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Mathematical modeling and topological graph description of dominating David derived networks based on edge partitions

Shahid Zaman¹, Wakeel Ahmed¹, Atash Sakeena¹, Kavi Bahri Rasool² & Mamo Abebe Ashebo³✉

Chemical graph theory is a well-established discipline within chemistry that employs discrete mathematics to represent the physical and biological characteristics of chemical substances. In the realm of chemical compounds, graph theory-based topological indices are commonly employed to depict their geometric structure. The main aim of this paper is to investigate the degree-based topological indices of dominating David derived networks (DDDn) and assess their effectiveness. DDDNs are widely used in analyzing the structural and functional characteristics of complex networks in various fields such as biology, social sciences, and computer science. We considered the F_N^* , M_2^* , and HM_N topological indices for DDDNs. Our computations' findings provide a clear understanding of the topology of networks that have received limited study. These computed indices exhibit a high level of accuracy when applied to the investigation of QSPRs and QSARs, as they demonstrate the strongest correlation with the acentric factor and entropy.

In the field of graph theory, specifically in chemical graph theory, a chemical molecule is represented by a molecular graph, which is a simple graph. In this representation, vertices denote the atoms and edges represent bonds or connections. The edges goes beyond simple connectivity; it encompasses the type of bond as well. For instance, a single edge might denote a single covalent bond, while a double edge could represent a double bond involving the sharing of two pairs of electrons.

The emerging field of cheminformatics, which explores the relationship between quantitative structure–activity and structure–property, is gaining momentum as it aids in the prediction of biological activities. Topological indices are important invariants derived from graph theory that enable the characterization of a graph's topology. A topological index is a numerical value that provides information about the structure of a graph. Topological indices help in identifying various characteristics of a graph. Furthermore, the topology of a graph remains invariant under the automorphisms of graphs. Comparisons of the degree based topological indices hold a particularly significant place in research^{1,2}.

The first topological index introduced by Wiener, during the research of paraffin melting point. Initially termed “path number”, it was later renamed and has since become known as the Wiener index. Researchers have put a lot of effort into studying chemical graph theory. A key component of graph theory's work involves honeycomb networks. The honeycomb shape, with its hexagonal pattern of cells, finds a wide range of applications across various fields due to its unique structural and geometric properties. Some of the notable applications of the honeycomb shape include as: In structural engineering and architecture the honeycomb structure's hexagonal arrangement provides exceptional strength and stability while using minimal material. This makes it suitable for applications in construction, such as in lightweight yet strong support structures, building facades, and panels. On the other hands, in art and design, the visually appealing hexagonal pattern of the honeycomb has inspired artists, designers, and architects to incorporate it into their creations. From decorative elements in interior design to art installations, the honeycomb pattern adds a unique aesthetic.

In this article the notation E denotes an edge set and V denotes the vertex set of a graph G . The expression $\eta_G(v)$ is the number of edges overall connected to a particular vertex v .

¹Department of Mathematics, University of Sialkot, Sialkot 51310, Pakistan. ²Faculty of Science, University of Zakho, Duhok, Kurdistan Region, Iraq. ³Department of Mathematics, Wollega University, 395 Nekemte, Ethiopia. ✉email: mamo@wollegauniversity.edu.et

For the sake of simplicity, assume that a and b are two adjacent vertices and E is an edge between them, then the edge partition of E is denoted by $E_{a,b}$ and formulated as $E_{a,b} = \{\eta_G(a), \eta_G(b)\}$.

The degree-based topological indices shows a significant role in the field of mathematical chemistry³⁻⁷, and widely used to develop models that accurately predict the boiling points of alkanes with carbon atom⁸. Some current discovered degree-based neighborhood indices are presented in^{9,10} and shown strong connections between entropy and the acentric factor.

In¹¹⁻¹⁶, different chemical significant graphs' topological indices are considered. Baig et al.¹⁷ considered the topological indices for several silicates and oxide networks. Ullah et al.¹⁸, compared and examined the computational characteristics of two carbon nanosheets using some innovative topological indices. The topological characteristics of rhombus-type silicate and oxide networks were explored by Javaid et al.¹⁹. Recently, Koam et al.²⁰, established the entropy measures of Y-junction based nanostructures. Ali et al.²¹ give some properties of v -degree based topological indices for hex-derived networks. In this study, an examination was conducted on distance-based topological polynomials that are associated with zero-divisor graphs, as discussed in²². The authors of²³ obtained the polynomials of degree-based indices of metal-organic networks. Zaman et al., determined the kemeny's constant and spanning trees of hexagonal ring network²⁴. Some upper bound and lower bound of graphs and also the spectral analysis of graphs are discussed in²⁵⁻²⁸. In this research, inspired by earlier studies, we establish some exact expressions of the different types of Dominating David derived networks and their comparisons.

We have calculated the forgotten index (F_N^*)²⁹, the second zargab index (M_2^*)³⁰ and the Harmonic index (HM_N)³¹ for DDD networks. These topological indices are defined as $F_N^* = \sum_{uv \in E(G)} [\eta_G(u)^2 + \eta_G(v)^2]$,

$$HM_N(G) = \sum_{uv \in E(G)} [\eta_G(u) + \eta_G(v)]^2, M_2^* = \sum_{uv \in E(G)} [\eta_G(u) + \eta_G(v)].$$

Constructions of dominating David derived networks (DDD_N)

In the field of chemistry, honeycomb networks are utilized as representations for benzenoid hydrocarbons. Honeycomb networks find extensive applications in various domains, including graphics, such as cell phone base stations and image processing. The honeycomb network is formed by enclosing the boundaries with a layer of hexagons. Based on the honeycomb network, different types of Dominating David derived networks can be derived. One can follow the below steps to construct the DDD_N (t dimension):

Step 1: Consider a t -dimension honeycomb network (see Fig. 1a).

Step 2: Add another vertex to divide each edge into two pieces (see Fig. 1b).

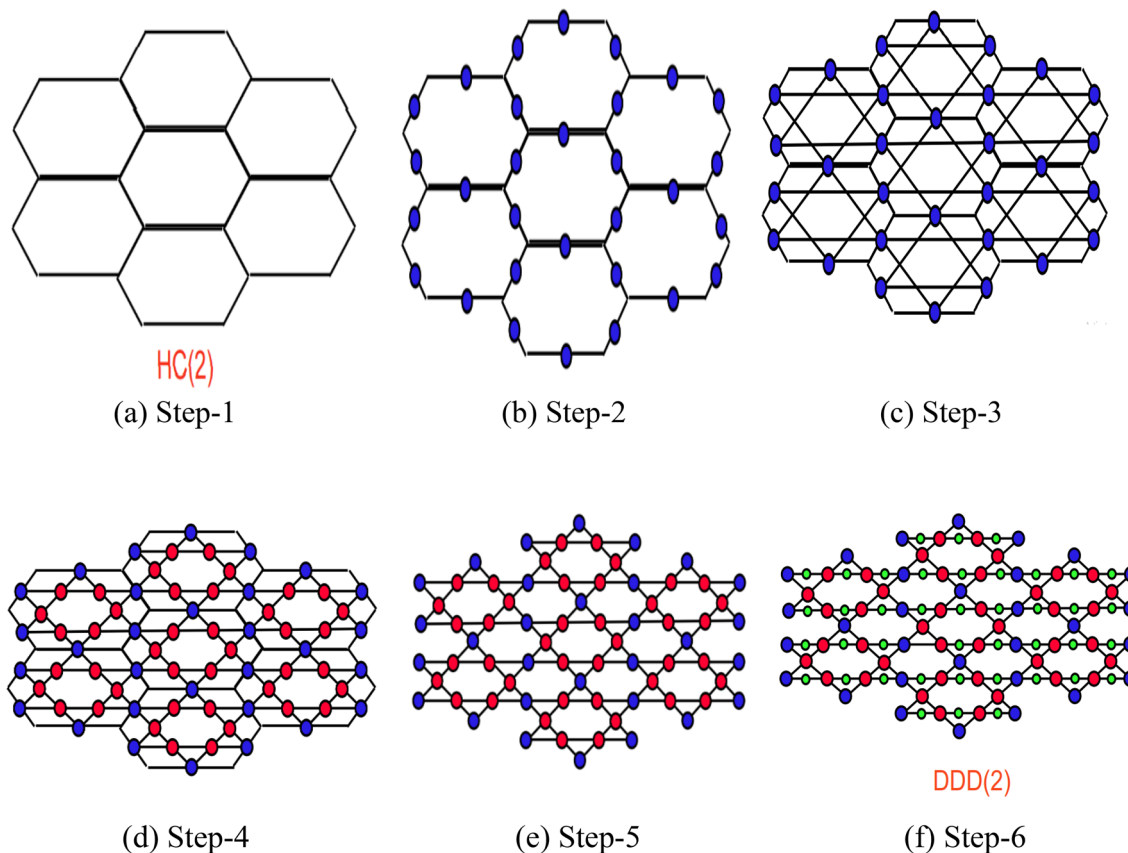


Figure 1. The steps to derive DDD (2).

Step 3: In each hexagonal cell, connect the new vertices by an edge if they are at a distance of 4 within a hexagon (see Fig. 1c).

Step 4: Add new vertices at new edge intersections. (see Fig. 1d).

Step 5: Remove the starting vertices and edges of the honeycomb (see Fig. 1e).

Step 6: Divide each horizontal edge into two parts by adding a new vertex (see Fig. 1f).

Main results

Our key findings rely on the edge partitions of Figs. 2, 3 and 4 as given below. We have calculated these edge partitions based on the degrees of the end vertices of each edge. For instance, the first row of Fig. 1 shows the degrees of the end vertices of edges, while the second row illustrates the count of edges with those specific degrees. In the same way, we have obtained the other tables.

The F_N^* topological index for dominating David derived networks. Let G be a graph in $D_1(t)$, $D_2(t)$ and $D_3(t)$ then according to the definition of F_N^* and Table 1, we have

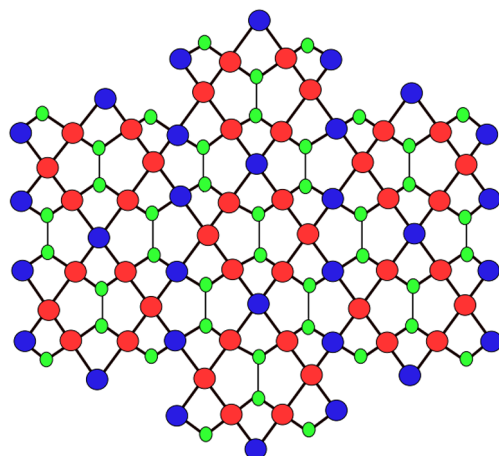


Figure 2. First type of $D_1(2)$ network.

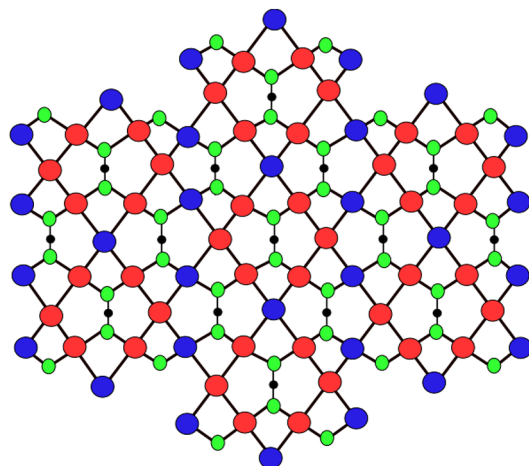


Figure 3. First type of $D_2(2)$ network.

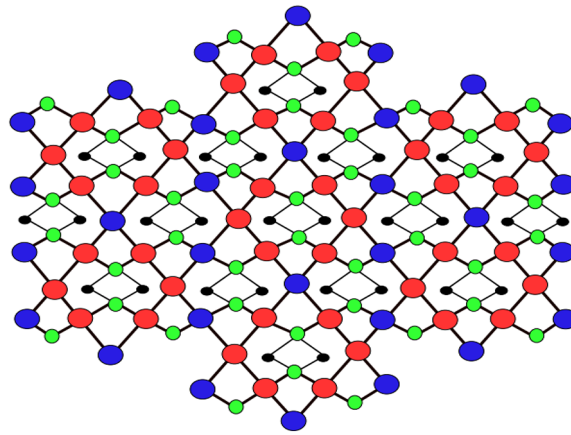


Figure 4. Third type of $D_3(2)$ network.

$(\eta_G(u), \eta_G(v))$	(2, 2)	(2, 3)	(2, 4)	(3, 3)	(3, 4)	(4, 4)
Frequency	$4t$	$4t - 4$	$28t - 16$	$9t^2 - 13t + 5$	$36t^2 - 56t + 24$	$36t^2 - 52t + 20$

Table 1. Edges partition $D_1(t)$.

$$\begin{aligned}
 F_N^*(G) &= \sum_{uv \in E(G)} [\eta_G(u)^2 + \eta_G(v)^2] \\
 &= |E_{(2,2)}| [(2)^2 + (2)^2] + |E_{(2,3)}| [(2)^2 + (3)^2] + |E_{(2,4)}| [(2)^2 + (4)^2] + |E_{(3,3)}| [(3)^2 + (3)^2] \\
 &\quad + |E_{(3,4)}| [(3)^2 + (4)^2] \\
 &= 4t(8) + 4t - 4(13) + 28t - 16(20) + 9t^2 - 13t + 5(18) + 36^2 - 56t + 24(25) + 36t^2 - 52t + 20(32) \\
 &= 32t + 52t - 52 + 560t - 320 + 162t^2 - 234t + 90 + 900t^2 - 1400t + 600 + 1152t^2 - 1664t + 640 \\
 &= 2214t^2 - 1951t + 958
 \end{aligned}$$

Similarly, from Table 2, we have

$$\begin{aligned}
 F_N^*(G) &= 32t + 234t^2 - 286t + 78 + 560t - 320 + 900t^2 - 1400t + 600 + 1152t^2 - 1664t + 640 \\
 &= 2286t^2 - 2758t + 998
 \end{aligned}$$

And from Table 3, one has

$$\begin{aligned}
 F_N^*(G) &= |E_{(2,2)}| (4 + 4) + |E_{(2,4)}| (4 + 16) + |E_{(4,4)}| (16 + 16) \\
 &= 32t + 720t^2 - 400t + 2304t^2 - 3456t + 1408 \\
 &= 3024t^2 - 3824t + 1408
 \end{aligned}$$

The M_2^* topological index for DDDN. Let G be a graph in $D_1(t)$, $D_2(t)$ and $D_3(t)$ then according to the definition of M_2^* and Table 1 we have

$(\eta_G(u), \eta_G(v))$	(2, 2)	(2, 3)	(2, 4)	(3, 4)	(4, 4)
Frequency	$4t$	$18t^2 - 22t + 6$	$28t - 16$	$36t^2 - 56t + 24$	$36t^2 - 52t + 20$

Table 2. Edge partition $D_2(t)$.

$(\eta_G(u), \eta_G(v))$	(2, 2)	(2, 4)	(4, 4)
Frequency	$4t$	$36t^2 - 20t$	$72t^2 - 108t + 44$

Table 3. Edge partition $D_3(t)$.

t	$F_N^*(D_1)$	$F_N^*(D_2)$	$F_N^*(D_3)$	$M_2^*(D_1)$	$M_2^*(D_2)$	$M_2^*(D_3)$	$HM_N(D_1)$	$HM_N(D_2)$	$HM_N(D_3)$
1	1221	526	608	233	236	272	2270	1493	1152
2	5912	4626	5856	2143	2188	2720	10,084	9992	11,296
3	15,031	13,298	17,152	6231	6372	8048	26,682	27,527	33,248
4	28,578	26,542	34,496	12,497	12,788	16,256	52,064	54,098	67,008
5	46,553	44,358	57,888	20,941	21,436	27,344	86,230	89,705	112,576
6	68,956	66,746	87,328	31,563	32,316	30,512	129,180	134,348	169,952

Table 4. The comparison of F_N^* , M_2^* and HM_N for $D_1(t)$, $D_2(t)$ and $D_3(t)$ graphs.

$$\begin{aligned} M_2^*(G) &= E_{(2,2)} | (2.2) + |E_{(2,3)} | (2.3) + |E_{(2,4)} | (2.4) + |E_{(3,3)} | (3.3) + |E_{(3,4)} | (3.4) + |E_{(4,4)} | (4.4) \\ &= 16t + 24t - 24 + 224t - 128 + 81t^2 - 117t + 45 + 432t^2 - 672t + 288 + 576t^2 - 832t + 320 \\ &= 1089t^2 - 1357t + 501 \end{aligned}$$

Likewise, based on the information presented in Table 2, we obtain

$$\begin{aligned} M_2^*(G) &= 16t + 108t^2 - 132t + 36 + 224t - 128 + 432t^2 - 672t + 288 + 576t^2 - 832t + 320 \\ &= 1116t^2 - 1396t + 516 \end{aligned}$$

And from Table 3, one has

$$\begin{aligned} M_2^*(G) &= |E_{(2,2)} | (2.2) + |E_{(2,4)} | (2.4) + |E_{(4,4)} | (4.4) \\ &= 16t + 288t^2 - 160t + 1152t^2 - 1728t + 704 \\ &= 1440t^2 - 1872t + 704 \end{aligned}$$

The HM_N topological index for DDDN. Let G be a graph in $D_1(t)$, $D_2(t)$ and $D_3(t)$ then according to the definition of HM_N and Table 1, we have

$$\begin{aligned} HM_N(G) &= 64t + 100t - 100 + 1008t - 576 + 324t^2 - 468t + 180 \\ &+ 1764t^2 - 2744t + 1176 + 2304t^2 - 3328t + 1280 \end{aligned}$$

Similarly, from Table 2, we have

$$\begin{aligned} HM_N(G) &= 4392t^2 - 5362t + 3240 \\ HM_N(G) &= 64t + 450t^2 - 55t + 150 + 1008t - 576 + 1764t^2 - 2744t + 1176 + 2304t^2 - 3328t + 1280 \\ HM_N(G) &= 4518t^2 - 5055t + 2030 \end{aligned}$$

And from Table 3, we have

$$\begin{aligned} HM_N(G) &= |E_{(2,2)} | (16) + |E_{(2,4)} | (36) + |E_{(4,4)} | (64) \\ &= 64t + 1296t^2 - 720t + 4608t^2 - 6912t + 2816 \\ &= 5904t^2 - 7568t + 2816 \end{aligned}$$

Concluding Remarks

In this study, we have considered the F_N^* , M_2^* and HM_N topological indices. Our simulated results help for the better comprehend topology and enhance physical properties of the honeycomb structure. The computed indices, and above, as previously mentioned, have the most closely relates to the acentric factor and entropy consequently, they are extremely accurate in QSPR and QSAR analysis.

In Table 4, the topological indices computed are represented mathematically. As we can see, increasing the values of t , increases the value of the indices as well. We have precise analytical formulations for the D_1 , D_2 and D_3 networks, considering various topological indices. In the rapidly expanding fields of nanotechnology and applications, such as networks, our current discoveries and techniques can be applied to other, more complex structures. The utilization of distance-based topological indices poses greater challenges and complexity, but they can be employed alongside existing methods. Exploring these types of studies will be the focus of future research endeavors. In Table 4 and Fig. 5, we computed the numerical comparison of the certain topological indices for D_1 , D_2 and D_3 networks, which shows that when we increase t as a result the values of the topological indices also increases. These numerical comparisons also shows that the increasing rate of HM_N for D_3 is greater than the other topological indices. Since, in graph theory, the HM_N is a mathematical concept used to describe the connectivity. Therefore, a higher HM_N reflects the more connectivity among the atoms of a molecule. This indicates that the D_3 molecule has a greater potential for forming diverse interactions with other molecules and participating in a wider range of chemical reactions.

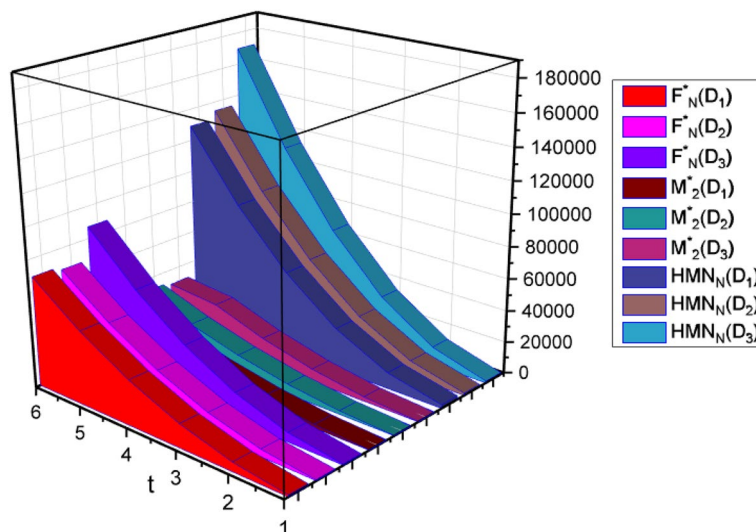


Figure 5. The comparison graph.

Data availability

All data generated or analysed during this study are included in this published article.

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Author contributions

All authors have made equal contributions to this paper at every stage, including conceptualization and the final drafting process. The manuscript has been approved by all authors and consent for publication has been granted.

Competing interests

The authors declare no competing interests.

Additional information

Correspondence and requests for materials should be addressed to M.A.A.

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