in \mathbb{N}, \ n \geq 2\). We calculated \(M_1^*\) as follows, using Table 2 edge partitioning and Equation (6):

\[
M_1^*(G) = \sum_{rs \in E(G)} [\mathcal{E}(r) + \mathcal{E}(s)].
\]

\[
M_1^*(HDN_1(n)) = \sum_{rs \in E_1(G)} [\mathcal{E}(r) + \mathcal{E}(s)] + \sum_{rs \in E_2(G)} [\mathcal{E}(r) + \mathcal{E}(s)]
\]

\[
= \sum_{n=1}^{n-1} \sum_{\beta=2}^{n} (3\beta - 4)(n + \beta - 2) + \sum_{n=1}^{n-1} \sum_{\beta=2}^{n} (24m - 6) \left( (n + \beta - 2) + (n + \beta - 2) \right)
\]

\[
= 6 \sum_{m=1}^{n-1} \sum_{\beta=2}^{n} (5m - 3) \left( (2m + 2\beta - 5) \right)
\]

\[
+ 12 \sum_{m=1}^{n-1} \sum_{\beta=2}^{n} (4m - 1) \left( (n + \beta - 1) \right).
\]

(16)

After calculations, we have

\[
\Rightarrow M_1^*(HDN_1(n)) = 3(n-1)^2 (27n^2 - 47n + 22).\]

(17)

**Theorem 3.1.4.** Consider HDN_1(n), \(\forall n \in \mathbb{N}, \ n \geq 2\), be the graph of first type of hex-derived network, then \(M_1^{**}\) index
of HDN₁(n) is
\[ M_1^{**}(HDN₁(n)) = \frac{1}{2}(51n^4 - 160n^3 + 179n^2 - 84n + 14). \]  
(18)

Proof. Consider HDN₁(n), ∀n ∈ N, n ≥ 2, be the hex-derivation network of first type. We calculated the second Zagreb eccentricity index as follows, using the vertices partitioned from Table 1 and Equation (7); the proof is analogue of Theorem 3.1.3.

Theorem 3.1.5. Consider HDN₁(n), ∀n ∈ N, n ≥ 2, be the graph of first type of hex-derivation network, then the M₂ index of HDN₁(n) is
\[ M_2^*(HDN₁(n)) = (n - 1)^2(63n^3 - 164n^2 + 145n - 42). \]  
(19)

Proof. Consider HDN₁(n), ∀n ∈ N, n ≥ 2, be the hex-derivation network of first type.

We calculated the third Zagreb eccentricity index as follows, using Table 2 edge partitioning and Equation (8):
\[ M_3^*(G) = \sum_{rst∈E(G)} [E(r), E(s)]. \]

\[ M_2^*(HDN₁(n)) = \sum_{rst∈E(G)} [E(r), E(s)] + \sum_{rst∈E(G)} [E(r), E(s)], \]
\[ = \sum_{m=1}^{n-1} \sum_{β=2}^{n} (30m - 18)(n + β - 3)(n + β - 2) \]
\[ + \sum_{m=1}^{n-1} \sum_{β=2}^{n} (24m - 6)(n + β - 2)(n + β - 2), \]
\[ = 6\sum_{m=1}^{n-1} \sum_{β=2}^{n} (5m - 3)(n + β - 3)(n + β - 2) \]
\[ + 6\sum_{m=1}^{n-1} \sum_{β=2}^{n} (4m - 1)(n + β - 2)^2. \]  
(20)

After calculations, we have
\[ ⇒M_2^*(HDN₁(n)) = (n - 1)^2(63n^3 - 164n^2 + 145n - 42). \]  
(21)

Theorem 3.1.6. Consider HDN₁(n), ∀n ∈ N, n ≥ 2, be the graph of first type of hex-derivation network, then the GA₄ index of HDN₁(n) is
\[ GA_4(HDN₁(n)) = 12n^2 - 30n^2 + 24n - 6 \]
\[ + 12\sum_{m=1}^{n-1} \sum_{β=2}^{n} (5m - 3) \frac{\sqrt{(n + β - 3)(n + β - 2)}}{2n + 2β - 5}. \]  
(22)

Proof. Consider HDN₁(n), ∀n ∈ N, n ≥ 2, be the hex-derivation network of first type. We calculated the eccentric GA₄ index as follows, using Table 2 edge partitioning and Equation (4):
\[ GA_4(HDN₁(n)) = \sum_{rst∈E(G)} \frac{2\sqrt{E(r), E(s)}}{E(r) + E(s)}. \]

\[ GA_4(HDN₁(n)) = \sum_{m=1}^{n-1} \sum_{β=2}^{n} (30m - 18) \frac{2\sqrt{(n + β - 3)(n + β - 2)}}{(n + β - 3) + (n + β - 2)} \]
\[ + \sum_{m=1}^{n-1} \sum_{β=2}^{n} (24m - 6) \frac{2\sqrt{(n + β - 2)(n + β - 2)}}{(n + β - 2) + (n + β - 2)}, \]
\[ = 12\sum_{m=1}^{n-1} \sum_{β=2}^{n} (5m - 3) \frac{2\sqrt{(n + β - 3)(n + β - 2)}}{2n + 2β - 5} \]
\[ + 6\sum_{m=1}^{n-1} \sum_{β=2}^{n} (4m - 1) \frac{2\sqrt{(n + β - 2)}}{2n + 2β - 5}. \]  
(23)

After calculations, we have
\[ ⇒GA_4(HDN₁(n)) = 12n^2 - 30n^2 + 24n - 6 \]
\[ + 12\sum_{m=1}^{n-1} \sum_{β=2}^{n} (5m - 3) \frac{\sqrt{(n + β - 3)(n + β - 2)}}{2n + 2β - 5}. \]  
(24)

Theorem 3.1.7. Consider HDN₁(n), ∀n ∈ N, n ≥ 2, be the graph of first type of hex-derivation network, then the ABC₅ index of HDN₁(n) is
\[ ABC_5(HDN₁(n)) = 6\sum_{m=1}^{n-1} \sum_{β=2}^{n} (5m - 3) \frac{\sqrt{2n + 2β - 7}}{(n + β - 3)(n + β - 2)} \]
\[ + \sum_{m=1}^{n-1} \sum_{β=2}^{n} (4m - 1) \frac{\sqrt{2n + 2β - 6}}{(n + β - 2)}. \]  
(25)

Proof. Consider HDN₁(n), ∀n ∈ N, n ≥ 2, be the hex-derivation network of first type. We calculated the eccentric ABC₅ index as follows, using Table 2 edge partitioning and Equation (5); the proof is analogue of Theorem 3.1.6.

4. Comparison and Discussion

The eccentricity-based TI’s of the HDN₁(n) first type of hex-derivation network for specific values of m and β are compared in Figures 3–5. It is obvious from the graphs that the values of indices are increasing for different m and β. So that it provides an indication that the results provided for different indices are true.
5. Conclusion

In this article, eccentricity-based TT's, the average eccentricity, eccentric version of Zagreb indices, total eccentricity index, eccentricity version of geometric-arithmetic index, and atom-bond connectivity index based on eccentricity for first type of hex-derived network are contempladed and investigate the basic topologies of these networks. Furthermore, we made a comparison in Figures 3–5 by the use of graph comparison. This analysis will facilitate researchers engaged in network science in recognizing the topology of the abovementioned networks. Furthermore, the results presented in this paper might be helpful in the QSRR/QSAR analysis to predict further structural and physicochemical properties of molecular graphs under discussion.

Data Availability

The data used to support the findings of this study are included within the article.

Conflicts of Interest

There is no conflict of interest among the authors.

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