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# TOPOLOGICAL CHARACTERIZATION AND GRAPH-THEORETICAL MODELING OF H-NAPHTHALENIC NANOSHEET USING CM-POLYNOMIAL

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**Abstract:** *The physico-chemical properties and biological activities of chemical compounds can be estimated using numerical descriptors known as topological indices. These indices transform molecular graph information into numerical values, thereby enhancing the analysis of structure–property and structure–activity relationships. The present study focuses on deriving the CM-polynomial for H-naphthalenic nanosheet, subdivision graph of H-Naphtalenic nanosheet and the line graph of subdivision graph of H-Naphtalenic nanosheet. From these CM-polynomials, several degree-based topological indices are subsequently obtained. Using these indices, numerical results are obtained to explore the physical and chemical characteristics of the H-naphthalenic nanosheet under investigation.*

**Keywords:** *Topological indices, CM-polynomial, Subdivision graph, Line graph, H-Naphtalenic Nanosheet.*

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## 1. Introduction

Graph theory has emerged as a powerful mathematical framework with extensive applications across numerous scientific disciplines, among which chemistry holds a prominent position. Within the realm of chemical graph theory, topological indices (TIs) serve as quantitative descriptors of molecular topology, enabling the prediction and analysis of various physico-chemical and biological properties of chemical compounds [15].

Over the years, TIs have attracted significant interest in fields such as pharmacology, bioinorganic chemistry, toxicity assessment, and theoretical modeling. These indices are fundamental to the development of Quantitative Structure–Activity Relationship (QSAR) and Quantitative Structure–Property Relationship (QSPR) models, which provide efficient computational methods for forecasting molecular behavior [9,10,18]. The effectiveness of TIs arises from their strong mathematical foundation and their ability to minimize experimental limitations, making them essential tools in modern theoretical chemistry. Furthermore, the accuracy of QSAR/QSPR predictions depends largely on the selection of molecular datasets, algorithms, and descriptors employed.

Graph theory employs several analytical tools that play a vital role in its diverse applications, among which graph polynomials are particularly significant. For instance, the Hosoya Polynomial [17] is essential in studying distance-based topological indices. In recent years, two important advancements have emerged. The M-polynomial [8] introduced in 2015 and the NM-polynomial [20] introduced in 2021, both of which serve as powerful tools for deriving closed-form expressions of various degree-based topological indices.

Numerous graph polynomials have been proposed in the literature to simplify and accelerate the computation of different graph indices. Due to their wide-ranging applications, these polynomials have been extensively used to formulate expressions for degree-based topological indices, which are crucial for understanding the structural and chemical properties of molecules [1,2]. Among these, the M-polynomial is particularly valuable, as it provides a unified framework for generating several topological indices. With ongoing advancements in this field, novel indices are being introduced continually. Recently, researchers have focused on neighborhood degree sum-based indices, leading to

increased interest in the NM-polynomial, which serves a similar function to the M-polynomial but specifically for neighborhood degree-based indices. Essentially, the M-polynomial acts as a general framework from which degree-based indices can be derived, while the NM-polynomial extends this concept to neighborhood degree-based indices. Typically, connectivity indices are computed directly from their definitions; however, using a single, unified polynomial to derive multiple indices is a more efficient approach. The M-polynomial provides such a compact and versatile method, and analyzing its properties offers deeper insights into degree-based topological indices.

In nanoscience and nanotechnology, Carbon nanotubes have proven especially valuable as nanoprobe in Atomic Force Microscopy (AFM), addressing key challenges in experimental modeling and nanoscale surface analysis. They also play an essential role in nanoelectromechanical systems (NEMS), including nanoscale memory devices and electrical motors. CNTs have attracted immense research interest, particularly in the computation of topological indices that describe their molecular structure and properties within the framework of chemical graph theory. These indices provide mathematical representations that help predict and analyze the physicochemical behavior of nanomaterials.

In recent years, two-dimensional (2D) nanomaterials, especially porphyrin-based naphthalenic nanosheets, have gained substantial attention for their potential applications in photodynamic therapy, nanodevices, and drug delivery systems. Such materials help overcome traditional challenges like poor solubility, toxicity, and inefficient release patterns in conventional drug formulations. Within chemical graph theory, numerous molecular descriptors derived from graph theory are employed to estimate the chemical and structural properties of these nanomaterials, forming the basis of QSAR/QSPR analyses. These approaches are instrumental in advancing research across materials science, chemical engineering, and pharmaceutical chemistry, underscoring the pivotal role of chemical graph theory in modern nanomaterial design and application [11,12,13,14,21].

## 2. H-naphthalenic Nanosheet and its Chemical Significance

The H-naphthalenic nanosheet is a trivalent molecular structure composed of alternating hexagonal ( $C_6$ ), square ( $C_4$ ), and octagonal ( $C_8$ ) carbon rings arranged in a periodic pattern. It is denoted as  $N(m,n)$ , where  $m$  represents the number of paired hexagons in each alternating row containing a  $C_4$  cycle, and  $n$  denotes the number of such rows. The topological indices of the H-naphthalenic nanosheet, which quantitatively describe its molecular structure, have been extensively studied in [7]. These indices play an essential role in chemical graph theory, as they help characterize the nanosheet's geometry and predict its physicochemical properties relevant to nanomaterial design and theoretical chemistry.

The H-naphthalenic nanosheet  $N(m,n)$  stands out from nanosheets like  $TUC_4C_8$ , graphene, and borophene due to its hybrid arrangement of hexagonal ( $C_6$ ), quadrilateral ( $C_4$ ), and octagonal ( $C_8$ ) rings. This mixed structure creates non-uniform vertex degrees and irregular edge connections, yielding a more complex molecular graph. In chemical graph theory, such diversity significantly alters topological indices, offering greater variability and analytical depth than the regular  $TUC_4C_8$  pattern. The parameters  $m$  and  $n$  enable scalable modeling, allowing exploration of how structural irregularities influence stability, reactivity, and electronic behavior, making  $N(m,n)$  a versatile and realistic model for nanoscale material studies.

## 3. Preliminaries

Let  $G$  be a finite, simple, undirected and connected graph with vertex set  $V(G)$  and edge set  $E(G)$ , having order  $r$  and size  $s$ . The edge  $uv$  connecting the two vertices  $u$  and  $v$ . The degree of vertex  $u$  is denoted by  $d(u)$ , and is defined as the number of edges incident to  $u$ . The neighborhood of  $u$  is denoted by  $N(u)$ , is the set of vertices adjacent to  $u$ , and the degree

sum of neighbor of a vertex  $u$  is  $S(u) = \sum_{v \in N(u)} d(v)$ . The closed neighborhood  $N_c[u] = N(u) \cup \{u\}$  includes  $u$  and its neighbors. The degree sum of closed neighbor of a vertex  $u$  is  $S_c[u] = \sum_{v \in N(u)} d(v) + d(u)$  [5]. We refer [16] for undefined graph terminologies and notations.

#### 4. Methodology

Motivated by the degree-based topological indices and neighborhood degree-based topological indices, we introduced some closed neighborhood degree-based topological indices and studied its QSPR analysis on octane isomers [5,6]. The closed neighborhood degree-based topological indices are defined as follows:

The *first closed neighborhood Zagreb index* is defined as

$$CM_1(G) = \sum_{uv \in E(G)} (S_c[u] + S_c[v]).$$

The *second closed neighborhood Zagreb index* is defined as

$$CM_2(G) = \sum_{uv \in E(G)} (S_c[u] \cdot S_c[v]).$$

The *closed neighborhood harmonic index* is defined as

$$CH(G) = \sum_{uv \in E(G)} \frac{2}{S_c[u] + S_c[v]}.$$

The *closed neighborhood inverse sum index* is defined as

$$CIS(G) = \sum_{uv \in E(G)} \frac{S_c[u] \cdot S_c[v]}{S_c[u] + S_c[v]}.$$

The *closed neighborhood forgotten index* is defined as

$$CF(G) = \sum_{uv \in E(G)} (S_c[u]^2 + S_c[v]^2).$$

The *first closed neighborhood hyper Zagreb index* is expressed as

$$CHM_1(G) = \sum_{uv \in E(G)} (S_c[u] + S_c[v])^2.$$

The *first closed neighborhood Gourava index* is defined as

$$CGO_1(G) = \sum_{uv \in E(G)} (S_c[u] + S_c[v] + S_c[u] \cdot S_c[v]).$$

**Definition 4.1.** [8] For a simple connected graph  $G$ , the *M-polynomial* is defined as

$$M(G; p, q) = \sum_{i \leq j} m_{ij}(G) p^i q^j,$$

where  $m_{ij}(G)$  represents the number of edges  $uv \in E(G)$  such that  $\{d(u), d(v)\} = \{i, j\}$ .

Inspired by the operator-based formulation of the M-polynomial and NM-polynomial, we defined new descriptor termed the *CM-polynomial*, which is defined using the closed neighborhood degree of a vertex [6].

**Definition 4.2.** For a simple connected graph  $G$ , the CM-polynomial is defined as

$$CM(G; p, q) = \sum_{i \leq j} c_{ij}(G) p^i q^j,$$

where  $c_{ij}(G)$  represents the number of edges  $uv \in E(G)$  such that  $\{S_c[u], S_c[v]\} = \{i, j\}$ .

**Table 1.** Operator-based derivation of closed neighborhood degree-based indices from the CM-polynomial

Index	$f(p, q)$	Derivation from $CM(G; p, q)$
$CM_1(G)$	$p + q$	$(D_p + D_q)CM(G; p, q) _{p=q=1}$
$CM_2(G)$	$pq$	$(D_p \cdot D_q)CM(G; p, q) _{p=q=1}$
$CH(G)$	$\frac{2}{p + q}$	$(2S_p J)CM(G; p, q) _{p=q=1}$
$CIS(G)$	$\frac{pq}{p + q}$	$(S_p J D_p D_q)CM(G; p, q) _{p=q=1}$
$CF(G)$	$p^2 + q^2$	$(D_p^2 + D_q^2)CM(G; p, q) _{p=q=1}$
$CHM_1(G)$	$(p + q)^2$	$(D_p^2 J)CM(G; p, q) _{p=q=1}$
$CGO_1(G)$	$p + q + pq$	$(D_p + D_q + D_p D_q)CM(G; p, q) _{p=q=1}$

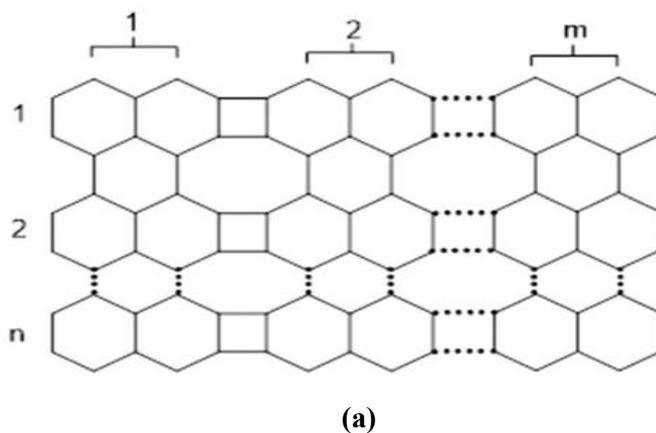
**Operator definitions:**

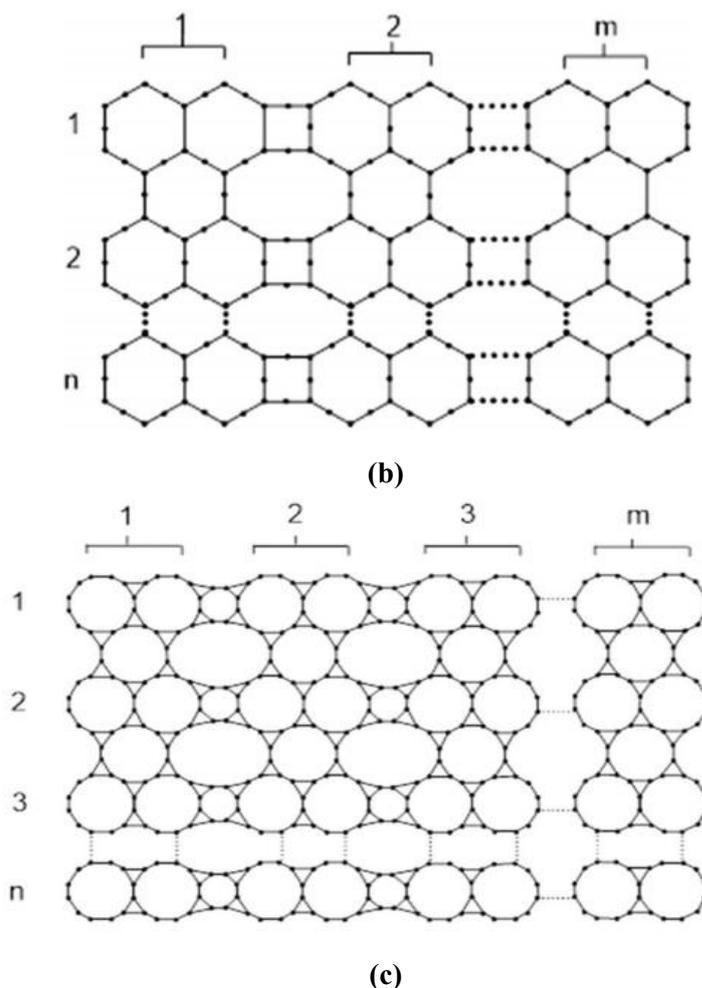
$$D_p f(p, q) = p \frac{\partial f(p, q)}{\partial p}, \quad D_q f(p, q) = q \frac{\partial f(p, q)}{\partial q}, \quad S_p f(p, q) = \int_0^p \frac{f(t, q)}{t} dt, \quad S_q f(p, q) = \int_0^q \frac{f(p, t)}{t} dt,$$

$$Jf(p, q) = f(p, p).$$

**5. Main results**

In our present work, we computed some closed neighborhood degree-based topological indices for H-naphtalenic nanosheet  $N(m, n)$ , subdivision graph of H-naphtalenic nanosheet  $S(N(m, n))$  and the line graph of subdivision graph of H-naphtalenic nanosheet  $L(S(N(m, n)))$  using CM-polynomial. The graph is shown in Figure 1.





**Figure 1.** (a) H-naphthalenic nanosheet  $N(m,n)$ , (b) Subdivision graph of H-naphthalenic nanosheet  $S(N(m,n))$ , (c) Line graph of subdivision graph of H-naphthalenic nanosheet  $L(S(N(m,n)))$ .

**Theorem 5.1:** Let  $N(m,n)$  be the graph of H-naphthalenic nanosheet. Then

$$CM(N(m,n); p, q) = 8p^6q^7 + 2np^7q^7 + 4(m-1)p^8q^7 + 2mp^7q^{12} + 4(m-1)p^8q^{11} + (2m+2n-4)p^{11}q^{11} + (4m+4n-8)p^{11}q^{12} + (15mn-18m-10n+12)p^{12}q^{12}.$$

**Proof:** The graph  $N(m,n)$  has  $10nm$  vertices and  $15nm-2(n+m)$  edges. The Edge partition of  $N(m,n)$  is given in Table 2. By applying, Table 2 in the definition of CM-polynomial, we obtain the desired result.

**Table 2.** Edge partition of  $N(m,n)$  based on closed neighborhood degree

$(S_c[u], S_c[v]), uv \in E(G)$	No. of edges
(6, 7)	8
(7, 7)	$2n$
(8, 7)	$4(m-1)$
(7, 12)	$2m$
(8, 11)	$4(m-1)$
(11, 11)	$2m+2n-4$
(11, 12)	$4m+4n-8$
(12, 12)	$15mn-18m-10n+12$

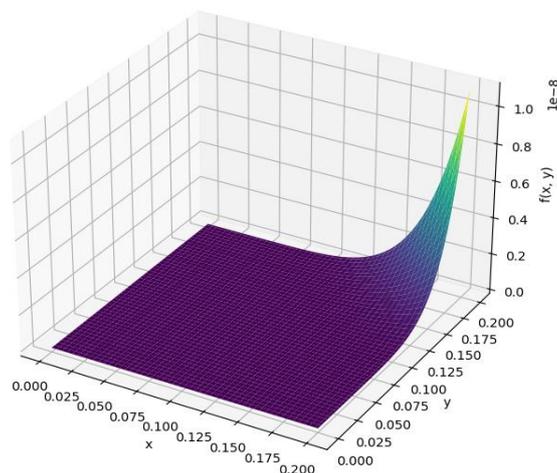


Figure 1. CM-polynomial of  $N(m,n)$  Graph for  $m=n=10$

**Corollary 5.2:** If  $N(m,n)$  be the graph of  $H$ -naphthalenic nanosheet, then

1.  $CM_1(N(m,n)) = 360mn - 122m - 76n - 16,$
2.  $CM_2(N(m,n)) = 2160mn - 1078m - 572n - 52,$
3.  $CH(N(m,n)) = \frac{5}{4}mn + \frac{28057}{144210}m - \frac{191}{10626}n + \frac{203497}{937365},$
4.  $CIS(N(m,n)) = 90mn - \frac{208067}{6555}m - \frac{438}{23}n - \frac{300514}{85215},$
5.  $CF(N(m,n)) = 4320mn - 2062m - 1140n - 144,$
6.  $CHM_1(N(m,n)) = 8640mn - 4218m - 2284n - 248,$
7.  $CGO_1(N(m,n)) = 2520mn - 1200m - 648n - 68.$

**Proof:** The CM-polynomial of a  $N(m,n)$  graph is

$$CM(N(m,n); p, q) = 8p^6q^7 + 2np^7q^7 + 4(m-1)p^8q^7 + 2mp^7q^{12} + 4(m-1)p^8q^{11} + (2m+2n-4)p^{11}q^{11} + (4m+4n-8)p^{11}q^{12} + (15mn-18m-10n+12)p^{12}q^{12}. \text{ Then}$$

$$D_p(N(m,n); p, q) = 180mnp^{12}q^{12} - 216mp^{12}q^{12} + 44mp^{11}q^{12} + 22mp^{11}q^{11} + 32mp^8q^{11} + 32mp^8q^7 + 14mp^7q^{12} - 120np^{12}q^{12} + 44np^{11}q^{12} + 22np^{11}q^{11} + 14np^7q^7 + 144p^{12}q^{12} - 88p^{11}q^{12} - 44p^{11}q^{11} - 32p^8q^{11} - 32p^8q^7 + 48p^6q^7,$$

$$D_q(N(m,n); p, q) = 180mnp^{12}q^{12} - 216mp^{12}q^{12} + 48mp^{11}q^{12} + 22mp^{11}q^{11} + 44mp^8q^{11} + 28mp^8q^7 + 24mp^7q^{12} - 120np^{12}q^{12} + 48np^{11}q^{12} + 22np^{11}q^{11} + 14np^7q^7 + 144p^{12}q^{12} - 96p^{11}q^{12} - 44p^{11}q^{11} - 44p^8q^{11} - 28p^8q^7 + 56p^6q^7,$$

$$S_p(N(m,n); p, q) = \frac{4}{3}p^6q^7 - \frac{2n}{7}p^7q^7 + \frac{(m-1)}{2}p^8q^7 + \frac{m}{6}p^7q^{12} + \frac{(m-1)}{2}p^8q^{11} + \frac{(2m+2n-4)}{11}p^{11}q^{11} + \frac{(4m+4n-8)}{11}p^{11}q^{12} + \frac{(15mn-18m-10n+12)}{12}p^{12}q^{12} - 120np^{12}q^{12},$$

$$S_q(N(m,n); p, q) = \frac{8}{7} p^6 q^7 + \frac{2n}{7} p^7 q^7 + \frac{4(m-1)}{7} p^8 q^7 + \frac{m}{6} p^7 q^{12} + \frac{4(m-1)}{11} p^8 q^{11} + \frac{(2m+2n-4)}{11} p^{11} q^{11} + \frac{(4m+4n-8)}{11} p^{11} q^{12} + \frac{(15mn-18m-10n+12)}{12} p^{12} q^{12},$$

$$J(N(m,n); p, q) = 15mnp^{24} - 18mp^{24} + 4mp^{23} + 2mp^{22} + 6mp^{19} + 4mp^{15} - 10np^{24} + 4np^{23} + 2np^{22} + 2np^{14} + 12p^{24} - 8p^{23} - 4p^{22} - 4p^{19} - 4p^{15} + 8p^{13},$$

By applying all these values in Table 1, we obtain the required result.

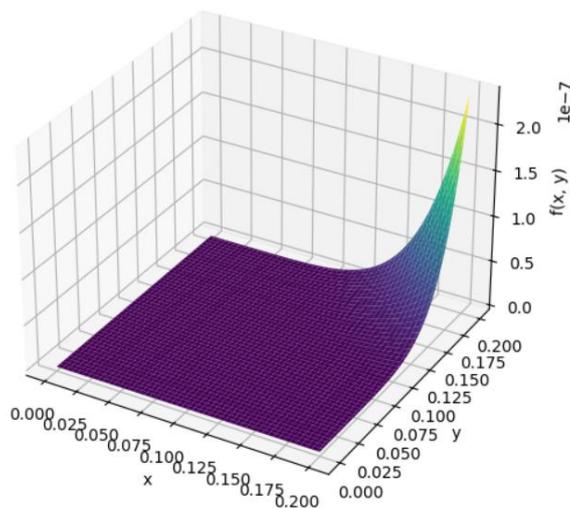
**Theorem 5.3:** Let  $S(N(m,n))$  be the subdivision graph of  $H$ -naphthalenic nanosheet. Then

$$CM(S(N(m,n)); p, q) = (2n+14)p^6q^6 + (8m+4n-8)p^6q^7 + (8m+2n-2)p^7q^9 + (30mn-20m-12n-4)p^8q^9.$$

**Proof:** The graph  $S(N(m,n))$  has  $20nm$  vertices and  $30nm-4(n+m)$  edges. The Edge partition of  $S(N(m,n))$  is given in Table 3. By using these values in definition of CM-polynomial, we obtain the desired result.

**Table 3.** Edge partition of  $S(N(m,n))$  based on closed neighborhood degree

$(S_c[u], S_c[v]), uv \in E(G)$	No. of edges
(6, 6)	$2n+14$
(6, 7)	$8m+4n-8$
(7, 9)	$8m+2n-2$
(8, 9)	$30mn-20m-12n-4$



**Figure 2.** CM-polynomial of  $S(N(m,n))$  Graph for  $m=n=10$

**Corollary 5.4:** If  $S(N(m,n))$  be the subdivision graph of  $H$ -naphthalenic nanosheet, then

1.  $CM_1(S(N(m,n))) = 510mn - 108m - 96n - 36,$
2.  $CM_2(S(N(m,n))) = 2160mn - 600m - 498n - 246,$
3.  $CH(S(N(m,n))) = \frac{60}{17}mn - \frac{27}{221}m - \frac{565}{2652}n + \frac{1013}{2652},$

4.  $CIS(S(N(m,n))) = \frac{2160}{17}mn - \frac{12093}{442}m - \frac{42477}{1768}n - \frac{15315}{1768}$ ,
5.  $CF(S(N(m,n))) = 4350mn - 1180m - 996n - 512$ ,
6.  $CHM_1(S(N(m,n))) = 8670mn - 2380m - 1992n - 1004$ ,
7.  $CGO_1(S(N(m,n))) = 2670mn - 708m - 594n - 282$ .

**Proof:** The CM-polynomial of a  $S(N(m,n))$  graph is

$$CM(S(N(m,n)); p, q) = (2n + 14)p^6q^6 + (8m + 4n - 8)p^6q^7 + (8m + 2n - 2)p^7q^9 + (30mn - 20m - 12n - 4)p^8q^9. \text{ Then}$$

$$D_p(S(N(m,n)); p, q) = 240mnp^8q^9 - 160mp^8q^9 + 56mp^7q^9 + 48mp^6q^7 - 96np^8q^9 + 14np^7q^9 + 24np^6q^7 + 12np^6q^6 - 32p^8q^9 - 14p^7q^9 - 48p^6q^7 + 84p^6q^6,$$

$$D_q(S(N(m,n)); p, q) = 270mnp^8q^9 - 180mp^8q^9 + 72mp^7q^9 + 56mp^6q^7 - 108np^8q^9 + 18np^7q^9 + 28np^6q^7 + 12np^6q^6 - 36p^8q^9 - 18p^7q^9 - 56p^6q^7 + 84p^6q^6,$$

$$S_p(S(N(m,n)); p, q) = \frac{(2n+14)}{6}p^6q^6 + \frac{(8m+4n-8)}{6}p^6q^7 + \frac{(8m+2n-2)}{7}p^7q^9 + \frac{(30mn-20m-12n-4)}{8}p^8q^9,$$

$$S_q(S(N(m,n)); p, q) = \frac{(2n+14)}{6}p^6q^6 + \frac{(8m+4n-8)}{7}p^6q^7 + \frac{(8m+2n-2)}{9}p^7q^9 + \frac{(30mn-20m-12n-4)}{9}p^8q^9,$$

$$J(S(N(m,n)); p, q) = 30mnp^{17} - 20mp^{17} + 8mp^{16} + 8mp^{13} - 12np^{17} + 2np^{16} + 4np^{13} + 2np^{12} - 4p^{17} - 2p^{16} - 8p^{13} + 14p^{12},$$

By applying all these values in Table 1, we obtain the desired result.

**Theorem 5.5:** Let  $L(S(N(m,n)))$  be the line graph of the subdivision graph of  $H$ -naphthalenic nanosheet. Then

$$CM(L(S(N(m,n))); p, q) = (2n + 8)p^6q^6 + 4np^6q^7 + (4m - 4)p^7q^7 + (8m + 4n - 8)p^7q^{11} + 2mp^{11}q^{11} + (12m - 8)p^{11}q^{12} + (45mn - 36m - 20n + 12)p^{12}q^{12}.$$

**Proof:** The graph  $L(S(N(m,n)))$  has  $30nm - 4m - 4n$  vertices and  $45nm - 10(n + m)$  edges. The Edge partition of  $L(S(N(m,n)))$  is given in Table 4. By using these values in definition of CM-polynomial, we obtain the desired result.

**Table 4.** Edge partition of nanosheet  $L(S(N(m,n)))$  based on closed neighborhood degree

$(S_c[u], S_c[v]), uv \in E(G)$	No. of edges
(6, 6)	$2n + 8$
(6, 7)	$4n$
(7, 7)	$4m - 4$
(7, 11)	$8m + 4n - 8$
(11, 11)	$2m$
(11, 12)	$12m - 8$
(12, 12)	$45mn - 36m - 20n + 12$

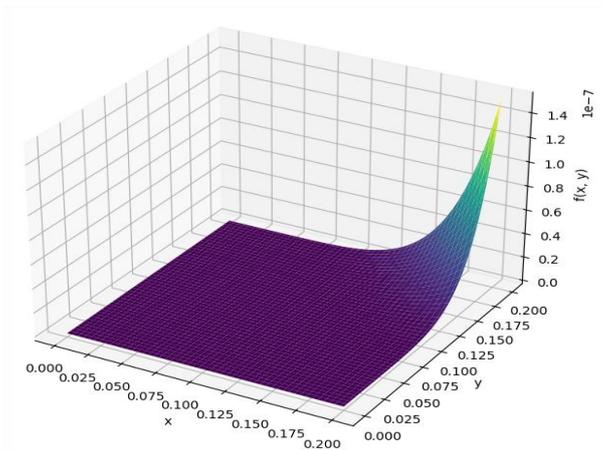


Figure 3. CM-polynomial of  $L(S(N(m,n)))$  Graph for  $m=n=10$

**Corollary 5.6:** If  $L(S(N(m,n)))$  be the Line graph of subdivision graph of H-Naphtalenic nanosheet, then

1.  $CM_1(L(S(N(m,n)))) = 1080mn - 344m - 332n$ ,
2.  $CM_2(L(S(N(m,n)))) = 6480mn - 2546m - 2332n + 148$ ,
3.  $CH(L(S(N(m,n)))) = \frac{15}{4}mn - \frac{5011}{15939}m - \frac{32}{117}n + \frac{257}{1449}$ ,
4.  $CIS(L(S(N(m,n)))) = 270mn - \frac{18197}{207}m - \frac{9824}{117}n + \frac{386}{207}$ ,
5.  $CF(L(S(N(m,n)))) = 12960mn - 4952m - 4596n + 160$ ,
6.  $CHM_1(L(S(N(m,n)))) = 25920mn - 10044m - 9260n + 456$ ,
7.  $CGO_1(L(S(N(m,n)))) = 7560mn - 2890m - 2664n + 148$ .

**Proof:** The CM-polynomial of a  $L(S(N(m,n)))$  graph is

$$CM(L(S(N(m,n))); p, q) = (2n + 8)p^6q^6 + 4np^6q^7 + (4m - 4)p^7q^7 + (8m + 4n - 8)p^7q^{11} + 2mp^{11}q^{11} + (12m - 8)p^{11}q^{12} + (45mn - 36m - 20n + 12)p^{12}q^{12}. \text{ Then}$$

$$D_p(L(S(N(m,n))); p, q) = 6480mnp^{12}q^{12} - 5184mp^{12}q^{12} + 1452mp^{11}q^{12} + 242mp^{11}q^{11} + 392mp^7q^{11} + 196mp^7q^7 - 2880np^{12}q^{12} + 196np^7q^{11} + 144np^6q^7 + 72np^6q^6 + 1728p^{12}q^{12} - 968p^{11}q^{12} - 392p^7q^{11} - 196p^7q^7 + 288p^6q^6,$$

$$D_q(L(S(N(m,n))); p, q) = 6480mnp^{12}q^{12} - 5184mp^{12}q^{12} + 1728mp^{11}q^{12} + 242mp^{11}q^{11} + 968mp^7q^{11} + 196mp^7q^7 - 2880np^{12}q^{12} + 484np^7q^{11} + 196np^6q^7 + 72np^6q^6 + 1728p^{12}q^{12} - 1152p^{11}q^{12} - 968p^7q^{11} - 196p^7q^7 + 288p^6q^6,$$

$$S_p(L(S(N(m,n))); p, q) = \frac{(2n + 8)}{6}p^6q^6 + \frac{2n}{3}p^6q^7 + \frac{(4m - 4)}{7}p^7q^7 + \frac{(8m - 4n - 8)}{7}p^7q^{11} + \frac{2m}{11}p^{11}q^{11} + \frac{(12m - 8)}{11}p^{11}q^{12} + \frac{(45mn - 36m - 20n + 12)}{12}p^{12}q^{12},$$

$$S_q(L(S(N(m,n))); p, q) = \frac{(2n+8)}{6} p^6 q^6 + \frac{4n}{7} p^6 q^7 + \frac{(4m-4)}{7} p^7 q^7 + \frac{(8m-4n-8)}{11} p^7 q^{11} + \frac{2m}{11} p^{11} q^{11} + \frac{(12m-8)}{12} p^{11} q^{12} + \frac{(45mn-36m-20n+12)}{12} p^{12} q^{12},$$

$$J(L(S(N(m,n))); p, q) = 45mnp^{24} - 36mp^{24} + 12mp^{23} + 2mp^{22} + 8mp^{18} + 4mp^{14} - 20np^{24} + 4np^{18} + 4np^{13} + 2np^{12} + 12p^{24} - 8p^{23} - 8p^{18} - 4p^{14} + 8p^{12},$$

By applying all these values in Table 1, we obtain the required result.

## 6. Numerical Results and Discussion

**Table 5:** Numerical comparison of closed neighborhood degree-based indices of  $N(m,n)$  for  $m=n=5$

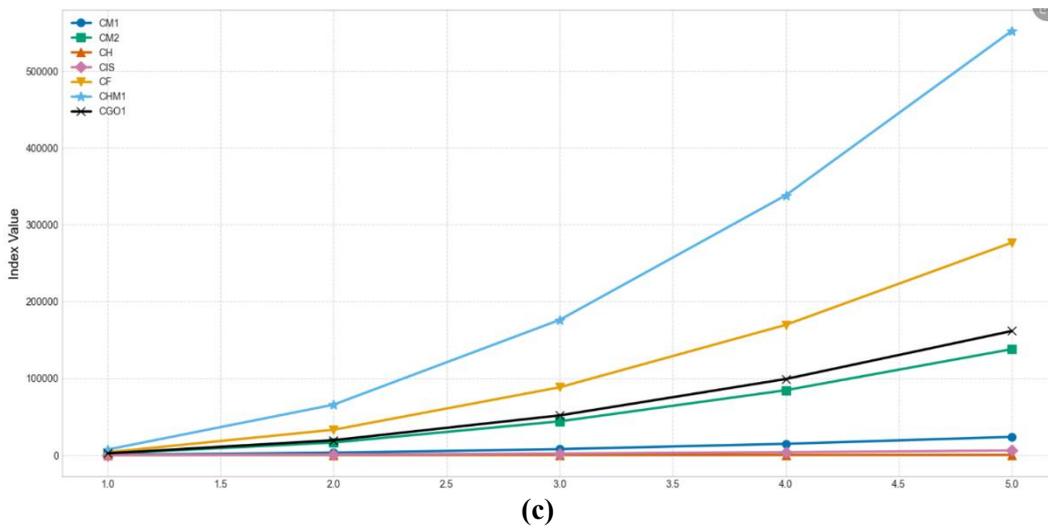
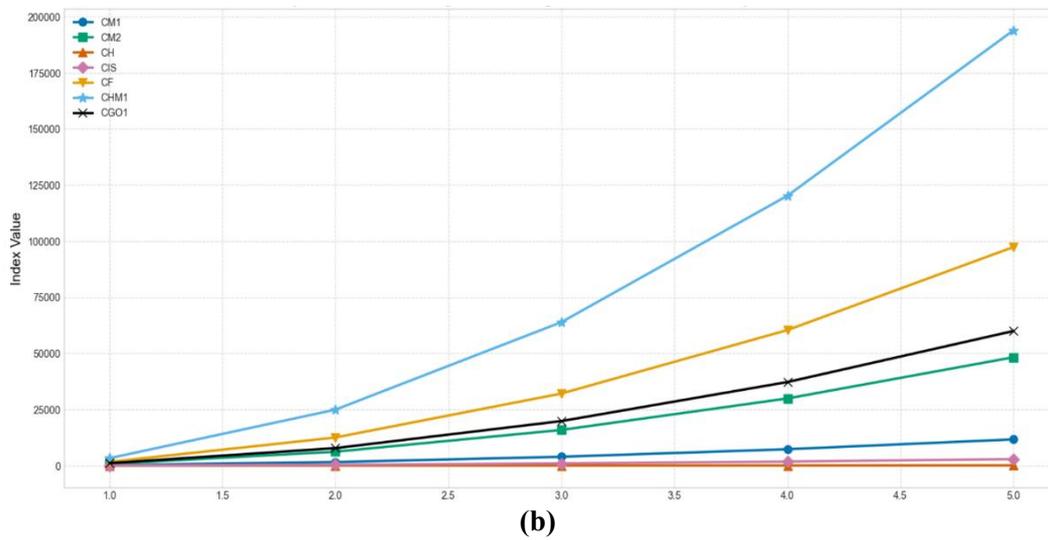
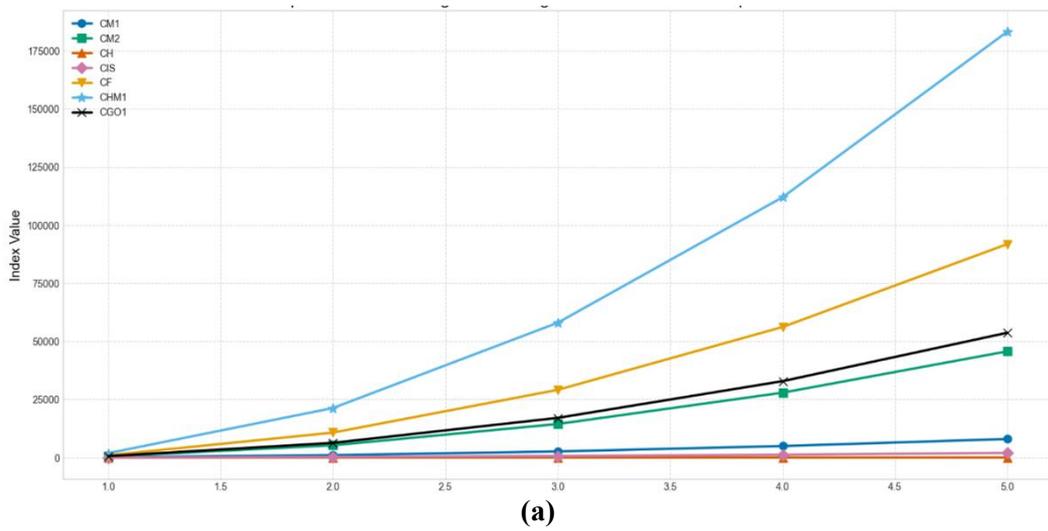
$[m,n]$	$CM_1$	$CM_2$	$CH$	$CIS$	$CF$	$CHM_1$	$CGO_1$
[1,1]	146	458	1.643	35.688	974	1890	604
[2,2]	1028	5288	5.570	254.903	10732	21308	6316
[3,3]	2630	14438	11.996	654.117	29130	58006	17068
[4,4]	4952	27908	20.923	1233.332	56168	111984	32860
[5,5]	7994	45698	32.350	1992.547	91846	183242	53692

**Table 6:** Numerical comparison of closed neighborhood degree-based indices of  $S(N(m,n))$  for  $m=n=5$

$[m,n]$	$CM_1$	$CM_2$	$CH$	$CIS$	$CF$	$CHM_1$	$CGO_1$
[1,1]	270	816	3.576	67.011	1662	3294	1086
[2,2]	1596	6198	13.829	396.802	12536	24932	7794
[3,3]	3942	15900	31.141	980.711	32110	63910	19842
[4,4]	7308	29922	55.511	1818.738	60384	120228	37230
[5,5]	11694	48264	86.941	2910.882	97358	193886	59958

**Table 7:** Numerical comparison of closed neighborhood degree-based indices of  $L(S(N(m,n)))$  for  $m=n=5$

$[m,n]$	$CM_1$	$CM_2$	$CH$	$CIS$	$CF$	$CHM_1$	$CGO_1$
[1,1]	404	1750	3.394	99.990	3572	7072	2154
[2,2]	2968	16312	14.001	738.116	32904	65528	19280
[3,3]	7692	43834	32.163	1916.242	88156	175824	51526
[4,4]	14576	84316	57.825	3634.368	169328	337960	98892
[5,5]	23620	137758	90.987	5892.494	276420	551936	161378



**Figure 4.** Comparison of indices (a)  $N(m, n)$  (b)  $S(N(m, n))$  (c)  $L(S(N(m, n)))$

To verify the behavior of molecular descriptor, different values of  $m=n$  are considered. It is noticed from Table 5, 6 and 7, the values of the topological indices increase as the  $m=n$  increases. The behavior of CM-polynomial is depicted in Figure 1, 2 and 3. The obtained topological indices are represented using 2D graphs for distinct values of  $m=n$  as shown in Figure 4. The variation of values of  $N(m, n)$ ,  $S(N(m, n))$  and  $L(S(N(m, n)))$  on closed neighborhood degree-based indices are observed and the following points are noted.

The 2D comparison plots illustrate how the topological indices change as the dimensions of the nanosheet increases. For the original H-naphthalenic nanosheet  $N(m, n)$ , all indices show a steady upward trend with larger values of  $m=n$ , indicating that molecular size enhances structural complexity. Among the indices,  $CHM_1$  and  $CF$  rise most sharply, reflecting their heightened sensitivity to variations in degree distribution and connectivity, whereas  $CH$  and  $CIS$  increase more gradually, suggesting a weaker dependence on high-degree vertices. In the subdivision graph  $S(N(m, n))$ , where each edge is split by an additional vertex, all indices generally exhibit higher magnitudes than in the original nanosheet.  $CHM_1$  and  $CF$  show a more pronounced increase due to the denser edge structure and more uniform vertex distribution, while the  $CGO_1$  index also grows substantially, highlighting the impact of added vertices on the sum of closed neighborhood degrees. In  $L(S(N(m, n)))$ , the indices reach their maximum values, as each edge of the subdivision graph is converted into a vertex, forming a highly interconnected network. The marked rise in  $CF$ ,  $CHM_1$ , and  $CM_2$  indicates that this transformation significantly intensifies neighborhood interactions and molecular compactness. Overall, in terms of closed neighborhood degree-based topological indices, the values of the graphs follow the hierarchy:  $CHM_1 > CF > CGO_1 > CM_2 > CM_1 > CIS > CH$  as  $m=n$  increases, demonstrating that each structural modification progressively increases molecular connectivity and complexity.

## 7. Conclusion

This research provides a comprehensive topological analysis of H-Naphthalenic nanosheet using the CM-polynomial framework. Based on the derived CM-polynomials, several closed neighborhood degree-based topological indices  $CM_1$ ,  $CM_2$ ,  $CH$ ,  $CIS$ ,  $CF$ ,  $CHM_1$ , and  $CGO_1$  were formulated and evaluated for three graph models such as nanosheet  $N(m, n)$ , its subdivision  $S(N(m, n))$  and the line graph of the subdivision  $L(S(N(m, n)))$ . The numerical analysis demonstrates that the values of all indices consistently rise with increasing  $m=n$ , confirming that the nanosheet's molecular complexity and interconnectivity expand with its structural growth. Overall, the CM-polynomial approach proves to be an effective algebraic method for exploring and comparing the structural and physico-chemical characteristics of nanoscale materials. This framework can be further extended to other molecular systems, offering valuable insights for QSAR/QSPR studies and theoretical modeling in chemical graph theory.

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