

On Some Neighbourhood Degree-Based Indices of Graphs Derived From Honeycomb Structure

Haidar Ali^{1*}, Usman Babar², Shahid Hussain Arshad³ and Ammara Sajjad⁴

¹Department of Mathematics, Government College University, Faisalabad, Pakistan

²Department of Mathematics, Government College University, Lahore, Pakistan

³Department of Applied Sciences, National Textile University, Faisalabad, Pakistan

⁴Government Public Girls High School, 214 RB, Faisalabad, Pakistan

*Corresponding author

Abstract

In mathematical chemistry, molecular structure of any chemical substance can be expressed by a numeric number or polynomial or sequence of numbers which represent the whole graph is called topological index. An important branch of graph theory is the chemical graph theory. Because of their worldwide uses, chemical networks have inspired researchers since their development. Determination of the expressions for topological indices of different derived graphs is a new and interesting problem in graph theory. In this article, some graphs which are derived from Honeycomb structure are studied and found their exact results for some neighbourhood degree-based topological indices. Additionally, a comparison is shown graphically among all the derived indices.

Keywords: Topological indices, Dominating David Derived network, M_N , F_N , F_N^* , M_2^* , HM_N

2010 Mathematics Subject Classification: 05C09, 05C12, 05C90, 05C92

1. Preliminaries

The molecular structures are those in which atoms are connected by covalent bonds. In graph theory, atoms are considered as vertices and covalent bonds are as edges. Cheminformatics is a new area of research in which the subjects Chemistry, Mathematics, and Information science are combined. That is why it attains the highly attention for researchers around the world. In this paper, we are considering Dominating David Derived networks which are derived from Honeycomb structure. Honeycomb structures, inspired from bee honeycombs, had found widespread applications in various fields, including architecture, transportation, mechanical engineering, chemical engineering, nanofabrication, and recently biomedicine. A major challenge in this field is to understand the unique properties of honeycomb structures, which depends on their structures, scales, and the materials used [13].

A Topological index TI, sometimes also known as a graph-theoretic index, is a numerical invariant of a chemical graph [24]. There are many types of TI's but most popular and authentic TI's are Distance-based, Degree-based, Neighbourhood Degree-Based indices. These indices contains a lot of information within themselves. In this paper, we are dealing with some newly derived Neighbourhood Degree-Based TI's [23, 27].

The method of drawing Dominating David Derived networks (dimension i) is as follows.

STEP 1:-Consider a Honeycomb network $HC(i)$ dimension i .

STEP 2:-Split each edge into two by embedding another vertex.

STEP 3:-In each hexagon cell, connect the new vertices by an edge if they are at a distance of 4 units within the cell.

STEP 4:-Place vertices at new edge crossings.

STEP 5:-Remove initial vertices and edges of Honeycomb network.

STEP 6:-Split each horizontal edge into two edges by inserting a new vertex. The resulting Graph is called Dominating David Derived system $DDD(i)$ of dimension i [25].

The First type of DDD network $D_1(i)$ can be obtained by connecting vertices of degree two by an edge, which are not in the boundary.

The second type of Dominating David Derived network $D_2(i)$ can be obtained by subdividing once the new edge introduced in $D_1(i)$.

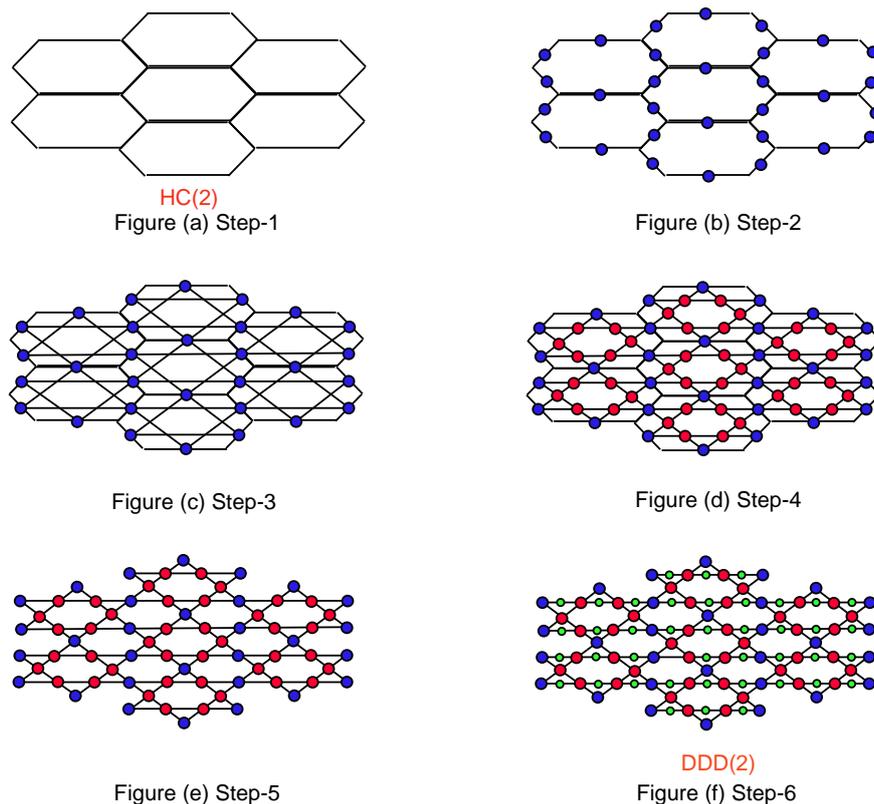


Figure 1.1: Construction Algorithm for DDD network $DDD(2)$.

The Third type of DDD network $D_3(i)$ can be obtained from $D_1(i)$ by introducing parallel path of length 2 between the vertices of degree two which are not in the boundary. See the figure 5, for third type Dominating David Derived network of dimension 2 $D_3(2)$.

Molecular graphs are pictorial models of chemical compounds. We consider only molecular graphs in this article, [7, 12, 28]. We consider $V(\eta)$ and $E(\eta)$ as vertex and edge sets, respectively, for a graph η . The degree of a vertex $i \in V(\eta)$, denoted by $d_{(\eta)}(i)$, is the number of edges that are incident to i in η . We say that a node i is a neighbor of another node j if i is adjacent to j in η . Here, $\delta_{(\eta)}(j)$ represents the totality of degrees of all neighbors of j in η , i.e.,

$$\delta_{(\eta)}(j) = \sum_{i \in N_{(\eta)}(j)} d_{(\eta)}(i),$$

where $N_{\eta}(j) = \{i \in V(\eta) : ij \in E(\eta)\}$. A valuable tool called a topological index provides a connection between mathematics and chemistry. A topological index is a particular number connected with a graph, such that two graphs have the same topological index are isomorphic. Topological indices play an important role in the quantitative structure–property (QSPR) and the quantitative structure–activity relationship (QSAR) models to predict different physico-chemical properties. This is also noteworthy for its use in various areas, including nanoscience, biotechnology. Topological indices began with the creation of the Wiener index in 1947 by chemist Harold Wiener [30]. Several topological indices have been introduced over the past decades based on the vertex degree. We worked some new Neighbourhood degree-based topological indices [22, 23] having nice correlations with entropy and the acentric factor. These indices are defined as follows.

The neighborhood Zagreb index is denoted by $M_N(\eta)$ and is defined as:

$$M_N(\eta) = \sum_{i \in V(\eta)} \delta_{(\eta)}(i)^2. \tag{1.1}$$

The neighborhood version of the forgotten topological index is denoted by $F_N(\eta)$ and is defined as:

$$F_N(\eta) = \sum_{i \in V(\eta)} \delta_{(\eta)}(i)^3. \tag{1.2}$$

The modified neighborhood version of the forgotten topological index is denoted by $F_N^*(\eta)$ and is defined as:

$$F_N^*(\eta) = \sum_{ij \in E(\eta)} [\delta_{(\eta)}(i)^2 + \delta_{(\eta)}(j)^2]. \tag{1.3}$$

The neighborhood version of the second Zagreb index is denoted by $M_2^*(\eta)$ and is defined by:

$$M_2^*(\eta) = \sum_{ij \in E(\eta)} [\delta_{(\eta)}(i) \times \delta_{(\eta)}(j)]. \tag{1.4}$$

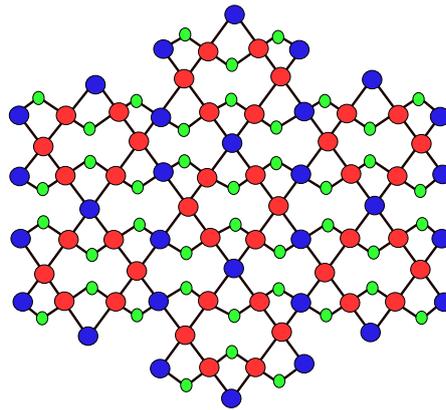


Figure 1.2: Isomorphic graph of DDD(2).

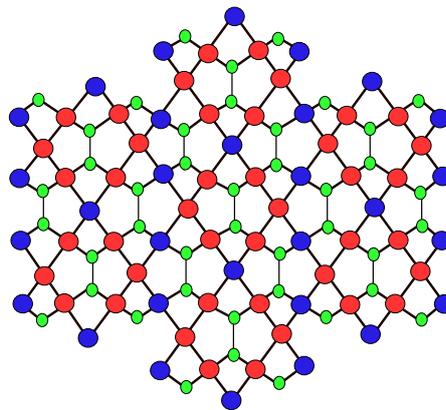


Figure 1.3: First type of DDD network $D_1(2)$.

The neighborhood version of the hyper Zagreb index is denoted by $HM_N(\eta)$ and is defined by:

$$HM_N(\eta) = \sum_{ij \in E(\eta)} [\delta_{(\eta)}(i) + \delta_{(\eta)}(j)]^2. \tag{1.5}$$

2. Main results

We study the Neighbourhood indices such as Neighbourhood Zagreb Index, neighborhood version of the forgotten index, modified neighborhood version of the forgotten index, neighborhood version of the second Zagreb index, neighborhood version of the hyper Zagreb index and give closed formulae of these indices for Some Derived networks. For further study of topological indices of various graph families see, [1, 2, 3, 4, 5, 6, 8, 9, 10, 11, 14, 15, 16, 17, 18, 19, 20, 21, 25, 26, 29].

2.1. Results for First type of DDD network

In this section, we calculate Neighbourhood degree-based topological indices of the dimension i for first type of Dominating David Derived networks. In the coming theorems, we compute some important neighbourhood degree based indices.

Theorem 2.1. Consider the DDD network of the first type $\eta_1 \cong D_1(i)$ for $i \in \mathbb{N}$. Neighbourhood Zagreb index is equal to

$$M_N(\eta_1) = 22(11 + i(27i - 31)).$$

Proof. Let η_1 be the $D_1(i)$. From equation 1, we have

$$M_N(\eta_1) = \sum_{j \in V(\eta_1)} \delta_{(\eta_1)}(j)^2.$$

By using neighbourhood vertex partition in table 1, where V_2, V_3 and V_4 are a vertices of degree 2, 3 and 4 respectively, we have

$$\begin{aligned} M_N(\eta_1) &= \sum_{j \in V_2} \delta_{(\eta_1)}(j)^2 + \sum_{j \in V_3} \delta_{(\eta_1)}(j)^2 + \sum_{j \in V_4} \delta_{(\eta_1)}(j)^2, \\ &= |V_2|(2)^2 + |V_3|(3)^2 + |V_4|(4)^2, \\ &= 4(20i - 10) + 9(18i^2 - 26i + 10) + 16(27i^2 - 33i + 12), \end{aligned}$$

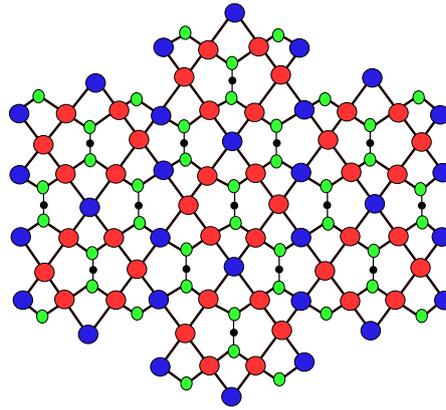


Figure 1.4: Second type of DDD network $D_2(2)$.

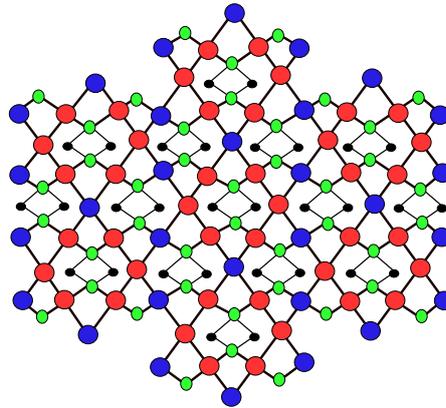


Figure 1.5: Third type of DDD network $D_3(2)$.

This value is what, we get after calculations

$$\implies M_N(\eta_1) = 22(11 + i(27i - 31)).$$

□

Theorem 2.2. Consider the DDD network of the first type $\eta_1 \cong D_1(i)$ for $i \in \mathbb{N}$. Neighborhood version of the Forgotten TI is equal to

$$F_N(\eta_1) = 2214i^2 - 2654i + 958.$$

Proof. Let η_1 be the $D_1(i)$. From equation 2, we have

$$F_N(\eta_1) = \sum_{j \in V(\eta_1)} \delta(\eta_1)(j)^3.$$

By using Neighbourhood vertex partition in table 1, we have

$$\begin{aligned} F_N(\eta_1) &= \sum_{j \in V_2} \delta(\eta_1)(j)^3 + \sum_{j \in V_3} \delta(\eta_1)(j)^3 + \sum_{j \in V_4} \delta(\eta_1)(j)^3, \\ &= |V_2|(2)^3 + |V_3|(3)^3 + |V_4|(4)^3, \\ &= 8(20i - 10) + 27(18i^2 - 26i + 10) + 64(27i^2 - 33i + 12), \end{aligned}$$

This value is what, we get after calculations

$$\implies F_N(\eta_1) = 2214i^2 - 2654i + 958.$$

□

Theorem 2.3. For DDD network $\eta_1 \cong D_1(i)$ for $i \in \mathbb{N}$. Then its modified neighborhood version of forgotten index is equal to

$$F_N^*(\eta_1) = 2214i^2 - 2654i + 958.$$

| Vertices with degrees | Number of vertices |
|-----------------------|--------------------|
| V_2 | $20i - 10$ |
| V_3 | $18i^2 - 26i + 10$ |
| V_4 | $27i^2 - 33i + 12$ |

Table 1: Neighbourhood vertex partition for $D_1(i)$

| (d_i, d_j) where $ij \in E(\eta_1)$ | Number of Edges |
|---------------------------------------|--------------------|
| (2,2) | $4i$ |
| (2,3) | $4i - 4$ |
| (2,4) | $28i - 16$ |
| (3,3) | $9i^2 - 13i + 5$ |
| (3,4) | $36i^2 - 56i + 24$ |
| (4,4) | $36i^2 - 52i + 20$ |

Table 2: Neighbourhood edge partition for $D_1(i)$

Proof. Let η_1 be the $D_1(i)$. From equation 3, we have

$$F_N^*(\eta_1) = \sum_{ij \in E(\eta_1)} [\delta_{(\eta_1)}(i)^2 + \delta_{(\eta_1)}(j)^2].$$

By using Neighbourhood edge partition in table 2, we have

$$\begin{aligned} F_N^*(\eta_1) &= \sum_{ij \in (2,2)} [\delta_{(\eta_1)}(i)^2 + \delta_{(\eta_1)}(j)^2] + \sum_{ij \in (2,3)} [\delta_{(\eta_1)}(i)^2 + \delta_{(\eta_1)}(j)^2] + \sum_{ij \in (2,4)} [\delta_{(\eta_1)}(i)^2 + \delta_{(\eta_1)}(j)^2] \\ &\quad + \sum_{ij \in (3,3)} [\delta_{(\eta_1)}(i)^2 + \delta_{(\eta_1)}(j)^2] + \sum_{ij \in (3,4)} [\delta_{(\eta_1)}(i)^2 + \delta_{(\eta_1)}(j)^2] \\ &\quad + \sum_{ij \in (4,4)} [\delta_{(\eta_1)}(i)^2 + \delta_{(\eta_1)}(j)^2], \\ &= |E_{2,2}|(2^2 + 2^2) + |E_{2,3}|(2^2 + 3^2) + |E_{2,4}|(2^2 + 4^2) + |E_{3,3}|(3^2 + 3^2) + \\ &\quad |E_{3,4}|(3^2 + 4^2) + |E_{4,4}|(4^2 + 4^2), \\ &= 8(4i) + 13(4i - 4) + 20(28i - 16) + 18(9i^2 - 13i + 5) + 25(36i^2 - 56i \\ &\quad + 24) + 32(36i^2 - 52i + 20), \end{aligned}$$

This value is what, we get after calculations

$$\implies F_N^*(\eta_1) = 2214i^2 - 2654i + 958.$$

□

Theorem 2.4. For DDD network $\eta_1 \cong D_1(i)$ for $i \in \mathbb{N}$. Then its modified neighborhood version of Second Zagreb index is equal to

$$M_2^*(\eta_1) = 501 + i(1089i - 1357).$$

Proof. Let η_1 be the $D_1(i)$. From equation 4, we have

$$M_2^*(\eta_1) = \sum_{ij \in E(\eta_1)} [\delta_{(\eta_1)}(i) \times \delta_{(\eta_1)}(j)].$$

By using Neighbourhood edge partition in table 2, we have

$$\begin{aligned} M_2^*(\eta_1) &= \sum_{ij \in (2,2)} [\delta_{(\eta_1)}(i) \times \delta_{(\eta_1)}(j)] + \sum_{ij \in (2,3)} [\delta_{(\eta_1)}(i) \times \delta_{(\eta_1)}(j)] + \sum_{ij \in (2,4)} [\delta_{(\eta_1)}(i) \times \delta_{(\eta_1)}(j)] \\ &\quad + \sum_{ij \in (3,3)} [\delta_{(\eta_1)}(i) \times \delta_{(\eta_1)}(j)] + \sum_{ij \in (3,4)} [\delta_{(\eta_1)}(i) \times \delta_{(\eta_1)}(j)] \\ &\quad + \sum_{ij \in (4,4)} [\delta_{(\eta_1)}(i) \times \delta_{(\eta_1)}(j)], \\ &= |E_{2,2}|(2 \times 2) + |E_{2,3}|(2 \times 3) + |E_{2,4}|(2 \times 4) + |E_{3,3}|(3 \times 3) + |E_{3,4}|(3 \\ &\quad \times 4) + |E_{4,4}|(4 \times 4), \\ &= 4(4i) + 6(4i - 4) + 8(28i - 16) + 9(9i^2 - 13i + 5) + 12(36i^2 - 56i \\ &\quad + 24) + 16(36i^2 - 52i + 20), \end{aligned}$$

This value is what, we get after calculations

$$\implies M_2^*(\eta_1) = 501 + i(1089i - 1357).$$

□

| Vertices with degree | Number of vertices |
|----------------------|--------------------|
| V_2 | $9i^2 + 7i - 5$ |
| V_3 | $18i^2 - 26i + 10$ |
| V_4 | $27i^2 - 33i + 12$ |

Table 3: Neighbourhood vertex partition for $D_2(i)$

Theorem 2.5. For DDD network $\eta_1 \cong D_1(i)$ for $i \in \mathbb{N}$. Then its neighborhood version of Hyper Zagreb index is equal to $HM_N(\eta_1) = 8(245 + 61i(9i - 11))$.

Proof. Let η_1 be the $D_1(i)$. From equation 5, we have

$$HM_N(\eta_1) = \sum_{ij \in E(\eta_1)} [\delta_{(\eta_1)}(i) + \delta_{(\eta_1)}(j)]^2.$$

By using Neighbourhood edge partition in table 2, we have

$$\begin{aligned} HM_N(\eta_1) &= \sum_{ij \in (2,2)} [\delta_{(\eta_1)}(i) + \delta_{(\eta_1)}(j)]^2 + \sum_{ij \in (2,3)} [\delta_{(\eta_1)}(i) + \delta_{(\eta_1)}(j)] + \sum_{ij \in (2,4)} [\delta_{(\eta_1)}(i) + \delta_{(\eta_1)}(j)]^2 + \sum_{ij \in (3,3)} [\delta_{(\eta_1)}(i) + \delta_{(\eta_1)}(j)]^2 + \sum_{ij \in (3,4)} [\delta_{(\eta_1)}(i) + \delta_{(\eta_1)}(j)]^2 + \sum_{ij \in (4,4)} [\delta_{(\eta_1)}(i) + \delta_{(\eta_1)}(j)]^2, \\ &= |E_{2,2}|(2+2)^2 + |E_{2,3}|(2+3)^2 + |E_{2,4}|(2+4)^2 + |E_{3,3}|(3+3)^2 + |E_{3,4}|(3+4)^2 + |E_{4,4}|(4+4)^2, \\ &= 16(4i) + 25(4i - 4) + 36(28i - 16) + 36(9i^2 - 13i + 5) + 49(36i^2 - 56i + 24) + 64(36i^2 - 52i + 20), \end{aligned}$$

This value is what, we get after calculations

$$\implies HM_N(\eta_1) = 8(245 + 61i(9i - 11)).$$

□

2.2. Results for Second Type of DDD network

Now, we are calculating Some new Neighborhood degree-based TI's of the $\eta_2 \cong D_2(i)$, where $i \in \mathbb{N}$ for second type of DDD network.

Theorem 2.6. Consider the Dominating David Derived network of the Second type $\eta_2 \cong D_2(i)$ for $i \in \mathbb{N}$. Neighbourhood Zagreb index is equal to

$$M_N(\eta_2) = 630i^2 - 734i + 262.$$

Proof. Let η_2 be the $D_2(i)$. From equation 1, we have

$$M_N(\eta_2) = \sum_{j \in V(\eta_2)} \delta_{(\eta_2)}(j)^2.$$

By using Neighbourhood vertex partition in table 3 we have,

$$\begin{aligned} M_N(\eta_2) &= \sum_{j \in V_2} \delta_{(\eta_2)}(j)^2 + \sum_{j \in V_3} \delta_{(\eta_2)}(j)^2 + \sum_{j \in V_4} \delta_{(\eta_2)}(j)^2, \\ &= |V_2|(2)^2 + |V_3|(3)^2 + |V_4|(4)^2, \\ &= 4(9i^2 + 7i - 5) + 9(18i^2 - 26i + 10) + 16(27i^2 - 33i + 12), \end{aligned}$$

This value is what, we get after calculations

$$\implies M_N(\eta_2) = 630i^2 - 734i + 262.$$

□

Theorem 2.7. Consider the DDD network of the Second type $\eta_2 \cong D_2(i)$ for $i \in \mathbb{N}$. Neighborhood version of forgotten index is equal to

$$F_N(\eta_2) = 2286i^2 - 2758i + 998.$$

Proof. Let η_2 be the $D_2(i)$. From equation 2, we have

$$F_N(\eta_2) = \sum_{j \in V(\eta_2)} \delta(\eta_2)(j)^3.$$

By using Neighbourhood vertex partition in table 3, we have

$$\begin{aligned} F_N(\eta_2) &= \sum_{j \in V_2} \delta(\eta_2)(j)^3 + \sum_{j \in V_3} \delta(\eta_2)(j)^3 + \sum_{j \in V_4} \delta(\eta_2)(j)^3, \\ &= |V_2|(2)^3 + |V_3|(3)^3 + |V_4|(4)^3, \\ &= 8(9i^2 + 7i - 5) + 27(18i^2 - 26i + 10) + 64(27i^2 - 33i + 12), \end{aligned}$$

This value is what, we get after calculations

$$\implies F_N(\eta_2) = 2286i^2 - 2758i + 998.$$

□

Theorem 2.8. Consider the DDD network of the Second type $\eta_2 \cong D_2(i)$ for $i \in \mathbb{N}$. Modified neighborhood version of forgotten index is equal to

$$F_N^*(\eta_2) = 2286i^2 - 2758i + 998.$$

Proof. Let η_2 be the $D_2(i)$. From equation 3, we have

$$F_N^*(\eta_2) = \sum_{ij \in E(\eta_2)} [\delta(\eta_2)(i)^2 + \delta(\eta_2)(j)^2].$$

By using Neighbourhood edge partition in table 4, we have

| $(d_i, d_j), ij \in E(\eta_2)$ | Number of Edges |
|--------------------------------|--------------------|
| (2,2) | $4i$ |
| (2,3) | $18i^2 - 22i + 6$ |
| (2,4) | $28i - 16$ |
| (3,4) | $36i^2 - 56i + 24$ |
| (4,4) | $36i^2 - 52i + 20$ |

Table 4: Neighbourhood edge partition for $D_2(i)$

$$\begin{aligned} F_N^*(\eta_2) &= \sum_{ij \in (2,2)} [\delta(\eta_2)(i)^2 + \delta(\eta_2)(j)^2] + \sum_{ij \in (2,3)} [\delta(\eta_2)(i)^2 + \delta(\eta_2)(j)^2] + \sum_{ij \in (2,4)} \\ &\quad [\delta(\eta_2)(i)^2 + \delta(\eta_2)(j)^2] + \sum_{ij \in (3,4)} [\delta(\eta_2)(i)^2 + \delta(\eta_2)(j)^2] + \sum_{ij \in (4,4)} [\delta(\eta_2)(i)^2 \\ &\quad + \delta(\eta_2)(j)^2], \\ &= |E_{2,2}|(2^2 + 2^2) + |E_{2,3}|(2^2 + 3^2) + |E_{2,4}|(2^2 + 4^2) + |E_{3,4}|(3^2 + 4^2) \\ &\quad + |E_{4,4}|(4^2 + 4^2), \\ &= 8(4i) + 13(18i^2 - 22i + 6) + 20(28i - 16) + 25(36i^2 - 56i + 24) \\ &\quad + 32(36i^2 - 52i + 20), \end{aligned}$$

This value is what, we get after calculations

$$\implies F_N^*(\eta_2) = 2286i^2 - 2758i + 998.$$

□

Theorem 2.9. Consider the DDD network of the Second type $\eta_2 \cong D_2(i)$ for $i \in \mathbb{N}$. Neighborhood version of second Zagreb index is equal to

$$M_2^*(\eta_2) = 4(209 - 557i + 423i^2).$$

Proof. Let η_2 be the $D_2(i)$. From equation 4, we have

$$M_2^*(\eta_2) = \sum_{ij \in E(\eta_2)} [\delta(\eta_2)(i) \times \delta(\eta_2)(j)].$$

By using Neighbourhood edge partition in table 4 we have,

$$\begin{aligned}
 M_2^*(\eta_2) &= \sum_{ij \in (2,2)} [\delta(\eta_2)(i) \times \delta(\eta_2)(j)] + \sum_{ij \in (2,3)} [\delta(\eta_2)(i) \times \delta(\eta_2)(j)] + \sum_{ij \in (2,4)} [\delta(\eta_2)(i) \times \delta(\eta_2)(j)] \\
 &\quad + \sum_{ij \in (3,4)} [\delta(\eta_2)(i) \times \delta(\eta_2)(j)] + \sum_{ij \in (4,4)} [\delta(\eta_2)(i) \times \delta(\eta_2)(j)], \\
 &= |E_{2,2}|(2 \times 2) + |E_{2,3}|(2 \times 3) + |E_{2,4}|(2 \times 4) + |E_{3,4}|(3 \times 4) \\
 &\quad + |E_{4,4}|(4 \times 4), \\
 &= 4(4i) + 6(18i^2 - 22i + 6) + 8(28i - 16) + 12(36i^2 - 56i + 24) \\
 &\quad + 16(36i^2 - 52i + 20),
 \end{aligned}$$

This value is what, we get after calculations

$$\implies M_2^*(\eta_2) = 4(209 - 557i + 423i^2).$$

□

Theorem 2.10. Consider the DDD network of the Second type $\eta_2 \cong D_2(i)$ for $i \in \mathbb{N}$. Neighborhood version of hyper Zagreb index is equal to

$$HM_N(\eta_2) = 4518i^2 - 5550i + 2030.$$

Proof. Let η_2 be the $D_2(i)$. From equation 5, we have

$$HM_N(\eta_2) = \sum_{ij \in E(\eta_2)} [\delta(\eta_2)(i) + \delta(\eta_2)(j)]^2.$$

By using Neighbourhood edge partition in table 4, we have

$$\begin{aligned}
 HM_N(\eta_2) &= \sum_{ij \in (2,2)} [\delta(\eta_2)(i) + \delta(\eta_2)(j)]^2 + \sum_{ij \in (2,3)} [\delta(\eta_2)(i) + \delta(\eta_2)(j)] + \sum_{ij \in (2,4)} [\delta(\eta_2)(i) + \delta(\eta_2)(j)] \\
 &\quad + \sum_{ij \in (3,4)} [\delta(\eta_2)(i) + \delta(\eta_2)(j)]^2 + \sum_{ij \in (4,4)} [\delta(\eta_2)(i) + \delta(\eta_2)(j)]^2, \\
 &= |E_{2,2}|(2 + 2)^2 + |E_{2,3}|(2 + 3)^2 + |E_{2,4}|(2 + 4)^2 + |E_{3,4}|(3 + 4)^2 \\
 &\quad + |E_{4,4}|(4 + 4)^2, \\
 &= 16(4i) + 25(18i^2 - 22i + 6) + 36(28i - 16) + 49(36i^2 - 56i + 24) \\
 &\quad + 64(36i^2 - 52i + 20),
 \end{aligned}$$

This value is what, we get after calculations

$$\implies HM_N(\eta_2) = 4518i^2 - 5550i + 2030.$$

□

2.3. Results for Third Type of DDD Network

In this section, we calculate the Neighbourhood based topological indices for third type of DDD network $D_3(i)$ of dimension i .

| Vertices with degrees | Number of degrees |
|-----------------------|--------------------|
| V_2 | $18i^2 - 6i$ |
| V_4 | $45i^2 - 59i + 22$ |

Table 5: Neighbourhood vertex partition for $D_3(i)$

Theorem 2.11. Consider the DDD network of the Second type $\eta_3 \cong D_3(i)$ for $i \in \mathbb{N}$. Neighborhood Zagreb index is equal to

$$M_N(\eta_3) = 88(9i^2 - 11i + 4).$$

Proof. Let η_3 be the $D_3(i)$. From equation 1, we have

$$M_N(\eta_3) = \sum_{j \in V(\eta_3)} \delta(\eta_3)(j)^2.$$

| $(d_i, d_j), ij \in E(\eta_3)$ | Number of edges |
|--------------------------------|---------------------|
| (2,2) | $4i$ |
| (2,4) | $36i^2 - 20i$ |
| (4,4) | $72i^2 - 108i + 44$ |

Table 6: Neighbourhood edge partition for $D_3(i)$

By using Neighbourhood vertex partition in table 5 we have,

$$\begin{aligned} M_N(\eta_3) &= \sum_{j \in V_2} \delta(\eta_3)(j)^2 + \sum_{j \in V_4} \delta(\eta_3)(j)^2, \\ &= |V_2|(2)^2 + |V_4|(4)^2, \\ &= 4(18i^2 - 6i) + 16(45i^2 - 59i + 22), \end{aligned}$$

This value is what, we get after calculations

$$\implies M_N(\eta_3) = 88(9i^2 - 11i + 4).$$

□

Theorem 2.12. Consider the DDD network of the Second type $\eta_3 \cong D_3(i)$ for $i \in \mathbb{N}$. Neighborhood version of forgotten index is equal to

$$F_N(\eta_3) = 16(88 - 239i + 189i^2).$$

Proof. Let η_3 be the $D_3(i)$. From equation 2, we have

$$F_N(\eta_3) = \sum_{j \in V(\eta_3)} \delta(\eta_3)(j)^3$$

By using Neighbourhood vertex partition in table 5, we have

$$\begin{aligned} F_N(\eta_3) &= \sum_{j \in V_2} \delta(\eta_3)(j)^3 + \sum_{j \in V_4} \delta(\eta_3)(j)^3, \\ &= |V_2|(2)^3 + |V_4|(4)^3, \\ &= 8(18i^2 - 6i) + 64(45i^2 - 59i + 22), \end{aligned}$$

This value is what, we get after calculations

$$\implies F_N(\eta_3) = 16(88 - 239i + 189i^2).$$

□

Theorem 2.13. Consider the DDD network of the Second type $\eta_3 \cong D_3(i)$ for $i \in \mathbb{N}$. Modified neighborhood version of forgotten index is equal to

$$F_N^*(\eta_3) = 16(88 - 239i + 189i^2).$$

Proof. Let η_3 be the $D_3(i)$. From equation 3, we have

$$F_N^*(\eta_3) = \sum_{ij \in E(\eta_3)} [\delta(\eta_3)(i)^2 + \delta(\eta_3)(j)^2].$$

By using Neighbourhood edge partition in table 6, we have

$$\begin{aligned} F_N^*(\eta_3) &= \sum_{ij \in (2,2)} [\delta(\eta_3)(i)^2 + \delta(\eta_3)(j)^2] + \sum_{ij \in (2,4)} [\delta(\eta_3)(i)^2 + \delta(\eta_3)(j)^2] \\ &\quad + \sum_{ij \in (4,4)} [\delta(\eta_3)(i)^2 + \delta(\eta_3)(j)^2], \\ &= |E_{2,2}|(2^2 + 2^2) + |E_{2,4}|(2^2 + 4^2) + |E_{4,4}|(4^2 + 4^2), \\ &= 8(4i) + 20(36i^2 - 20i) + 32(72i^2 - 108i + 44), \end{aligned}$$

This value is what, we get after calculations

$$\implies F_N^*(\eta_3) = 16(88 - 239i + 189i^2).$$

□

Theorem 2.14. Consider the DDD network of the Second type $\eta_3 \cong D_3(i)$ for $i \in \mathbb{N}$. Neighborhood version of second Zagreb index is equal to

$$M_2^*(\eta_3) = 16(90i^2 - 117i + 44).$$

Proof. Let η_3 be the $D_3(i)$. From equation 4, we have

$$M_2^*(\eta_3) = \sum_{ij \in E(\eta_3)} [\delta_{(\eta_3)}(i) \times \delta_{(\eta_3)}(j)].$$

By using Neighbourhood edge partition in table 6, we have

$$\begin{aligned} M_2^*(\eta_3) &= \sum_{ij \in (2,2)} [\delta_{(\eta_3)}(i) \times \delta_{(\eta_3)}(j)] + \sum_{ij \in (2,4)} [\delta_{(\eta_3)}(i) \times \delta_{(\eta_3)}(j)] + \sum_{ij \in (4,4)} [\delta_{(\eta_3)}(i) \times \delta_{(\eta_3)}(j)], \\ &= |E_{2,2}|(2 \times 2) + |E_{2,4}|(2 \times 4) + |E_{4,4}|(4 \times 4), \\ &= 4(4i) + 8(36i^2 - 20i) + 16(72i^2 - 108i + 44), \end{aligned}$$

This value is what, we get after calculations

$$\implies M_2^*(\eta_3) = 16(90i^2 - 117i + 44).$$

□

Theorem 2.15. Consider the DDD network of the Second type $\eta_3 \cong D_3(i)$ for $i \in \mathbb{N}$. Neighborhood version of hyper Zagreb index is equal to

$$HM_N(\eta_3) = 16(369i^2 - 473i + 176).$$

Proof. Let η_3 be the $D_3(i)$. From equation 5, we have

$$HM_N(\eta_3) = \sum_{ij \in E(\eta_3)} [\delta_{(\eta_3)}(i) + \delta_{(\eta_3)}(j)]^2.$$

By using Neighbourhood edge partition in table 6, we have

$$\begin{aligned} HM_N(\eta_3) &= \sum_{ij \in (2,2)} [\delta_{(\eta_3)}(i) + \delta_{(\eta_3)}(j)]^2 + \sum_{ij \in (2,4)} [\delta_{(\eta_3)}(i) + \delta_{(\eta_3)}(j)]^2 + \sum_{ij \in (4,4)} [\delta_{(\eta_3)}(i) + \delta_{(\eta_3)}(j)]^2, \\ &= |E_{2,2}|(2 + 2)^2 + |E_{2,4}|(2 + 4)^2 + |E_{4,4}|(4 + 4)^2, \\ &= 16(4i) + 36(36i^2 - 20i) + 64(72i^2 - 108i + 44), \end{aligned}$$

This value is what, we get after calculations

$$\implies HM_N(\eta_3) = 16(369i^2 - 473i + 176).$$

□

In figures 4, 5 and 5, there is a comparison of TI's of DDD network of first, second and third type for certain values of i . These graphs shows the correctness of results, because the graph of TI's are increasing for the different values of i .

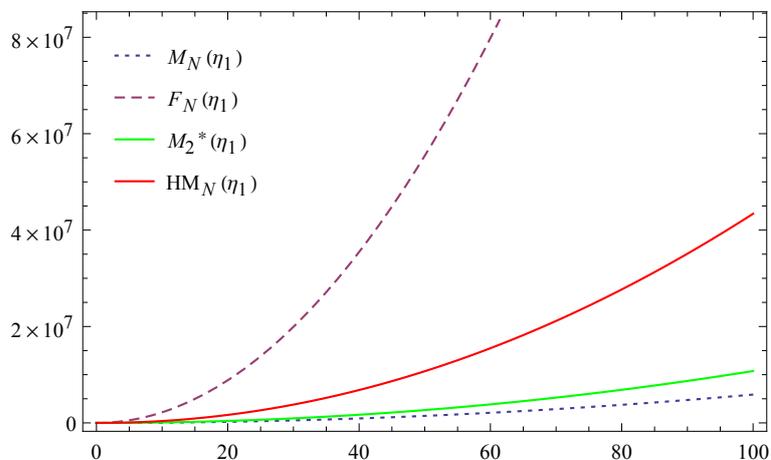


Figure 2.1: First type of Dominating David Derived network $D_1(2)$.

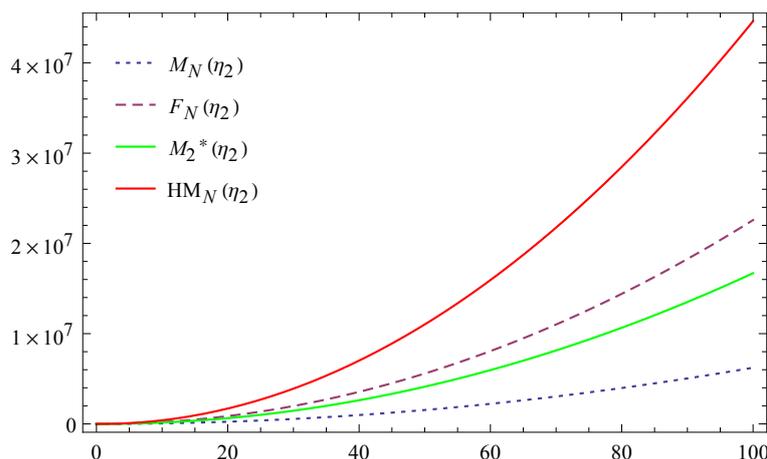


Figure 2.2: Second type of Dominating David Derived network $D_2(2)$.

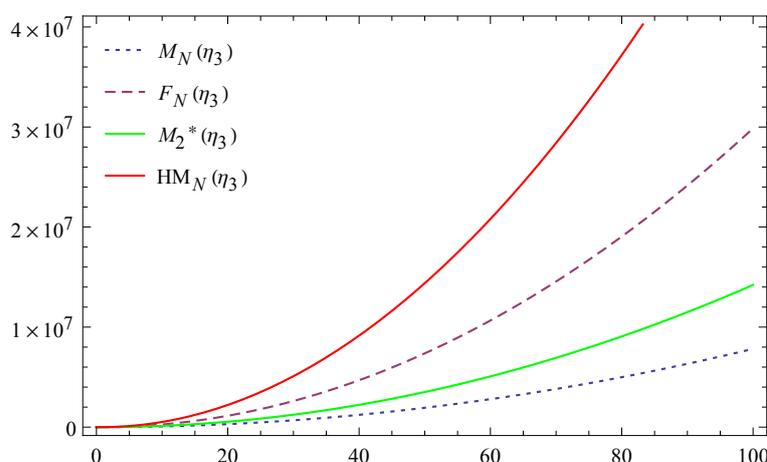


Figure 2.3: Third type of Dominating David Derived network $D_3(2)$.

Conclusion:

In this paper, some new Neighborhood-degree based topological indices, to be specific the Neighborhood versions Zagreb, Forgotten, Modified version of Forgotten, second Zagreb, Hyper-Zagreb indices for three kinds of DDD networks contemplated and investigate the basic topologies of these networks. Furthermore, we made a comparison in figure 4, 5, and 6 by the use of graph comparison. The neighborhood edition of the forgotten index F_N had the most powerful influence relative to other indices. The Zagreb neighborhood index M_N rose more slowly but surely than the others. The nature of the neighborhood version of the second Zagreb index M_2^* was close to the F_N . This analysis will facilitate researchers engaged in network science in recognizing the topology of the above-mentioned networks. For some other chemical networks, we would like to obtain such indices in the future.

References

- [1] Ali, H.; Sajjad, A. On further results of hex derived networks. *Open J. Discret. Appl. Math.* **2019**, *2(1)*, 32-40.
- [2] Ali, H.; Binyamin, M. A.; Shafiq, M. K.; Gao, W. On the Degree-Based Topological Indices of Some Derived Networks. *Mathematics* **2019**, *7*, 612.
- [3] Akhtar, S.; Imran, M. On molecular topological properties of benzenoid structures. *Can. J. Chem.* **2016**, *94*, 687-698.
- [4] Babar, U.; Ali, H.; Arshad, S.H. and Sheikh, U., Multiplicative topological properties of graphs derived from honeycomb structure. *AIMS Mathematics*, **2020**, *5(2)*, 1562.
- [5] Baig, A.Q.; Imran M.; Ali, H. On topological indices of poly oxide, poly silicate, DOX, and DSL networks. *Can. J. Chem.* **2015**, *93*, 730-739.
- [6] Baig, A. Q.; Naeem, M.; Gao, W. Revan and hyper-Revan indices of Octahedral and icosahedral networks. *Applied Mathematics and Nonlinear Sciences*, **2018**, *3(1)*, 33-40.
- [7] Diudea, M.V.; Gutman, I.; Lorentz, J. Molecular Topology; Babes-Bolyai University: Cluj-Napoca, Romania, **2001**.
- [8] Dustigeer, G., Ali, H., Khan, M. I., & Chu, Y. M. On multiplicative degree based topological indices for planar octahedron networks. *Main Group Metal Chemistry*, **2020**, *43(1)*, 219-228.
- [9] Furtula, B.; Gutman, I. Forgotten topological index. *J. Math. Chem.* **2015**, *53*, doi:10.1007/s10910-015-0480-z.
- [10] Gao, W.; Baig, A. Q.; Khalid, W.; Farahani, M. R. Molecular description of copper(II) oxide. *Maced. J. Chem. Chem. Eng.* **2017**, *36*, 93-99.
- [11] Ghorbani, M.; Hosseinzadeh, M.A. The third version of Zagreb index. *Discret. Math. Algorithms Appl.* **2013**, *5*, doi:10.1142/S1793830913500390.
- [12] Gutman, I.; Polansky, O.E. *Mathematical Concepts in Organic Chemistry*; Springer: Berlin, Germany, **1986**.
- [13] HoneyComb Structure [online]. Available from <https://www.sciencedirect.com/topics/materials-science/honeycomb-structure>
- [14] Hu, M., Ali, H., Binyamin, M. A., Ali, B., Liu, J. B., & Fan, C. On Distance-Based Topological Descriptors of Chemical Interconnection Networks. *Journal of Mathematics*, **2021**.
- [15] Imran, M.; Baig, A. Q.; Ali, H. On topological properties of dominating David derived networks, *Can. J. Chem.* **94**, 137-148, **2016**.
- [16] Liu, J. B.; Chunxiang W.; Shaohui W.; Bing W. Zagreb indices and multiplicative Zagreb indices of eulerian graphs. *Bulletin of the Malaysian Mathematical Sciences Society*, **2019**, *42(1)*, 67-78.
- [17] Liu, J. B., Zhao, J., He, H., & Shao, Z. Valency-based topological descriptors and structural property of the generalized sierpiński networks. *Journal of Statistical Physics*, **2019**, *177(6)*, 1131-1147.
- [18] Liu, J. B., Zhao, J., Min, J., & Cao, J. The hosoya index of graphs formed by a fractal graph. *Fractals*, **2019**, *27(08)*, 1950135.

- [19] Liu, J. B.; Zhi Y. S.; Ying H. P.; Jinde C.; M. Abdel-Aty; Udai Al-Juboori. Computing the Laplacian spectrum of linear octagonal-quadrilateral networks and its applications. *Polycyclic Aromatic Compounds*, **2020**, 1-12.
- [20] Liu, J. B.; Jing Z.; Zheng Q. C. On the generalized adjacency, Laplacian and signless Laplacian spectra of the weighted edge corona networks. *Physica A: Statistical Mechanics and Its Applications*, **2020**, 540, 123073.
- [21] Liu, J. B.; Jing Z.; Zhongxun Z. On the number of spanning trees and normalized Laplacian of linear octagonal-quadrilateral networks. *International Journal of Quantum Chemistry*, **2019**, 119(17), e25971.
- [22] Mondal, S.; De, N.; Pal, A. The Neighborhood Zagreb index of product graphs and its chemical interest. arXiv 2018, arXiv:1805.05273.
- [23] Mondal, S., De, N., & Pal, A. (2019). On some new neighborhood degree-based indices for some oxide and silicate networks. *J—Multidisciplinary Scientific Journal*, 2(3), 384-409.
- [24] Plavšić, D.; Nokolić, S.; Trinajstić, Mihalić, Z. On the Haray index for the Characterization of Chemical Graphs, *J. Math. Chem.* 12, 235-250, **1993**.
- [25] Simonraj, F.; George, A. Embedding of poly honeycomb networks and the metric dimension of star of david network, *GRAPH-HOC*, 4(**2012**), 11 – 28.
- [26] Shirdel, G.H.; Rezapour, H.; Sayadi, A.M. The hyper Zagreb index of graph operations. *Iran. J. Math. Chem.* **2013**, 4, 213–220.
- [27] Smith K. M. On neighbourhood degree sequences of complex networks. *Scientific reports*. **2019**, 6:9(1), 8340.
- [28] Trinajstić, N. *Chemical Graph Theory*; CRC Press: Boca Raton, FL, USA, **1983**.
- [29] Wei, C.C.; Ali, H.; Binyamin, M.A.; Naem, M.N.; Liu, J.B. Computing Degree Based Topological Properties of Third Type of Hex-Derived Networks. *Mathematics*, **2019**, 7, 368.
- [30] Wiener, H. Structural determination of the paraffin boiling points. *J. Am. Chem. Soc.* **1947**, 69, 17–20.