



# A new perspective on the modeling and topological characterization of H-Naphtalenic nanosheets with applications

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## Abstract

In the past few years, two-dimensional (2D) layered nanomaterials have greatly attracted the scientific community. Among 2D nanomaterials, the porphyrin-based Naphtalenic nanosheets have been the subject of intense research due to their utilization in photo-dynamic therapy and nanodevices. New technologies based on nanomaterials or Naphtalenic nanosheet are advantageous in overcoming the problems in conventional drug delivery like poor solubility, toxicity and poor release pattern of drugs. In chemical network theory, various molecular descriptors are used to predict the chemical properties of molecules; these molecular descriptors are found to be very useful for Quantitative Structure–Activity/ Quantitative Structure–Property (QSAR/QSPR) relationship analysis in materials engineering, chemical and pharmaceutical industries. Researchers have computed the molecular descriptors for various nanostructures; however, despite intense research, the topology of nanostructures is not yet well understood. Specially, to our knowledge, the computation of topological indices for the line graph of subdivision graph of H-Naphtalenic nanosheet has not been discussed so far, which may open new perspectives for a more accurate and reliable topological characterization of this nanosheet.

In this article, we employed some important degree-based topological indices to study the chemical structure of Naphtalenic nanosheet as a chemical network for QSAR/QSPR analysis. We have computed these degree-based topological indices for the line graph of subdivision graph of H-Naphtalenic nanosheet and derived formulas for them. Based on the derived formulas, numerical results are obtained and the physical and chemical properties of the under study nanosheet are investigated.

**Keywords** Nanostructures · Graph theory · Mathematical chemistry · Topological indices · QSAR · QSPR

## Introduction

The popular 2D nanomaterial graphene, the thinnest 2D material (0.34 nm) in the world [1–3] containing of a single layer of carbon atoms with hexagonal lattice, is currently the subject of intense research. Inspired by graphene, there is a rising interest in new 2D inorganic, organic and hybrid nanomaterials development. Since their invention [4, 5], carbon nanotubes have gained much attention. Carbon nanotubes

(CNTs) are made of carbon with nanometer-sized diameters. These are often refer to single-wall carbon nanotubes with diameter in the range of nanometer and were discovered by Iijima and Ichihashi [4], and Bethune et al. [5] independently. Nanosheets are 2D nanostructures with a thickness ranging from 1 to 100 nm (nanometer) [6–9]. These 2D nanosheets exhibit interesting physical, electronic, biological and chemical properties which are very important for catalysis, storage, biomaterials, nano (bio)-technology, sensing, electronics, optical and dielectric-related applications. Therefore, it is very important to predict these nanostructures in order to gain insight into the topology and enhance their physical properties.

Mathematical chemistry techniques are used to model and characterize molecules in order to better understand the physical properties of chemical compounds [10]. Graphs are mathematical structures which are used to model pairwise relation between objects. Chemical graphs are simple finite graphs in which the vertices represent atoms while the edges

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represent chemical bonds in underlying chemical/ molecular structures. Line graph is one of the well-known and most studied graphs linked with a graph. Let  $H$  be a non-empty graph, then its line graph  $L(H)$  has the set of edges in  $H$  as its vertex set and two vertices of  $L(H)$  are adjacent if the corresponding edges of  $G$  are adjacent. Alexandru Balaban, Ante Graovac, Ivan Gutman, Harao Hosoya, Milan Randić and Nenad Trinajstić [11] laid foundations of chemical graph theory. Due to its vast applications in different fields of life such as materials science, drug design, chemistry, biological networks, electrical networks and computer science, chemical graph theory has currently attracted much attention of researchers [12, 13]. Recently, a blend field of mathematics, chemistry and information science has been introduced, namely chem-informatics.

A numeric or arithmetic value that characterizes the entire chemical or molecular structure is called a topological index. Topological index describes some salient features (melting point, boiling point, stability and connectivity) of molecular graphs of some chemical compounds. These descriptors play a vital role in biological, chemical, materials sciences and drug design. In QSAR modeling, the predictors consist of physico-chemical properties or theoretical molecular descriptor [14–16], while the term QSPR models as response variable [17–20]. Wiener [21] introduced the concept of topological index while working on boiling point of paraffin and named it as path number. It is the first and most studied topological index both from application and theoretical point of view. It is defined as the sum of distance between all pairs of vertices in a graph  $G$ ; further details can be found in ref. [22]. Degree-based topological indices are commonly used and play a significant role in chemical graph theory, especially in chemistry. Gutman and Trinajstić established the earliest topological indices, the Zagreb indices [23–26], which have been utilized to investigate molecular difficulty, boiling point and chirality. The degree-based concept has recently been transformed into Ev-degree, Ve-degree, degree-based entropy, M-polynomial and NM-polynomials [27].

In the present study, we have represented the degree of  $u$  and  $v$  as  $\zeta_u$  and  $\zeta_v$ , respectively, where  $uv \in E(G)$ . The topological indices based on vertex degree are as follows:

For any graph  $G$ , the first Zagreb index  $M_1(G)$  and second Zagreb index  $M_2(G)$  are given as:

$$M_1(G) = \sum_{uv \in E(G)} [\zeta_u + \zeta_v] \quad (1)$$

$$M_2(G) = \sum_{uv \in E(G)} [\zeta_u \zeta_v] \quad (2)$$

Shirdel, Rez and Sayadi [27] presented the idea of a new degree-based index, and it was termed as “hyper-Zagreb index” which is defined as:

$$HM(G) = \sum_{uv \in E(G)} [\zeta_u + \zeta_v]^2 \quad (3)$$

Ghorbani and Azimi formulated two new versions of degree-based indices for any graph  $G$  [28] and named as the first multiple Zagreb index  $PM_1(G)$  and second multiple Zagreb index  $PM_2(G)$  which are formulated as:

$$PM_1(G) = \prod_{uv \in E(G)} [\zeta_u + \zeta_v] \quad (4)$$

$$PM_2(G) = \prod_{uv \in E(G)} [\zeta_u \zeta_v] \quad (5)$$

The first Zagreb polynomial  $M_1(G, x)$  and second Zagreb polynomial  $M_2(G, x)$  are formulated as:

$$M_1(G, x) = \sum_{uv \in E(G)} x^{[\zeta_u + \zeta_v]} \quad (6)$$

$$M_2(G, x) = \sum_{uv \in E(G)} x^{[\zeta_u \zeta_v]} \quad (7)$$

Augmented Zagreb Index is defined as [29]

$$A(G) = \sum_{uv \in E(G)} \left[ \frac{\zeta_u \zeta_v}{\zeta_u + \zeta_v - 2} \right]^3 \quad (8)$$

ABC (atom-bond connectivity) index is proposed by Estrada et al. [30]. It is the widely used connectivity index. The mathematical formula for ABC is as follows:

$$ABC(G) = \sum_{uv \in E(G)} \sqrt{\frac{\zeta_u + \zeta_v - 2}{\zeta_u \zeta_v}} \quad (9)$$

Sum connectivity index is almost associated variant of the Randić index. It is formulated by Zhou [31] and is defined as:

$$SCI(G) = \sum_{uv \in E(G)} \frac{1}{\sqrt{\zeta_u + \zeta_v}} \quad (10)$$

Vukičević and Furtula suggested a geometric–arithmetic index [29] and is defined as:

$$GA(G) = \sum_{uv \in E(G)} \frac{2\sqrt{\zeta_u \zeta_v}}{\zeta_u + \zeta_v} \quad (11)$$

Harmonic index is formulated by [32],

$$H(G) = \sum_{uv \in E(G)} \frac{2}{\zeta_u + \zeta_v} \tag{12}$$

Randic [32] suggested a structural descriptor, known as the branching index. Later on, it was termed as famous Randic index. It is one of the most favorable molecular descriptors in QSPR and QSAR analysis. It is satisfactory to measure the level of branching of carbon atom sketch of saturated hydrocarbon. Randic index is defined as:

$$R_\alpha(G) = \sum_{uv \in E(G)} (\zeta_u \zeta_v)^\alpha \tag{13}$$

V. S. Shigehalli and Rachanna Kanabur proposed the following new degree-based indices, namely arithmetic–geometric (AG1) index, SK, SK<sub>1</sub>, SK<sub>2</sub> indices and are defined as, respectively [33],

$$AG_1(G) = \sum_{uv \in E(G)} \frac{\zeta_u + \zeta_v}{2\sqrt{\zeta_u \zeta_v}} \tag{14}$$

$$SK(G) = \sum_{uv \in E(G)} \frac{\zeta_u + \zeta_v}{2} \tag{15}$$

$$SK_1(G) = \sum_{uv \in E(G)} \frac{\zeta_u \times \zeta_v}{2} \tag{16}$$

$$SK_2(G) = \sum_{uv \in E(G)} \left( \frac{\zeta_u + \zeta_v}{2} \right)^2 \tag{17}$$

Kalli introduced the below listed indices [34]:

$$(i) \ GO_1(G) = \sum_{uv \in E(G)} [(\zeta_u + \zeta_v) + (\zeta_u \zeta_v)] \tag{18}$$

$$(ii) \ GO_2(G) = \sum_{uv \in E(G)} [(\zeta_u + \zeta_v) + (\zeta_u \zeta_v)] \tag{19}$$

In addition to above, Kalli has also introduced the following indices [35]:

$$(i) \ HGO_1(G) = \sum_{uv \in E(G)} [(\zeta_u + \zeta_v) + (\zeta_u \zeta_v)]^2 \tag{20}$$

$$(ii) \ HGO_2(G) = \sum_{uv \in E(G)} [(\zeta_u + \zeta_v) + (\zeta_u \zeta_v)]^2 \tag{21}$$

Among 2D nanomaterials, the porphyrin-based Naphtalenic nanosheets have been the subject of intense research due to their utilization in photo-dynamic therapy and nanodevices. New technologies based on nanomaterials or Naphtalenic nanosheet are good in overcoming the problems in conventional drug delivery like poor solubility, toxicity and poor release pattern of drugs. The physical and chemical properties of these nanosheets depend on their structure.

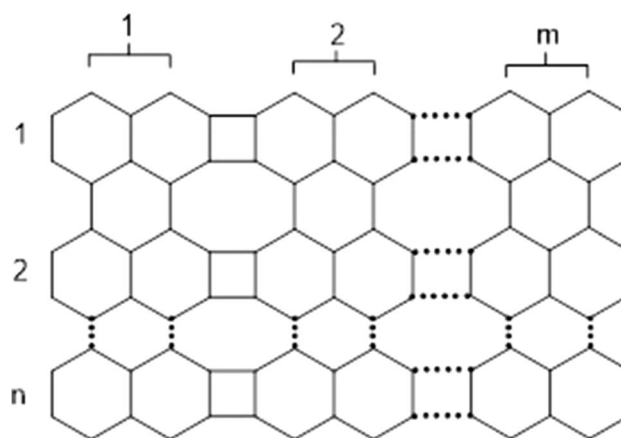


Fig. 1 H-Naphtalenic nanosheet H(m, n)

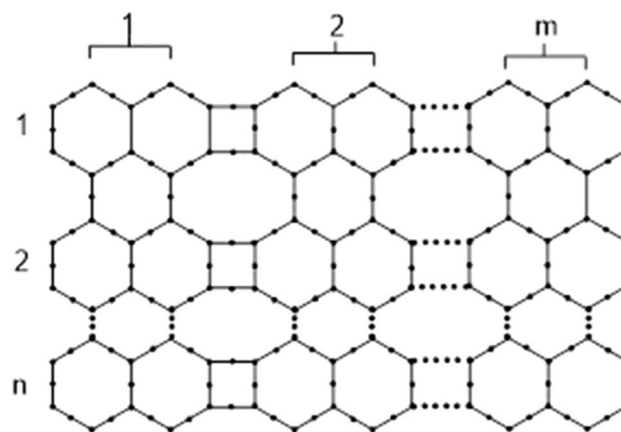
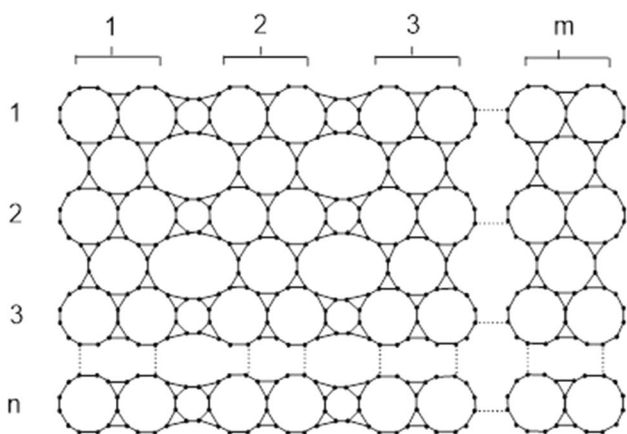


Fig. 2 Subdivision graph of H-Naphtalenic nanosheet S(H(m, n))

Researchers have computed the molecular descriptors for various nanostructures. Deng et al. investigated the molecular descriptors of pent-heptagonal nanosheets [36]. Szeged and PI Indices of VC<sub>5</sub>C<sub>7</sub>[p, q] and HC<sub>5</sub>C<sub>7</sub>[p, q] are discussed in [37]. In [38–42], the topological properties of H-Naphtalenic nanosheets are studied. Jane Olive Sharon et al. investigated the transmission of every vertex in H-Naphtalenic nanosheet [43]. In [13, 44], scientists investigated the topological modeling and characterization of antiviral medications used for the COVID-19 treatment, such as bevacizumab, hydroxy chloroquine, umifenovir, ritonavir, remdesivir, nafamostat, theaflavin, lopinavir and camostat. Further details on the topological characterization of nano- and microstructures can be found in refs. [45–54]. However, despite intense research, the topology of nanostructures is



**Fig. 3** Line graph of subdivision graph of H-Naphtalenic nanosheet  $L(S(H(m, n)))$

not yet well understood. Specially, the computation of topological indices for the line graph of subdivision graph of H-Naphtalenic nanosheet has not been discussed so far. This investigation focuses on the computation of the above-mentioned degree-based topological indices for the line graph of H-Naphtalenic nanosheet in order to better predict the nanostructure for QSAR/QSPR analysis.

### H-Naphtalenic nanosheet

H-Naphtalenic nanosheet is formed by alternating hexagons  $C_6$ ,  $C_4$  and Octagons  $C_8$ . H-Naphtalenic nanosheet  $H(m, n)$  contains 10 nm number of vertices,  $m$  represents the number of paired hexagons in each alternate row with  $C_4$  cycle, and  $n$  represents the number of rows consisting  $C_4$ . Topological indices of H-Naphtalenic nanosheet are studied in [38].

In the present calculations, we employed edge partition and vertex partition tools of graph theory. The graph of H-Naphtalenic nanosheet is denoted by  $H(m, n)$ , and its subdivision graph is denoted by  $S(H(m, n))$ , whereas line graph of subdivision graph is denoted by  $L(S(H(m, n)))$ . The respective graphs are shown in Figs. 1, 2, 3, respectively. There are a total of  $30mn - 4m - 4n$  vertices in  $L(S(H(m, n)))$ , out of which  $8(m + n)$  vertices are having degree 2 and  $30mn - 12m - 12n$  are having degree 3. Also the sum of degrees of all vertices in  $L(S(H(m, n)))$  is  $90mn - 20m - 20n$ . It is easy to observe from Handshaking lemma that the total number of edges in  $L(S(H(m, n)))$  is  $45mn - 10m - 10n$ . The edge set  $E(L(S(H(m, n))))$  is split up into three edge partitions  $E_1, E_2$  and  $E_3$ , based on degree of end vertices. The details of these partitions are shown in Table 1.

**Table 1** Edge partition of nanosheet  $L(S(H(m, n)))$  on the degree of end vertices of each edge

Types of edges	$E_1(2, 2)$	$E_2(2, 3)$	$E_3(3, 3)$
$(\zeta_u, \zeta_v), uv \in E(L(S(H)))$	(2, 2)	(2, 3)	(3, 3)
Number of edges	$6n + 4m + 4$	$4n + 8m - 8$	$45mn - 20n - 22m + 4$

### Main results

In this section, we have computed some important degree-based topological indices for  $L(S(H(m, n)))$ ; the graph is shown in Fig. 3. The computational results are as follows:

**Theorem 3.1:** Let the line graph of subdivision graph of H-Naphtalenic nanosheet be  $L(S(H(m, n)))$ , then.

$$M_1(L(S(H))) = 270mn - 76m - 76n$$

**Proof:** Together with Eq. 1 and Table 1, we have.

$$\begin{aligned} &= \sum_{uv \in E_1(L(S(H)))} [\zeta_u + \zeta_v] + \sum_{uv \in E_2(L(S(H)))} [\zeta_u + \zeta_v] + \sum_{uv \in E_3(L(S(H)))} [\zeta_u + \zeta_v] \\ &= (2 + 2)|E_1(L(S(H)))| + (2 + 3)|E_2(L(S(H)))| + (3 + 3)|E_3(L(S(H)))| \\ &= 4(6n + 4m + 4) + 5(4n + 8m - 8) + 6(45mn - 20n - 22m + 4) \\ &= 24n + 16m + 16 + 20n + 40m - 40 + 230mn - 120n - 132m + 24 \end{aligned}$$

$$M_1(L(S(H))) = 270mn - 76m - 76n$$

**Theorem 3.2:** Let  $L(S(H(m, n)))$  denote the line graph of subdivision graph of H-Naphtalenic nanosheet, then its second Zagreb index is as follows.

$$M_2(L(S(H))) = 405mn - 134m - 132n + 4$$

**Proof:** Together with Eq. 2 and Table 1, we have.

$$\begin{aligned} &= \sum_{uv \in E_1(L(S(H)))} [\zeta_u + \zeta_v] + \sum_{uv \in E_2(L(S(H)))} [\zeta_u + \zeta_v] + \sum_{uv \in E_3(L(S(H)))} [\zeta_u + \zeta_v] \\ &= (2 \times 2)|E_1(L(S(H)))| + (2 \times 3)|E_2(L(S(H)))| + (3 \times 3)|E_3(L(S(H)))| \\ &= 4(6n + 4m + 4) + 6(4n + 8m - 8) + 9(45mn - 20n - 22m + 4) \\ &= 24n + 16m + 16 + 24n + 48m - 48 + 405mn - 180n - 198m + 36 \end{aligned}$$

$$M_1(L(S(H))) = 405mn - 134m - 132n + 4$$

Hence, it is proved.

**Theorem 3.3:** Denote the line graph of subdivision graph of H-Naphtalenic nanosheet by  $L(S(H(m, n)))$ , then its hyper-Zagreb index is as follows.

$$HM(\mathbf{L}(\mathbf{S}(\mathbf{H}))) = 1620mn - 528m - 524n + 8$$

**Proof:** Together with Eq. 3 and Table 1, we have.

$$\begin{aligned} &= \sum_{uv \in E_1(\mathbf{L}(\mathbf{S}(\mathbf{H})))} [\zeta_u + \zeta_v]^2 + \sum_{uv \in E_2(\mathbf{L}(\mathbf{S}(\mathbf{H})))} [\zeta_u + \zeta_v]^2 + \sum_{uv \in E_3(\mathbf{L}(\mathbf{S}(\mathbf{H})))} [\zeta_u + \zeta_v]^2 \\ &= (2 + 2)^2 |E_1(\mathbf{L}(\mathbf{S}(\mathbf{H})))| + (2 + 3)^2 |E_2(\mathbf{L}(\mathbf{S}(\mathbf{H})))| + (3 + 3)^2 |E_3(\mathbf{L}(\mathbf{S}(\mathbf{H})))| \\ &= 16(6n + 4m + 4) + 25(4n + 8m - 8) + 36(45mn - 20n - 22m + 4) \end{aligned}$$

$$HM(\mathbf{L}(\mathbf{S}(\mathbf{H}))) = 1620mn - 528m - 524n + 8$$

**Theorem 3.4:** Assume  $L(S(H(m, n)))$  denotes the line graph of subdivision graph of H-Naphtalenic nanosheet, then its first multiple Zagreb index is as follows.

$$PM_1(\mathbf{L}(\mathbf{S}(\mathbf{H}))) = 4^{(6n+4m+4)} \times 5^{(4n+8m-8)} \times 6^{(45mn-20n-22m+4)}$$

**Proof:** From Eq. 4 and Table 1, we have.

$$\begin{aligned} &= \prod_{uv \in E_1(\mathbf{L}(\mathbf{S}(\mathbf{H})))} [\zeta_u + \zeta_v] \times \prod_{uv \in E_2(\mathbf{L}(\mathbf{S}(\mathbf{H})))} [\zeta_u + \zeta_v] \times \prod_{uv \in E_3(\mathbf{L}(\mathbf{S}(\mathbf{H})))} [\zeta_u + \zeta_v] \\ &= (2 + 2)^{E_1(\mathbf{L}(\mathbf{S}(\mathbf{H})))} \times (2 + 3)^{E_2(\mathbf{L}(\mathbf{S}(\mathbf{H})))} \times (3 + 3)^{E_3(\mathbf{L}(\mathbf{S}(\mathbf{H})))} \end{aligned}$$

$$PM_1(\mathbf{L}(\mathbf{S}(\mathbf{H}))) = 4^{(6n+4m+4)} \times 5^{(4n+8m-8)} \times 6^{(45mn-20n-22m+4)}$$

**Theorem 3.5:** Let  $L(S(H(m, n)))$  denote the line graph of subdivision graph of H-Naphtalenic nanosheet, then its second multiple Zagreb index is as follows.

$$PM_2(\mathbf{L}(\mathbf{S}(\mathbf{H}))) = 4^{(6n+4m+4)} \times 6^{(4n+8m-8)} \times 9^{(45mn-20n-22m+4)}$$

**Proof:** Using Eq. 5 and Table 1, we have.

$$\begin{aligned} &= \prod_{uv \in E_1(\mathbf{L}(\mathbf{S}(\mathbf{H})))} [\zeta_u + \zeta_v] \times \prod_{uv \in E_2(\mathbf{L}(\mathbf{S}(\mathbf{H})))} [\zeta_u + \zeta_v] \times \prod_{uv \in E_3(\mathbf{L}(\mathbf{S}(\mathbf{H})))} [\zeta_u + \zeta_v] \\ &= (2 \times 2)^{E_1(\mathbf{L}(\mathbf{S}(\mathbf{H})))} \times (2 \times 3)^{E_2(\mathbf{L}(\mathbf{S}(\mathbf{H})))} \times (3 \times 3)^{E_3(\mathbf{L}(\mathbf{S}(\mathbf{H})))} \end{aligned}$$

$$PM_2(\mathbf{L}(\mathbf{S}(\mathbf{H}))) = 4^{(6n+4m+4)} \times 6^{(4n+8m-8)} \times 9^{(45mn-20n-22m+4)}$$

**Theorem 3.6:** Assume  $L(S(H(m, n)))$  denotes the line graph of subdivision graph of H-Naphtalenic nanosheet, then its first Zagreb polynomial is as follows.

$$M_1(\mathbf{L}(\mathbf{S}(\mathbf{H}), x)) = (6n + 4m + 4)x^4 + (4n + 8m - 8)x^5 + (45mn - 20n - 22m + 4)x^6$$

**Proof:** Together with Eq. 6 and Table 1, we have.

$$= \sum_{uv \in E_1(\mathbf{L}(\mathbf{S}(\mathbf{H})))} x^{[\zeta_u + \zeta_v]} + \sum_{uv \in E_2(\mathbf{L}(\mathbf{S}(\mathbf{H})))} x^{[\zeta_u + \zeta_v]} + \sum_{uv \in E_3(\mathbf{L}(\mathbf{S}(\mathbf{H})))} x^{[\zeta_u + \zeta_v]}$$

$$\begin{aligned} &= \sum_{uv \in E_1(\mathbf{L}(\mathbf{S}(\mathbf{H})))} x^{2+2} + \sum_{uv \in E_2(\mathbf{L}(\mathbf{S}(\mathbf{H})))} x^{2+3} + \sum_{uv \in E_3(\mathbf{L}(\mathbf{S}(\mathbf{H})))} x^{3+3} \\ &= \sum_{uv \in E_1(\mathbf{L}(\mathbf{S}(\mathbf{H})))} x^4 + \sum_{uv \in E_2(\mathbf{L}(\mathbf{S}(\mathbf{H})))} x^5 + \sum_{uv \in E_3(\mathbf{L}(\mathbf{S}(\mathbf{H})))} x^6 \\ &= |E_1(\mathbf{L}(\mathbf{S}(\mathbf{H})))| x^4 + |E_2(\mathbf{L}(\mathbf{S}(\mathbf{H})))| x^5 + |E_3(\mathbf{L}(\mathbf{S}(\mathbf{H})))| x^6 \end{aligned}$$

$$M_1(\mathbf{L}(\mathbf{S}(\mathbf{H}), x)) = (6n + 4m + 4)x^4 + (4n + 8m - 8)x^5 + (45mn - 20n - 22m + 4)x^6$$

**Theorem 3.7:** Let  $L(S(H(m, n)))$  denote the line graph of subdivision graph of H-Naphtalenic nanosheet, then its second Zagreb polynomial is equal to.

$$M_2(\mathbf{L}(\mathbf{S}(\mathbf{H}), x)) = (6n + 4m + 4)x^4 + (4n + 8m - 8)x^6 + (45mn - 20n - 22m + 4)x^9$$

**Proof:** Together with Eq. 7 and Table 1, we have.

$$\begin{aligned} &= \sum_{uv \in E_1(\mathbf{L}(\mathbf{S}(\mathbf{H})))} x^{[\zeta_u \times \zeta_v]} + \sum_{uv \in E_2(\mathbf{L}(\mathbf{S}(\mathbf{H})))} x^{[\zeta_u \times \zeta_v]} + \sum_{uv \in E_3(\mathbf{L}(\mathbf{S}(\mathbf{H})))} x^{[\zeta_u \times \zeta_v]} \\ &= \sum_{uv \in E_1(\mathbf{L}(\mathbf{S}(\mathbf{H})))} x^{2 \times 2} + \sum_{uv \in E_2(\mathbf{L}(\mathbf{S}(\mathbf{H})))} x^{2 \times 3} + \sum_{uv \in E_3(\mathbf{L}(\mathbf{S}(\mathbf{H})))} x^{3 \times 3} \end{aligned}$$

$$= \sum_{uv \in E_1(\mathbf{L}(\mathbf{S}(\mathbf{H})))} x^4 + \sum_{uv \in E_2(\mathbf{L}(\mathbf{S}(\mathbf{H})))} x^6 + \sum_{uv \in E_3(\mathbf{L}(\mathbf{S}(\mathbf{H})))} x^9$$

$$M_2(\mathbf{L}(\mathbf{S}(\mathbf{H}), x)) = (6n + 4m + 4)x^4 + (4n + 8m - 8)x^6 + (45mn - 20n - 22m + 4)x^9$$

**Theorem 3.8:** Let  $L(S(H(m, n)))$  denote the line graph of subdivision graph of H-Naphtalenic nanosheet, then its augmented Zagreb index is as follows.

$$A(\mathbf{L}(\mathbf{S}(\mathbf{H}))) = \frac{32805}{64}mn - \frac{4947}{32}m - \frac{2365}{16}n + \frac{217}{16}$$

**Proof:** From Eq. 8 and Table 1, we have.

$$\begin{aligned} &= \sum_{uv \in E_1(\mathbf{L}(\mathbf{S}(\mathbf{H})))} \left[ \frac{\zeta_u \zeta_v}{\zeta_u + \zeta_v - 2} \right]^3 + \sum_{uv \in E_2(\mathbf{L}(\mathbf{S}(\mathbf{H})))} \left[ \frac{\zeta_u \zeta_v}{\zeta_u + \zeta_v - 2} \right]^3 \\ &\quad + \sum_{uv \in E_3(\mathbf{L}(\mathbf{S}(\mathbf{H})))} \left[ \frac{\zeta_u \zeta_v}{\zeta_u + \zeta_v - 2} \right]^3 \\ &= |E_1(\mathbf{L}(\mathbf{S}(\mathbf{H})))| \left[ \frac{2 \times 2}{2 + 2 - 2} \right]^3 + |E_2(\mathbf{L}(\mathbf{S}(\mathbf{H})))| \left[ \frac{2 \times 3}{2 + 3 - 2} \right]^3 \\ &\quad + |E_3(\mathbf{L}(\mathbf{S}(\mathbf{H})))| \left[ \frac{3 \times 3}{3 + 3 - 2} \right]^3 \end{aligned}$$

$$\begin{aligned}
 &= (6n + 4m + 4)8 + (4n + 8m - 8)8 + (45mn - 20n - 22m + 4) \frac{729}{64} \\
 &= \frac{(6n + 4m + 4)512 + (4n + 8m - 8)512 + (45mn - 20n - 22m + 4)729}{64} \\
 &= \frac{3072n + 256m + 256 + 2048n + 4096m - 4096 + 32805mn - 14580n - 16038 + 2916}{64} \\
 &= \frac{32805}{64}mn - \frac{9894}{64}m - \frac{9460}{64}n + \frac{868}{64} \\
 A(\mathbf{L}(\mathbf{S}(\mathbf{H}))) &= \frac{32805}{64}mn - \frac{4947}{32}m - \frac{2365}{16}n + \frac{217}{16}
 \end{aligned}$$

**Theorem 3.9:** Consider  $L(S(H(m, n)))$  for the line graph of subdivision graph of H-Naphtalenic nanosheet, then its ABC (atom-bond connectivity) index is as follows.

$$ABC(\mathbf{L}(\mathbf{S}(\mathbf{H}))) = 30mn + m \left( \frac{36 - 44\sqrt{2}}{3\sqrt{2}} \right) + n \left( \frac{30 - 40\sqrt{2}}{3\sqrt{2}} \right) + \left( \frac{8\sqrt{2} - 12}{3\sqrt{2}} \right)$$

**Proof:** Using Eq. 9 and Table 1, we have.

$$\begin{aligned}
 &= \sum_{uv \in E_1(\mathbf{L}(\mathbf{S}(\mathbf{H})))} \sqrt{\frac{\zeta_u + \zeta_v - 2}{\zeta_u \zeta_v}} + \sum_{uv \in E_2(\mathbf{L}(\mathbf{S}(\mathbf{H})))} \sqrt{\frac{\zeta_u + \zeta_v - 2}{\zeta_u \zeta_v}} \\
 &\quad + \sum_{uv \in E_3(\mathbf{L}(\mathbf{S}(\mathbf{H})))} \sqrt{\frac{\zeta_u + \zeta_v - 2}{\zeta_u \zeta_v}} \\
 &= |E_1(\mathbf{L}(\mathbf{S}(\mathbf{H})))| \sqrt{\frac{2+2-2}{2 \times 2}} + |E_2(\mathbf{L}(\mathbf{S}(\mathbf{H})))| \sqrt{\frac{2+3-2}{2 \times 3}} \\
 &\quad + |E_3(\mathbf{L}(\mathbf{S}(\mathbf{H})))| \sqrt{\frac{3+3-2}{3 \times 3}} \\
 &= (6n + 4m + 4) \frac{1}{\sqrt{2}} + (4n + 8m - 8) \frac{1}{\sqrt{2}} + (45mn - 20n - 22m + 4) \frac{2}{3} \\
 &= \frac{6n}{\sqrt{2}} + \frac{4m}{\sqrt{2}} + \frac{4}{\sqrt{2}} + \frac{4n}{\sqrt{2}} + \frac{8m}{\sqrt{2}} - \frac{8}{\sqrt{2}} + \frac{90mn}{3} - \frac{40n}{3} - \frac{44m}{3} + \frac{8}{3} \\
 &= \frac{90mn}{3} + \frac{18n - 40\sqrt{2}n + 12n}{3\sqrt{2}} \\
 &\quad + \frac{12m + 24m - 44\sqrt{2}m}{3\sqrt{2}} + \frac{12 - 24 + 8\sqrt{2}}{3\sqrt{2}}
 \end{aligned}$$

$$\begin{aligned}
 ABC(\mathbf{L}(\mathbf{S}(\mathbf{H}))) &= 30mn + m \left( \frac{36 - 44\sqrt{2}}{3\sqrt{2}} \right) \\
 &\quad + n \left( \frac{30 - 40\sqrt{2}}{3\sqrt{2}} \right) + \left( \frac{8\sqrt{2} - 12}{3\sqrt{2}} \right)
 \end{aligned}$$

**Theorem 3.10:** Assume that  $L(S(H(m, n)))$  denotes the line graph of subdivision graph of H-Naphtalenic nanosheet, then its sum connectivity index (SCI) is as follows.

$$\begin{aligned}
 SCI(\mathbf{L}(\mathbf{S}(\mathbf{H}))) &= \frac{45}{\sqrt{6}}mn + m \left( \frac{2\sqrt{30} + 8\sqrt{6} - 22\sqrt{5}}{\sqrt{30}} \right) + n \left( \frac{4\sqrt{6} + 3\sqrt{30} - 20\sqrt{5}}{\sqrt{30}} \right) \\
 &\quad + \left( \frac{2\sqrt{30} - 8\sqrt{6} - 4\sqrt{5}}{\sqrt{30}} \right)
 \end{aligned}$$

**Proof:** Together with Eq. 10 and Table 1, we have.

$$\begin{aligned}
 &= \sum_{uv \in E_1(\mathbf{L}(\mathbf{S}(\mathbf{H})))} \frac{1}{\sqrt{\zeta_u + \zeta_v}} + \sum_{uv \in E_2(\mathbf{L}(\mathbf{S}(\mathbf{H})))} \frac{1}{\sqrt{\zeta_u + \zeta_v}} + \sum_{uv \in E_3(\mathbf{L}(\mathbf{S}(\mathbf{H})))} \frac{1}{\sqrt{\zeta_u + \zeta_v}} \\
 &= |E_1(\mathbf{L}(\mathbf{S}(\mathbf{H})))| \frac{1}{\sqrt{2+2}} + |E_2(\mathbf{L}(\mathbf{S}(\mathbf{H})))| \frac{1}{\sqrt{2+3}} + |E_3(\mathbf{L}(\mathbf{S}(\mathbf{H})))| \frac{1}{\sqrt{3+3}} \\
 &= (6n + 4m + 4) \frac{1}{\sqrt{4}} + (4n + 8m - 8) \frac{1}{\sqrt{5}} + (45mn - 20n - 22m + 4) \frac{1}{\sqrt{6}} \\
 &= 3n + 2m + 2 + \frac{4}{\sqrt{5}}n + \frac{8}{\sqrt{5}}m - \frac{8}{\sqrt{5}} + \frac{45}{\sqrt{6}}mn - \frac{20}{\sqrt{6}}n - \frac{22}{\sqrt{6}}m + \frac{4}{\sqrt{6}}
 \end{aligned}$$

$$\begin{aligned}
 SCI(\mathbf{L}(\mathbf{S}(\mathbf{H}))) &= \frac{45}{\sqrt{6}}mn + m \left( \frac{2\sqrt{30} + 8\sqrt{6} - 22\sqrt{5}}{\sqrt{30}} \right) \\
 &\quad + n \left( \frac{4\sqrt{6} + 3\sqrt{30} - 20\sqrt{5}}{\sqrt{30}} \right) + \left( \frac{2\sqrt{30} - 8\sqrt{6} - 4\sqrt{5}}{\sqrt{30}} \right)
 \end{aligned}$$

**Theorem 3.11:** Let  $L(S(H(m, n)))$  denote the line graph of subdivision graph of H-Naphtalenic nanosheet, then its geometric–arithmetic index is as follows.

$$GA(\mathbf{L}(\mathbf{S}(\mathbf{H}))) = 45mn + m \left( \frac{216\sqrt{6} - 2}{5} \right) + n \left( \frac{8\sqrt{6} + 10}{5} \right) + \left( \frac{40 - 16\sqrt{6}}{5} \right)$$

**Proof:** From Eq. 11 and Table 1, we have.

$$\begin{aligned}
 &= \sum_{uv \in E_1(\mathbf{L}(\mathbf{S}(\mathbf{H})))} \frac{2\sqrt{\zeta_u \zeta_v}}{\zeta_u + \zeta_v} + \sum_{uv \in E_2(\mathbf{L}(\mathbf{S}(\mathbf{H})))} \frac{2\sqrt{\zeta_u \zeta_v}}{\zeta_u + \zeta_v} + \sum_{uv \in E_3(\mathbf{L}(\mathbf{S}(\mathbf{H})))} \frac{2\sqrt{\zeta_u \zeta_v}}{\zeta_u + \zeta_v} \\
 &= |E_1(\mathbf{L}(\mathbf{S}(\mathbf{H})))| \frac{2\sqrt{\zeta_u \zeta_v}}{\zeta_u + \zeta_v} + |E_2(\mathbf{L}(\mathbf{S}(\mathbf{H})))| \frac{2\sqrt{\zeta_u \zeta_v}}{\zeta_u + \zeta_v} \\
 &\quad + |E_3(\mathbf{L}(\mathbf{S}(\mathbf{H})))| \frac{2\sqrt{\zeta_u \zeta_v}}{\zeta_u + \zeta_v} \\
 &= (6n + 4m + 4) \frac{2\sqrt{2 \times 2}}{2+2} + (4n + 8m - 8) \frac{2\sqrt{2 \times 3}}{2+3} \\
 &\quad + (45mn - 20n - 22m + 4) \frac{2\sqrt{3 \times 3}}{3+3} \\
 &= (6n + 4m + 4) + (4n + 8m - 8) \frac{2\sqrt{6}}{5} + (45mn - 20n - 22m + 4) \\
 &= 6n + 4m + 4 + \frac{8\sqrt{6}n}{5} + \frac{16\sqrt{6}m}{5} - \frac{16\sqrt{6}}{5} \\
 &\quad + 45mn - 20n - 22m + 4
 \end{aligned}$$

$$= 45mn + 6n + \frac{8\sqrt{6}n}{5} - 20n + 4m + \frac{16\sqrt{6}m}{5} - 22m + 4 - \frac{16\sqrt{6}}{5} + 4$$

$$= 45mn + \frac{30n + 8\sqrt{6}n - 100n}{5} + \frac{20m + 16\sqrt{6}m - 110m}{5} + \frac{20 - 16\sqrt{6} + 20}{5}$$

$$GA(\mathbf{L}(\mathbf{S}(\mathbf{H}))) = 45mn + m\left(\frac{216\sqrt{6} - 2}{5}\right) + n\left(\frac{8\sqrt{6} + 10}{5}\right) + \left(\frac{40 - 16\sqrt{6}}{5}\right)$$

**Theorem 3.12:** Let  $L(S(H(m, n)))$  denote the line graph of subdivision graph of H-Naphtalenic nanosheet, then its harmonic index is as follows.

$$H(\mathbf{L}(\mathbf{S}(\mathbf{H}))) = 15mn - \frac{32}{15}m - \frac{31}{15}n + \frac{2}{15}$$

**Proof:** Together with Eq. 12 and Table 1, we have.

$$= \sum_{uv \in E_1(\mathbf{L}(\mathbf{S}(\mathbf{H})))} \frac{2}{\zeta_u + \zeta_v} + \sum_{uv \in E_2(\mathbf{L}(\mathbf{S}(\mathbf{H})))} \frac{2}{\zeta_u + \zeta_v} + \sum_{uv \in E_3(\mathbf{L}(\mathbf{S}(\mathbf{H})))} \frac{2}{\zeta_u + \zeta_v}$$

$$= |E_1(\mathbf{L}(\mathbf{S}(\mathbf{H})))| \frac{2}{\zeta_u + \zeta_v} + |E_2(\mathbf{L}(\mathbf{S}(\mathbf{H})))| \frac{2}{\zeta_u + \zeta_v} + |E_3(\mathbf{L}(\mathbf{S}(\mathbf{H})))| \frac{2}{\zeta_u + \zeta_v}$$

$$= |E_1(\mathbf{L}(\mathbf{S}(\mathbf{H})))| \frac{2}{2+2} + |E_2(\mathbf{L}(\mathbf{S}(\mathbf{H})))| \frac{2}{2+3} + |E_3(\mathbf{L}(\mathbf{S}(\mathbf{H})))| \frac{2}{3+3}$$

$$= (6n + 4m + 4) \frac{1}{2} + (4n + 8m - 8) \frac{2}{5} + (45mn - 20n - 22m + 4) \frac{1}{3}$$

$$= \frac{6n}{2} + \frac{4m}{2} + \frac{4}{2} + \frac{8n}{5} + \frac{16m}{5} - \frac{16}{5} + \frac{45mn}{3} - \frac{20n}{3} - \frac{22m}{3} + \frac{4}{3}$$

$$= \frac{45mn}{3} + \frac{4m}{2} + \frac{16m}{5} - \frac{22m}{3} + \frac{8n}{5} + \frac{6n}{2} - \frac{20n}{3} - \frac{16}{5} + \frac{4}{3} + \frac{4}{2}$$

$$= 15mn + \frac{60m + 96m - 220m}{30} + \frac{48n + 90n - 100n}{30} - \frac{96 + 40 + 60}{5}$$

$$H(\mathbf{L}(\mathbf{S}(\mathbf{H}))) = 15mn - \frac{32}{15}m - \frac{31}{15}n + \frac{2}{15}$$

**Theorem 3.13:** Let  $L(S(H(m, n)))$  denote the line graph of subdivision graph of H-Naphtalenic nanosheet, then its Randic index is as follows.

$$R_\alpha(\mathbf{L}(\mathbf{S}(\mathbf{H}))) = \begin{cases} 135mn + m(8\sqrt{6} - 58) + n(4\sqrt{6} - 48) + (20 - 8\sqrt{6}) & \text{for } \alpha = \frac{1}{2} \\ 15mn + m\left(\frac{24-16\sqrt{6}}{\sqrt{6}}\right) + n\left(\frac{12-11\sqrt{6}}{3\sqrt{6}}\right) + \left(\frac{10\sqrt{6}-24}{3\sqrt{6}}\right) & \text{for } \alpha = -\frac{1}{2} \end{cases}$$

**Proof:** Together with Eq. 13 and Table 1, for  $\alpha = \frac{1}{2}$  we have.

$$R_{\frac{1}{2}}(\mathbf{L}(\mathbf{S}(\mathbf{H}))) = \sum_{uv \in E_1(\mathbf{L}(\mathbf{S}(\mathbf{H})))} \sqrt{\zeta_u \zeta_v} + \sum_{uv \in E_2(\mathbf{L}(\mathbf{S}(\mathbf{H})))} \sqrt{\zeta_u \zeta_v} + \sum_{uv \in E_3(\mathbf{L}(\mathbf{S}(\mathbf{H})))} \sqrt{\zeta_u \zeta_v}$$

$$= |E_1(\mathbf{L}(\mathbf{S}(\mathbf{H})))| \sqrt{\zeta_u \zeta_v} + |E_2(\mathbf{L}(\mathbf{S}(\mathbf{H})))| \sqrt{\zeta_u \zeta_v} + |E_3(\mathbf{L}(\mathbf{S}(\mathbf{H})))| \sqrt{\zeta_u \zeta_v}$$

$$= (6n + 4m + 4) \sqrt{2 \times 2} + (4n + 8m - 8) \sqrt{2 \times 3} + (45mn - 20n - 22m + 4) \sqrt{3 \times 3}$$

$$= (6n + 4m + 4) \sqrt{2 \times 2} + (4n + 8m - 8) \sqrt{2 \times 3} + (45mn - 20n - 22m + 4) \sqrt{3 \times 3}$$

$$= 135mn + m(8 + 8\sqrt{6} - 66) + n(12 + 4\sqrt{6} - 60) + (8 - 8\sqrt{6} + 12)$$

$$R_{\frac{1}{2}}(\mathbf{L}(\mathbf{S}(\mathbf{H}))) = 135mn + m(8\sqrt{6} - 58) + n(4\sqrt{6} - 48) + (20 - 8\sqrt{6})$$

Now for  $\alpha = -\frac{1}{2}$ , we have

$$R_{\frac{1}{2}}(\mathbf{L}(\mathbf{S}(\mathbf{H}))) = \sum_{uv \in E_1(\mathbf{L}(\mathbf{S}(\mathbf{H})))} \frac{1}{\sqrt{\zeta_u \zeta_v}} + \sum_{uv \in E_2(\mathbf{L}(\mathbf{S}(\mathbf{H})))} \frac{1}{\sqrt{\zeta_u \zeta_v}} + \sum_{uv \in E_3(\mathbf{L}(\mathbf{S}(\mathbf{H})))} \frac{1}{\sqrt{\zeta_u \zeta_v}}$$

$$= |E_1(\mathbf{L}(\mathbf{S}(\mathbf{H})))| \frac{1}{\sqrt{2 \times 2}} + |E_2(\mathbf{L}(\mathbf{S}(\mathbf{H})))| \frac{1}{\sqrt{2 \times 3}} + |E_3(\mathbf{L}(\mathbf{S}(\mathbf{H})))| \frac{1}{\sqrt{3 \times 3}}$$

$$= (6n + 4m + 4) \frac{1}{\sqrt{4}} + (4n + 8m - 8) \frac{1}{\sqrt{6}} + (45mn - 20n - 22m + 4) \frac{1}{\sqrt{9}}$$

$$= 15mn + m\left(2 + \frac{8}{\sqrt{6}} - \frac{22}{3}\right) + n\left(3 + \frac{4}{\sqrt{6}} - \frac{20}{3}\right) + \left(2 - \frac{8}{\sqrt{6}} + \frac{4}{3}\right)$$

$$R_{\frac{1}{2}}(\mathbf{L}(\mathbf{S}(\mathbf{H}))) = 15mn + m\left(\frac{24 - 16\sqrt{6}}{3\sqrt{6}}\right) + n\left(\frac{12 - 11\sqrt{6}}{3\sqrt{6}}\right) + \left(\frac{10\sqrt{6} - 24}{3\sqrt{6}}\right)$$

Hence,

$$R_\alpha(\mathbf{L}(\mathbf{S}(\mathbf{H}))) = \begin{cases} 135mn + m(8\sqrt{6} - 58) + n(4\sqrt{6} - 48) + (20 - 8\sqrt{6}) & \text{for } \alpha = \frac{1}{2} \\ 15mn + m\left(\frac{24-16\sqrt{6}}{\sqrt{6}}\right) + n\left(\frac{12-11\sqrt{6}}{3\sqrt{6}}\right) + \left(\frac{10\sqrt{6}-24}{3\sqrt{6}}\right) & \text{for } \alpha = -\frac{1}{2} \end{cases}$$

**Theorem 3.14:** Let  $L(S(H(m, n)))$  denote the line graph of subdivision graph of H-Naphtalenic nanosheet, then its arithmetic-geometric ( $AG_1$ ) index is equal to.

$$AG_1(\mathbf{L}(\mathbf{S}(\mathbf{H}))) = 45mn + m\left(\frac{20 - 18\sqrt{6}}{\sqrt{6}}\right) + n\left(\frac{10 - 14\sqrt{6}}{\sqrt{6}}\right) + \left(\frac{8\sqrt{6} - 20}{\sqrt{6}}\right)$$

**Proof:** From Eq. 14 and Table 1, we have.

$$= \sum_{uv \in E_1(\mathbf{L}(\mathbf{S}(\mathbf{H})))} \frac{\zeta_u + \zeta_v}{2\sqrt{\zeta_u \zeta_v}} + \sum_{uv \in E_2(\mathbf{L}(\mathbf{S}(\mathbf{H})))} \frac{\zeta_u + \zeta_v}{2\sqrt{\zeta_u \zeta_v}} + \sum_{uv \in E_3(\mathbf{L}(\mathbf{S}(\mathbf{H})))} \frac{\zeta_u + \zeta_v}{2\sqrt{\zeta_u \zeta_v}}$$

$$= |E_1(\mathbf{L}(\mathbf{S}(\mathbf{H})))| \frac{\zeta_u + \zeta_v}{2\sqrt{\zeta_u \zeta_v}} + |E_2(\mathbf{L}(\mathbf{S}(\mathbf{H})))| \frac{\zeta_u + \zeta_v}{2\sqrt{\zeta_u \zeta_v}} + |E_3(\mathbf{L}(\mathbf{S}(\mathbf{H})))| \frac{\zeta_u + \zeta_v}{2\sqrt{\zeta_u \zeta_v}}$$

$$= (6n + 4m + 4) \frac{2+2}{2\sqrt{2} \times 2} + (4n + 8m - 8) \frac{2+3}{2\sqrt{2} \times 3} + (45mn - 20n - 22m + 4) \frac{3+3}{2\sqrt{3} \times 3}$$

$$= (6n + 4m + 4)1 + (4n + 8m - 8) \frac{5}{2\sqrt{6}} + (45mn - 20n - 22m + 4)1$$

$$= 6n + 4m + 4 + \frac{20n}{2\sqrt{6}} + \frac{40m}{2\sqrt{6}} - \frac{40}{2\sqrt{6}} + 45mn - 20n - 22m + 4$$

$$= 45mn + 4m + \frac{40m}{2\sqrt{6}} - 22m + \frac{20n}{2\sqrt{6}} + 6n - 20n - \frac{40}{2\sqrt{6}} + 4 + 4$$

$$AG_1(L(S(H))) = 45mn + m \left( \frac{20 - 18\sqrt{6}}{\sqrt{6}} \right) + n \left( \frac{10 - 14\sqrt{6}}{\sqrt{6}} \right) + \left( \frac{8\sqrt{6} - 20}{\sqrt{6}} \right)$$

**Theorem 3.15:** Let  $L(S(H(m, n)))$  denote the line graph of subdivision graph of H-Naphtalenic nanosheet, then its SK index is equal to.

$$SK(L(S(H))) = 135m - 38m - 38n$$

**Proof:** Together with Eq. 15 and Table 1, we have.

$$= \sum_{uv \in E_1(L(S(H)))} \frac{\zeta_u + \zeta_v}{2} + \sum_{uv \in E_2(L(S(H)))} \frac{\zeta_u + \zeta_v}{2} + \sum_{uv \in E_3(L(S(H)))} \frac{\zeta_u + \zeta_v}{2}$$

$$= |E_1(L(S(H)))| \frac{2+2}{2} + |E_2(L(S(H)))| \frac{2+3}{2} + |E_3(L(S(H)))| \frac{3+3}{2}$$

$$= (6n + 4m + 4)2 + (4n + 8m - 8) \frac{5}{2} + (45mn - 20n - 22m + 4)3$$

$$SK(L(S(H))) = 135m - 38m - 38n$$

**Theorem 3.16:** Consider  $L(S(H(m, n)))$  denotes the line graph of subdivision graph of H-Naphtalenic nanosheet, then its  $SK_1$  index is equal to.

$$SK_1(L(S(H))) = \frac{9}{2}m - 67m - 66n + 2$$

**Proof:** Together with Eq. 16 and Table 1, we have.

$$SK_1(L(S(H))) = \sum_{uv \in E_1(L(S(H)))} \frac{\zeta_u \times \zeta_v}{2} + \sum_{uv \in E_2(L(S(H)))} \frac{\zeta_u \times \zeta_v}{2} + \sum_{uv \in E_3(L(S(H)))} \frac{\zeta_u \times \zeta_v}{2}$$

$$= |E_1(L(S(H)))| \frac{2 \times 2}{2} + |E_2(L(S(H)))| \frac{2 \times 3}{2} + |E_3(L(S(H)))| \frac{3 \times 3}{2}$$

$$= (6n + 4m + 4)2 + (4n + 8m - 8)3 + (45mn - 20n - 22m + 4) \frac{9}{2}$$

$$= 12n + 8m + 8 + 12n + 24m - 24 + \frac{405mn}{2} - \frac{180n}{2} - \frac{198m}{2} + \frac{36}{2}$$

$$= 12n + 8m + 8 + 12n + 24m - 24 + \frac{405mn}{2}mn - 90n - 99m + 18$$

$$SK_1(L(S(H))) = \frac{405}{2}m - 67m - 66n + 2$$

**Theorem 6.17:** Assume  $L(S(H(m, n)))$  denotes the line graph of subdivision graph of H-Naphtalenic nanosheet, then its  $SK_2$  index is equal to.

$$SK_2(L(S(H))) = 405m - 132m - 131n + 2$$

**Proof:** Together with Eq. 17 and Table 1, we have.

$$SK_2(L(S(H))) = \sum_{uv \in E_1(L(S(H)))} \left( \frac{\zeta_u \times \zeta_v}{2} \right)^2 + \sum_{uv \in E_2(L(S(H)))} \left( \frac{\zeta_u \times \zeta_v}{2} \right)^2 + \sum_{uv \in E_3(L(S(H)))} \left( \frac{\zeta_u \times \zeta_v}{2} \right)^2$$

$$= |E_1(L(S(H)))| \left( \frac{2+2}{2} \right)^2 + |E_2(L(S(H)))| \left( \frac{2+3}{2} \right)^2 + |E_3(L(S(H)))| \left( \frac{3+3}{2} \right)^2$$

$$= (6n + 4m + 4)4 + (4n + 8m - 8) \frac{25}{4} + (45mn - 20n - 22m + 4)9$$

$$= 24n + 16m + 16 + 25n + 50m - 50 + 405mn - 180 - 198m + 36$$

$$SK_2(L(S(H))) = 405m - 132m - 131n + 2$$

**Theorem 3.18:** Assume  $L(S(H(m, n)))$  denotes the line graph of subdivision graph of H-Naphtalenic nanosheet, then its first Gourava index is equal to.

$$GO_1(L(S(H))) = 675m - 210m - 208n + 4$$

**Proof:** Using Eq. 18 and Table 1, we have.

$$= |E_1(L(S(H)))|[(2+2) + (2 \times 2)] + |E_2(L(S(H)))|[(2+3) + (2 \times 3)] + |E_3(L(S(H)))|[(3+3) + (3 \times 3)]$$

$$= (6n + 4m + 4)8 + (4n + 8m - 8)11 + (45mn - 20n - 22m + 4)15$$

$$= 48n + 32m + 32 + 44n + 88m - 88 + 675mn - 300n - 330m + 60$$

$$GO_1(L(S(H))) = 675m - 210m - 208n + 4$$

**Theorem 3.19:** Let  $L(S(H(m, n)))$  denote the line graph of subdivision graph of H-Naphtalenic nanosheet, then its second Gourava index is equal to.



$$GO_2(L(S(H))) = 2430m - 884m - 864n + 40$$

**Proof:** From Eq. 19 and Table 1, we have.

$$\begin{aligned} &= \sum_{uv \in E_1(L(S(H)))} [(\zeta_u + \zeta_v) + (\zeta_u \zeta_v)] + \sum_{uv \in E_2(L(S(H)))} [(\zeta_u + \zeta_v) + (\zeta_u \zeta_v)] \\ &\quad + \sum_{uv \in E_3(L(S(H)))} [(\zeta_u + \zeta_v) + (\zeta_u \zeta_v)] \\ &= |E_1(L(S(H)))|[(2 + 2) + (2 \times 2)] + |E_2(L(S(H)))|[(2 + 3) + (2 \times 3)] \\ &\quad + |E_3(L(S(H)))|[(3 + 3) + (3 \times 3)] \\ &= (6n + 4m + 4)16 + (4n + 8m - 8)30 + (45mn - 20n - 22m + 4)54 \\ &= 69n + 64m + 64 + 120n + 240m - 240 \\ &\quad + 2430mn - 1080n - 1188m + 216 \end{aligned}$$

$$GO_2(L(S(H))) = 2430m - 884m - 864n + 40$$

**Theorem 3.20:** Let  $L(S(H(m, n)))$  denote the line graph of subdivision graph of H-Naphtalenic nanosheet, then its first hyper-Gourava index is equal to.

$$HGO_1(L(S(H))) = 10125mn - 3726m - 3632n + 188$$

**Proof:** Together with Eq. 20 and Table 1, we have.

$$\begin{aligned} &= \sum_{uv \in E_1(L(S(H)))} [(\zeta_u + \zeta_v) + (\zeta_u \zeta_v)]^2 + \sum_{uv \in E_2(L(S(H)))} [(\zeta_u + \zeta_v) + (\zeta_u \zeta_v)]^2 \\ &\quad + \sum_{uv \in E_3(L(S(H)))} [(\zeta_u + \zeta_v) + (\zeta_u \zeta_v)]^2 \\ &= |E_1(L(S(H)))|[(2 + 2) + (2 \times 2)]^2 + |E_2(L(S(H)))|[(2 + 3) + (2 \times 3)]^2 \\ &\quad + |E_3(L(S(H)))|[(3 + 3) + (3 \times 3)]^2 \\ &= |E_1(L(S(H)))|[4 + 4]^2 + |E_2(L(S(H)))|[5 + 6]^2 + |E_3(L(S(H)))|[6 + 9]^2 \\ &= |E_1(L(S(H)))|[8]^2 + |E_2(L(S(H)))|[11]^2 + |E_3(L(S(H)))|[15]^2 \end{aligned}$$

$$\begin{aligned} &= (6n + 4m + 4)64 + (4n + 8m - 8)121 + (45mn - 20n - 22m + 4)225 \\ &= 384n + 256m + 256 + 484n + 968m - 968 \\ &\quad + 10125mn - 4500n - 4950m + 900 \end{aligned}$$

$$HGO_1(L(S(H))) = 10125mn - 3726m - 3632n + 188$$

**Theorem 3.21:** Let  $L(S(H(m, n)))$  denote the line graph of subdivision graph of H-Naphtalenic nanosheet, then its second hyper-Gourava index is equal to.

$$HGO_2(L(S(H))) = 131220mn - 55928m - 5318n + 5488$$

**Proof:** Together with Eq. 21 and Table 1, we have.

$$\begin{aligned} &= \sum_{uv \in E_1(L(S(H)))} [(\zeta_u + \zeta_v) + (\zeta_u \zeta_v)]^2 + \sum_{uv \in E_2(L(S(H)))} [(\zeta_u + \zeta_v) + (\zeta_u \zeta_v)]^2 \\ &\quad + \sum_{uv \in E_3(L(S(H)))} [(\zeta_u + \zeta_v) + (\zeta_u \zeta_v)]^2 \\ &= |E_1(L(S(H)))|[(2 + 2) + (2 \times 2)]^2 + |E_2(L(S(H)))|[(2 + 3) + (2 \times 3)]^2 \\ &\quad + |E_3(L(S(H)))|[(3 + 3) + (3 \times 3)]^2 \end{aligned}$$

$$\begin{aligned} &= (6n + 4m + 4)256 + (4n + 8m - 8)900 \\ &\quad + (45mn - 20n - 22m + 4)2916 \end{aligned}$$

$$\begin{aligned} &= 1536n + 1024m + 1024 + 3600n + 7200m - 7200 \\ &\quad + 131220mn - 58320n - 64152m + 11664 \end{aligned}$$

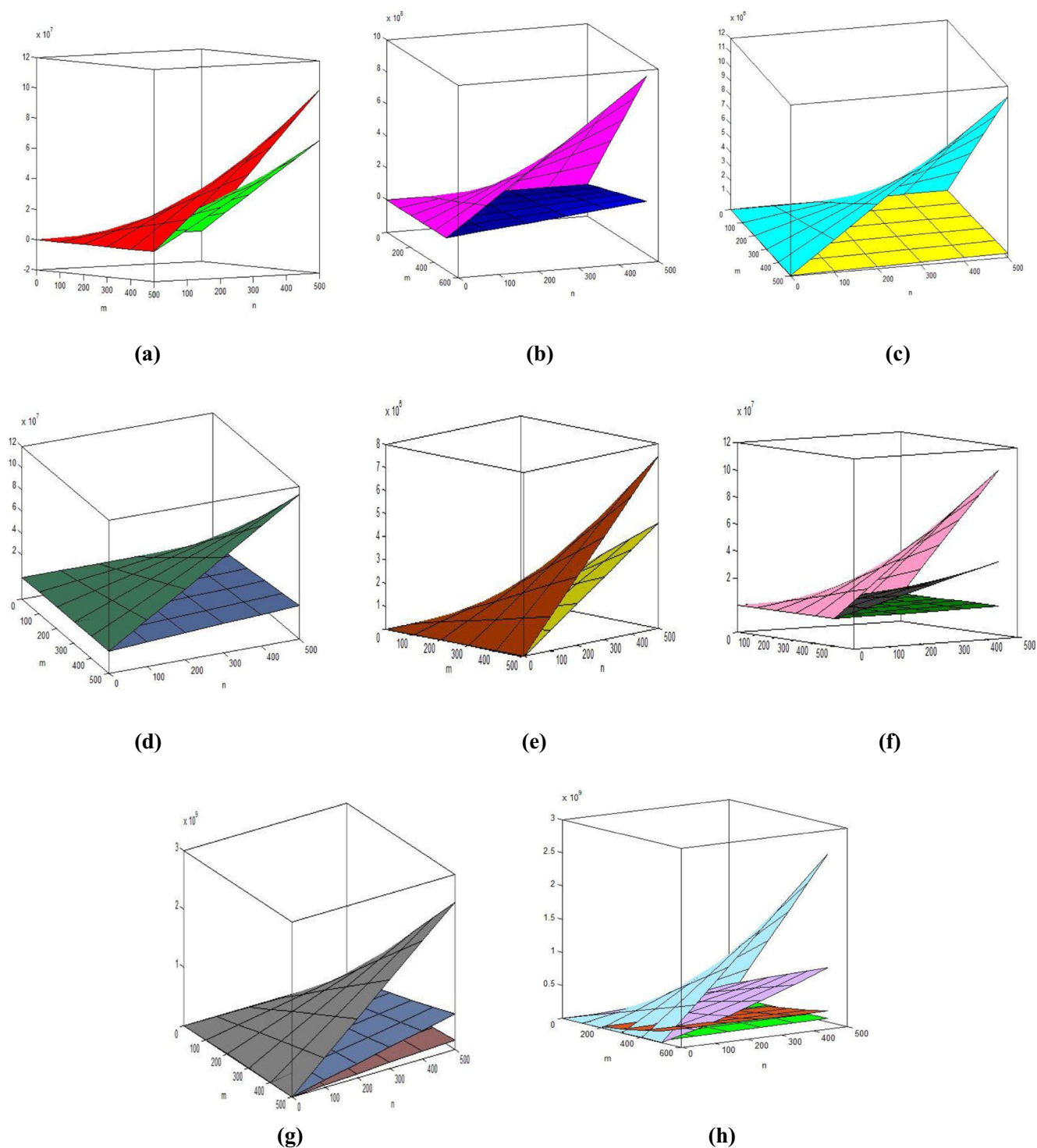
$$HGO_2(L(S(H))) = 131220mn - 55928m - 5318n + 5488$$

### Numerical results and discussion

In this section, all indices for different values of  $m, n$  for the structure  $L(S(H(m, n)))$  are computed. Bear in mind Table 2, it is easy to see that all the considered indices are raising with an increase in the amount of  $m, n$ . The structural

**Table 2** Numerical table associated with the structure of  $L(S(H(m, n)))$  of H-Naphtalenic nanosheet

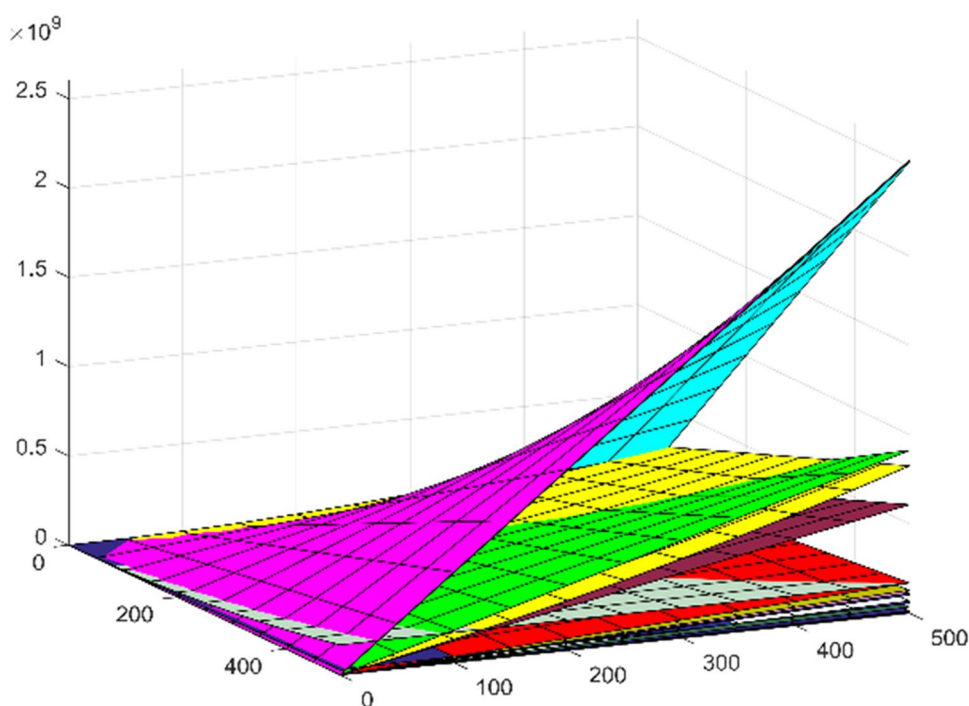
[m, n]	M1	M2	HM	PM1	PM2	M1(G, x)	M2(G, x)	A	ABC	SCI	
[1, 1]	118	143	2258	46,965	70,955	1095	955	715	1002	1955	
[2, 2]	776	1092	11,618	58,053	85,054	3055	1054	890	1123	2054	
[3, 3]	1974	2851	28,268	88,113	89,110	4911	2110	980	1457	2310	
[4, 4]	3712	5420	52,208	98,724	99,904	9944	3904	1151	1679	2990	
[m, n]	GA	H	Rα	AG1	SK	SK1	SK2	GO1	GO2	HGO1	HGO2
[1, 1]	109	955	965	6965	469	965	1450	19,965	66,960	1276	32,167
[2, 2]	254	1054	1053	8053	580	1053	23,618	28,054	78,052	1783	42,678
[3, 3]	310	1110	1113	8113	881	2113	32,261	37,112	88,114	2384	55,678
[4, 4]	504	1904	1724	9724	987	3724	41,205	56,721	98,726	3300	92,174



**Fig. 4** Comparison of indices (a)  $M_1$  and  $M_2$ , (b) HM and A, (c)  $PM_1$  and  $PM_2$ , (d)  $PM_1$  and  $PM_2$  (e) ABC, SCI and GA, (f) H,  $R_\alpha$  and  $AG_1$ , (g) SK,  $SK_1$  and  $SK_2$ , (h)  $GO_1$ ,  $GO_2$ ,  $HGO_1$  and  $HGO_2$

interpretations of all topological indices of  $L(S(H(m, n)))$  are shown in Fig. 4(a-h) for different amount of  $m, n$ . Similarly, by considering Table 2, the comparison of all topological indices for different values of  $m, n$  is presented in Fig. 5.

The Zagreb type indices as well as the Zagreb type polynomial indices are beneficial for the calculation of total  $\pi$ -electron energy of molecules. Thus, it is easy to see from Table 2 and Fig. 4(a-e) that in case of  $L(S(H(m, n)))$  the

**Fig. 5** Comparison of all considered indices

total  $\pi$ -electron energy increases for higher values of  $m$ ,  $n$ . Hence, we deduce that, to obtain the higher value of  $\pi$ -electron energy in  $L(S(H(m, n)))$ , we need to increase the amount of  $m$ ,  $n$ .

Since the augmented Zagreb index (AZI) demonstrates an excellent correlation with the formation heat of octane and heptanes, our computation for AZI index plays an important role for formation heat of octane and heptanes, as its values are in increasing order. The sum connectivity index is helpful for testing the pharmacological properties and substance of drug nuclear structures. So in the case of  $L(S(H(m, n)))$ , its increasing value is useful for quick action during chemical reaction for drugs.

Since the arithmetic–geometric (AG) index is well correlated with a range of physicochemical properties of molecule, in the case of  $L(S(H(m, n)))$ , the AG index well correlates with a range of physicochemical properties. Harmonic and Randic indices are important parameters to assess the operation of a power system. So in the case of  $L(S(H(m, n)))$ , its increasing values are helpful to make the system more powerful.

## Conclusion

In this paper, we have computed certain important degree-based topological indices, such as first Zagreb index, second Zagreb index, hyper-Zagreb index, first multiple Zagreb index, second multiple Zagreb index,

first Zagreb polynomial, second Zagreb polynomial, augmented Zagreb index, ABC (atom-bond connectivity) index, sum connectivity index (SCI), geometric–arithmetic index, harmonic index, Randic indices  $R_\alpha$  ( $L(H)$ ) where  $\alpha$  is the real number, arithmetic–geometric ( $AG_1$ ) index, SK,  $SK_1$ ,  $SK_2$  indices, first and second Gourava indices, first and second hyper-Gourava indices for the line graph of subdivision graph of H-Naphtalenic nanosheet, and derived formulas for them. Based on the derived formulas, numerical results are obtained, and the physical and chemical properties of the under study nanosheet are investigated. These topological indices proved to be very helpful in predicting the nanostructure for QSAR/QSPR analysis.

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**Code availability** Not applicable.

## Declarations

**Conflicts of interest/Competing interests** The authors declare no any conflict of interest/competing interests.

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