Research Article

Theoretical Analysis of Superphenalene Using Different Kinds of VDB Indices

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Topological indices (TIs) are numerical quantities that enable theoretical chemists to analyse molecular structures mathematically. These TIs are essential to exploring chemical compounds using theoretical techniques like QSAR/QSPR methods. Superphenalene is a large polycyclic aromatic hydrocarbon molecule which has been quickly gaining importance as a building block for alternate energy providers due to its photovoltaic properties. The exciting features of this compound, coupled with its potential applications, warrant an investigation of its nature and properties from a structural perspective. The objective of this research is to compute the proper analytical expressions of four kinds of vertex degree-based (VDB) indices for superphenalene. The numerical values of these indices and 3D graphical representations also help in understanding the relationship between the VDB indices of the compound and its underlying chemical structure quantitatively.

1. Introduction

Chemical graph theory enables mathematicians and chemists to represent the molecular structures of chemical compounds as graphs in order to analyse them theoretically. The vertices may represent atoms, molecules, or molecule collections in a chemical graph. The edges of a chemical graph indicate the relationships between the chemical objects and generally represent reactions, mechanisms of reactions, chemical bonds, or other transformations in chemical objects. The major applications of such graphs involve topological indices (TIs), which are used in Quantitative Structure-Property Relationships (QSPR) and Quantitative Structure-Activity Relationships (QSAR) [1]. A TI is a distinct numerical quantity which describes a molecular structure and its characteristics. It can also be considered a score function mapping each molecular graph to a distinct real number. The study of these indices is crucial to the theoretical analysis of chemical compounds without involving practical experiments, thus saving time and effort involved in their research.

There are several kinds of TIs defined in the literature, of which the degree-based indices are extensively studied and applied in molecular topology. A degree-based topological index is a type of TI which is determined on the basis of the degrees of a molecular graph. Among VDB indices, a few are connectivity-based TIs, namely, the generalized connectivity index [2], Randić connectivity index [3], Estrada's ABC index, sum-connectivity index, Zagreb index, geometric-arithmetic [4], and harmonic [5] indices. In modern-day mathematical chemistry, quite a number of these indices are recorded and studied.

There is evidence of a strong correlation between various physical, chemical, and biological properties of chemical compounds and a number of degree-based topological indices. For instance, the Randić and sum-connectivity indices exhibit a high correlation with the π-electron energy of benzenoid hydrocarbons and octanol partition and dermal penetration of benzenoid compounds [6–8]. Zagreb and its co indices have been used to predict total π-electron energy and heat of formation in heptanes and octanes [9, 10]. The total surface area of polychlorobiphenyls and the symmetric

division deg (SDD) index show a strong positive correlation [11, 12]. The ABC index has been applied in the study of the heat of formation and stability of alkanes [13]. The F-index is widely used in order to analyse drugs based on molecular structures using entropy and acentric factor [14].

As a result, VDB TIs have a multitude of applications in the pharmaceutical industry, particularly in drug discovery. Additionally, when compared with distance-based TIs and other sophisticated quantum chemical techniques, the VDB indices are also simpler to investigate, making the study of degree-based indices more lucrative. This research is focused on computing the VDB indices for superphenalene structure.

Superphenalene has been quickly gaining the attention of chemists as well as researchers studying alternative energy sources. Superphenalene ($C_{96}H_{30}$) is a very large PAH, made up of three interconnected hexa-peri-hexabenzocoronene structures that are uniformly joined around a central point. Hexa-peri-hexabenzocoronene (HBC), in turn, is made up of a coronene ring in the middle of the molecule, and along the molecule's periphery, an additional benzene ring is added to the top of each ring. It is a well-studied PAH with the empirical formula $C_{48}H_{24}$. The HBC adopts a doubly concave, D3d-symmetric structure due to steric constriction around the periphery [15]. It is also known as contorted hexabenzocoronene [16] because of its twisted structure. Zhang et al. [17] have successfully synthesised constrained hexabenzocoronene, which could be applied in photo-responsive transistors, and photovoltaic materials and exhibits chemoresponsive properties as well. As they support the creation of self-gathering columns and nanotubes, these structures have been known as molecular electronic building blocks since 2004 [18]. The molecular structure of super-phenalene is represented in Figure 1.

Due to the increasing interest in large PAHs like superphenalene, there is also a rising demand to study these structures from a structural viewpoint. The degree-based indices offer a convenient and efficient way to analyse the structures and predict their physical and chemical properties. Recently, Julietraja and Venugopal [19] determined the VDB indices for single-hole coronoids. Chu et al. [20] calculated the VDB and irregularity-based TIs for certain classes of PAHs. Julietraja et al. also estimated the VDB indices for some PAHs using the M-polynomial [21–23]. Radhakrishnan et al. studied distance-based indices for two different kinds of PAHs, including superphenalene in [24].

However, there are no studies till now that have attempted to describe the superphenalene structure using different kinds of VDB indices. Thus, the aim of this research work is to compute four different kinds of VDB indices, namely, VDB multiplicative TIs, irregularity indices, VDB entropy measures and other VDB indices derived using M-polynomial. The derived indices, when combined, can be used to predict several properties of the compound under study. This will help chemists not only understand super-phenalene but also explore similar large molecules using these indices.
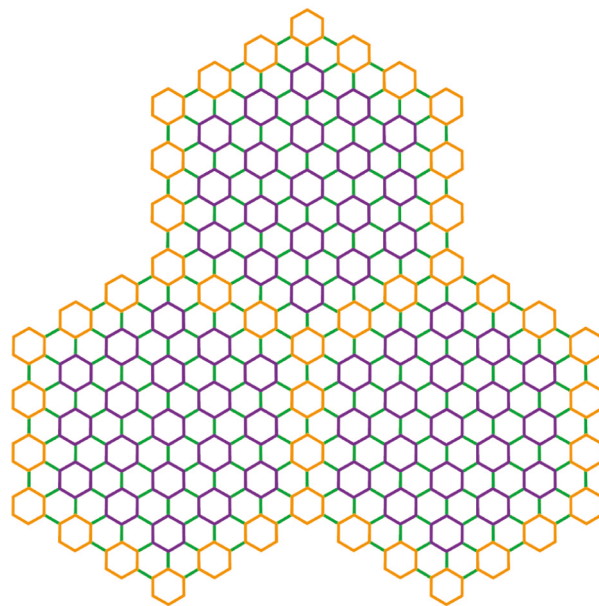

Figure 1: Molecular graph of superphenalene.

2. Mathematical Terminologies and Definitions

In this paper, Γ represents a connected graph, $V(\Gamma)$ and $E(\Gamma)$ refers to the vertex set and the edge set, respectively. The degree of a vertex $\mathfrak{d}_\mathfrak{v}$ in a graph Γ is the number of edges that are adjacent to that vertex $\mathfrak{v}$ [25].

3. Multiplicative Topological Indices

The multiplicative TIs are a recently introduced and studied class of VDB indices. The generic multiplicative topological index [26] is represented as

$$= - \sum_{\mathfrak{u}\mathfrak{v}\in E(\Gamma)} \frac{F(\mathfrak{d}_\mathfrak{u}, \mathfrak{d}_\mathfrak{v})}{\mathscr{X}(\Gamma)} \log \frac{F(\mathfrak{d}_\mathfrak{u}, \mathfrak{d}_\mathfrak{v})}{\mathfrak{X}(\Gamma)}, MTI(\Gamma) = \prod_{\mathfrak{u}\mathfrak{v}\in E(\Gamma)} F(\mathfrak{d}_\mathfrak{u}, \mathfrak{d}_\mathfrak{v}), \tag{1}$$

where Π denotes the product of the terms $F(\mathfrak{d}_\mathfrak{u}, \mathfrak{d}_\mathfrak{v})$. The multiplicative version of the Wiener index was the first topological index investigated by Das and Gutman [27].

The first and second versions of multiplicative F-indices [28] are described as follows:

$$MF_1I(\Gamma) = \prod_{\mathfrak{u}\mathfrak{v}\in E(\Gamma)} \mathfrak{d}_\mathfrak{u}^2 + \mathfrak{d}_\mathfrak{v}^2,$$
$$MF_2I(\Gamma) = \prod_{\mathfrak{u}\mathfrak{v}\in E(\Gamma)} \mathfrak{d}_\mathfrak{u}^2 \times \mathfrak{d}_\mathfrak{v}^2. \tag{2}$$

The first multiplicative hyper-Zagreb index is described [29] as

$$FMHZI(\Gamma) = \prod_{\mathfrak{u}\mathfrak{v}\in E(\Gamma)} (\mathfrak{d}_\mathfrak{u} + \mathfrak{d}_\mathfrak{v})^2 \mathfrak{A}. \tag{3}$$

The multiplicative harmonic index of a graph is defined [28] as

$$MHI(\Gamma) = \prod_{\mathfrak{uv} \in E(\Gamma)} \left(\frac{2}{\mathfrak{d}_\mathfrak{u} + \mathfrak{d}_\mathfrak{v}} \right). \qquad (4)$$

The multiplicative sum connectivity and Randić indices are represented [30] as

$$MSCI(\Gamma) = \prod_{\mathfrak{uv} \in E(\Gamma)} \frac{1}{\sqrt{\mathfrak{d}_\mathfrak{u} + \mathfrak{d}_\mathfrak{v}}},$$

$$MRI(\Gamma) = \prod_{\mathfrak{uv} \in E(\Gamma)} \frac{1}{\sqrt{\mathfrak{d}_\mathfrak{u} \times \mathfrak{d}_\mathfrak{v}}}. \qquad (5)$$

Multiplicative ABC index and multiplicative GA index are defined as

$$MABCI(\Gamma) = \prod_{\mathfrak{uv} \in E(\Gamma)} \sqrt{\frac{\mathfrak{d}_\mathfrak{u} + \mathfrak{d}_\mathfrak{v} - 2}{\mathfrak{d}_\mathfrak{u} \times \mathfrak{d}_\mathfrak{v}}},$$

$$MGAI(\Gamma) = \prod_{\mathfrak{uv} \in E(\Gamma)} \frac{2\sqrt{\mathfrak{d}_\mathfrak{u} \times \mathfrak{d}_\mathfrak{v}}}{\mathfrak{d}_\mathfrak{u} + \mathfrak{d}_\mathfrak{v}}. \qquad (6)$$

The multiplicative augmented Zagreb index is defined [28] as

$$MAZI(\Gamma) = \prod_{\mathfrak{uv} \in E(\Gamma)} \left(\frac{\mathfrak{d}_\mathfrak{u} \times \mathfrak{d}_\mathfrak{v}}{\mathfrak{d}_\mathfrak{u} + \mathfrak{d}_\mathfrak{v} - 2} \right)^3. \qquad (7)$$

4. Computing the VDB Multiplicative TIs for Superphenalene

In this section, the analytical expressions of VDB multiplicative TIs have been studied for superphenalene $SP(n)$. The cardinality of Γ is $V(\Gamma) = 54n^2 - 72n + 24$ and $E(\Gamma) = 81n^2 - 120n + 45$ [24]. The edge partition of $SP(n)$ is presented in Table 1.

Theorem 1. *If $\Gamma = SP(n)$ is a superphenalene, then the VDB multiplicative TIs are computed as*

(1) $MF_1I(\Gamma) =$
(1/142291965149018983699997094313984) ×
$5832^{(27n-25)(n-1)}$ ×
$37300984912024432463052038291845021696^n$

(2) $MF_2I(\Gamma) = (1/3766863772439521954013$
$06999861472444605792256) \times 531441^{(27n-25)(n-1)} \times$
$6319748715279270675921934218987893281199411530039296^n$

(3) $FMHZI(\Gamma) =$
(1/5960464477539062500000000000000000000000) ×

Table 1: Edge partition table for superphenalene [24].

S.no	Edge pairs	Edge frequency
1	$(2, 2)$	$12n - 6$
2	$(2, 3)$	$24n - 24$
3	$(3, 3)$	$81n^2 - 156n + 75$

$46656^{(27n-25)(n-1)} \times 1000000000000000000000000000000000000000000000000000000^n$

(4) $MHI(\Gamma) = (1/262144) \times 5^{-24n+24} \times 4096^n \times 27^{-(27n-25)(n-1)}$

(5) $MSCI(\Gamma) = 15625000000 \times 1000000000000^{-n} \times 36^{-(27n-25)(n-1)} \times 6^{(1/2(27n-25))(n-1)}$

(6) $MRI(\Gamma) = 139314069504 \times 27^{-(27n-25)(n-1)} \times 8916100448256^{-n}$

(7) $MABCI(\Gamma) = 6^{-12*n+12} \times 27^{-(27n-25)(n-1)}$

(8) $MGAI(\Gamma) = 5^{-24n+24} \times 24^{12n-12}$

(9) $MAZI(\Gamma) = (1/1237940039285380274899124224) \times 324518553658426726783156020576256^n \times 387420489^{(27n-25)(n-1)} \times 262144^{-(27n-25)(n-1)}$

Proof. Let $\Gamma = SP(n)$ be the molecular graph of superphenalene. The superphenalene contains vertices $V(\Gamma) = 54n^2 - 72n + 24$ and edges $E(\Gamma) = 81n^2 - 120n + 45$. By using the definitions of VDB multiplicative TIs and Table 1, the results are obtained as listed above. □

5. M-Polynomial and VDB Indices for Superphenalene

Several algebraic polynomials have been used to calculate the distance-based TIs. In the context of determining distance-based TIs, the Hosoya polynomial is said to be the most generic polynomial. The Hosoya polynomial can be used to calculate a significant number of distance-based indices via a single polynomial. Deutsch and Klavzar [31] had a similar breakthrough for VDB indices. The M-polynomial is used for the VDB indices in the same way as the Hosoya polynomial is used for distance-based indices. The M-polynomial has a unique advantage in providing a wealth of information on VDB graph invariants. The VDB indices for superphenalene are computed in this section using the M-polynomial. The derivation for computing M-polynomial can be seen in Table 2. The M-polynomial of Γ is defined as [31]

$$M(\Gamma; w, k) = \sum_{\delta \leq i \leq j \leq \Delta} m_{ij}(\Gamma) w^i k^j, \qquad (8)$$

TABLE 2: VDB TIs derived from M-polynomials.

S.no	VDB TIs derived from $M(\Gamma; w, k) = f(w, k)$
1	$ABC(\Gamma) = D_w^{1/2} Q_{-2} J S_w^{1/2} S_k^{1/2} (f(w, k))\vert_{w=1}$
2	$GA(\Gamma) = 2S_w J D_w^{1/2} D_k^{1/2} (f(w, k))\vert_{w=1}$
3	$B_1(\Gamma) = (D_w + D_k + 2D_w Q_{-2} J)(f(w, k))\vert_{w=k=1}$
4	$B_2(\Gamma) = D_w Q_{-2} J (D_w + D_k)(f(w, k))\vert_{w=1}$
5	$HB_1(\Gamma) = D_w^2 + D_k^2 + 2D_w^2 Q_{-2} J + 2D_w Q_{-2} J (D_w + D_k)(f(w, k))\vert_{w=k=1}$
6	$HB_2(\Gamma) = D_w^2 Q_{-2} J (D_w^2 + D_k^2)(f(w, k))\vert_{w=1}$
7	$MB_1(\Gamma) = S_w Q_{-2} J (L_w + L_k)(f(w, k))\vert_{w=1}$
8	$MB_2(\Gamma) = S_w Q_{-2} J (S_w + S_k)(f(w, k))\vert_{w=1}$
9	$H_b(\Gamma) = 2S_w Q_{-2} J (L_w + L_k)(f(w, k))\vert_{w=1}$

where $\delta = \text{Min}\{\mathfrak{d}_{\mathfrak{v}} : \mathfrak{v} \in V(\Gamma)\}$; $\Delta = \text{Max}\{\mathfrak{d}_{\mathfrak{v}} : \mathfrak{v} \in V(\Gamma)\}$, and $m_{ij}(\Gamma)$ is the edge $\mathfrak{v}\mathfrak{u} \in E(\Gamma)$ for which $\{\mathfrak{d}_{\mathfrak{v}}, \mathfrak{d}_{\mathfrak{u}}\} = \{i, j\}$.

$$D_w(f(w, k)) = w \frac{\partial f(w, k)}{\partial w},$$

$$D_k(f(w, k)) = k \frac{\partial f(w, k)}{\partial k},$$

$$L_w(f(w, k)) = f(w^2, k),$$

$$L_k(f(w, k)) = f(w, k^2),$$

$$S_w(f(w, k)) = \int_0^w \frac{f(t, k)}{t} dt,$$

$$S_k(f(w, k)) = \int_0^k \frac{f(w, t)}{t} dt,$$

$$J(f(w, k)) = f(w, w),$$

$$D_w^{1/2}(f(w, k)) = \sqrt{w \frac{\partial f(w, k)}{\partial w}} \cdot \sqrt{f(w, k)},$$

$$D_k^{1/2}(f(w, k)) = \sqrt{k \frac{\partial f(w, k)}{\partial k}} \cdot \sqrt{f(w, k)},$$

$$s_w^{1/2}(f(w, k)) = \sqrt{\int_0^w \frac{f(w, k)}{t} dt} \cdot \sqrt{f(w, k)},$$

$$s_k^{1/2}(f(w, k)) = \sqrt{\int_0^k \frac{f(w, k)}{t} dt} \cdot \sqrt{f(w, k)},$$

$$Q_\alpha(f(w, k)) = w^\alpha f(w, k),$$

$$\alpha \neq 0.$$

(9)

Theorem 2. *If $\Gamma = SP(n)$ is a superphenalene, then the M-polynomial is computed as*

$$M(\Gamma; w, k) = (12n - 6)w^2 k^2 + (24n - 24)w^2 k^3 \\ + (81n^2 - 156n + 75)w^3 k^3.$$

(10)

Proof. Using the definition of M-polynomial and Table 1, the result is obtained as

$$M(\Gamma; w, k) = (12n - 6)w^2 k^2 + (24n - 24)w^2 k^3 \\ + (81n^2 - 156n + 75)w^3 k^3.$$

(11)

Hence the proof. □

Theorem 3. *If $\Gamma = SP(n)$ is a superphenalene, then the VDB indices using M-polynomial are computed as*

(1) $ABC(\Gamma) = 18\sqrt{2}n + 54n^2 - 15\sqrt{2} - 104n + 50$

(2) $GA(\Gamma) = 81n^2 - 144n + 69 + (48/5)\sqrt{6}n - (48/5)\sqrt{6}$

(3) $B_1(\Gamma) = 1134n^2 - 1824n + 738$

(4) $B_2(\Gamma) = 1944n^2 - 3288n + 1392$

(5) $HB_1(\Gamma) = 7938n^2 - 13440n + 5694$

(6) $HB_2(\Gamma) = 23328n^2 - 41736n + 18600$

(7) $MB_1(\Gamma) = (162/7)n^2 - (1042/35)n + 337/35$

(8) $MB_2(\Gamma) = (27/2)n^2 - (40/3)n + 17/6$

(9) $H_b(\Gamma) = (324/7)n^2 - (2084/35)n + 674/35$

Proof. Consider $M(\Gamma; w, k) = f(w, k) = (12n - 6)w^2 k^2 + (24n - 24)w^2 k^3 + (81n^2 - 156n + 75)w^3 k^3$. Using Table 2 and the result obtained in Theorem 2, the indices are determined, as listed above. □

6. VDB Entropy Measures for Superphenalene

The intrinsic and extrinsic measures of graph entropy enable mathematicians to relate graph components such as edges and vertices to probability distributions. Graph entropies have found widespread use in numerous disciplines, including sociology, ecology, and biology, as well as chemistry [32, 33]. In the study of networks, the degree-based entropy measures, which are extensively studied and used in graph theory, are regarded as information functionals. Based on information functionals, Dehmer introduced graph entropies that captured structural information and studied their properties [34, 35]. Applications of entropy network measures range from quantitatively describing a molecular structure to investigate the biological and chemical properties of molecular graphs. The entropy measures can be applied in a variety of ways to different areas of chemical graph theory.

Let n be the order of a graph of size m and φ be some meaningful information function. The Shannon's entropy [36, 37] of a graph is depicted as follows.

Let Γ be a graph with vertex $\mathfrak{v}_i$ and $\mathfrak{d}_i$ be the degree of $\mathfrak{v}_i$ for the given edge $\mathfrak{u}_i\mathfrak{v}_j$, then one can define

$$\mathscr{P}_{ij} = \frac{\mathfrak{w}(\mathfrak{u}_i\mathfrak{v}_j)}{\sum_{j=1}^{\mathfrak{d}_i}\mathfrak{w}(\mathfrak{u}_i\mathfrak{v}_j)}, \tag{12}$$

where $\mathfrak{w}(\mathfrak{u}_i\mathfrak{v}_j)$ be the weight of the edge $\mathfrak{u}_i\mathfrak{v}_j$ and $\mathfrak{w}(\mathfrak{u}_i\mathfrak{v}_j) > 0$. The node entropy is defined as

$$\mathrm{ENT}_\Gamma(\mathfrak{v}_i) = -\sum_{j=1}^{\mathfrak{d}_i}\mathscr{P}_{ij}\log(\mathscr{P}_{ij}). \tag{13}$$

For an edge-weighted graph $\Gamma = (V, E, \mathfrak{w})$, the entropy measure of Γ is defined as

$$\mathrm{ENT}_\Gamma(\Gamma, \mathfrak{w}) = -\sum_{\mathfrak{u}\mathfrak{v} \in E(\Gamma)}\mathscr{P}_{\mathfrak{u}\mathfrak{v}}\log\mathscr{P}_{\mathfrak{u}\mathfrak{v}}, \tag{14}$$

where

$$\mathscr{P}_{\mathfrak{u}\mathfrak{v}} = \frac{\mathfrak{w}(\mathfrak{u}\mathfrak{v})}{\sum_{\mathfrak{u}\mathfrak{v} \in E(\Gamma)}\mathfrak{w}(\mathfrak{u}\mathfrak{v})},$$

$$
\begin{aligned}
\mathrm{ENT}_{\mathscr{X}}(\Gamma) &= -\sum_{\mathfrak{u}\mathfrak{v} \in E(\Gamma)}\mathscr{P}_{u,\mathfrak{v}}\log\mathscr{P}_{u,\mathfrak{v}} \\
&= -\sum_{\mathfrak{u}\mathfrak{v} \in E(\Gamma)}\frac{F(\mathfrak{d}_u, \mathfrak{d}_\mathfrak{v})}{\mathscr{X}(\Gamma)}\log\frac{F(\mathfrak{d}_u, \mathfrak{d}_\mathfrak{v})}{\mathscr{X}(\Gamma)} \\
&= -\frac{1}{\mathscr{X}(\Gamma)}\sum_{\mathfrak{u}\mathfrak{v} \in E(\Gamma)}F(\mathfrak{d}_u, \mathfrak{d}_\mathfrak{v})\log\frac{F(\mathfrak{d}_u, \mathfrak{d}_\mathfrak{v})}{\mathscr{X}(\Gamma)} \\
&= -\frac{1}{\mathscr{X}(\Gamma)}\sum_{\mathfrak{u}\mathfrak{v} \in E(\Gamma)}F(\mathfrak{d}_u, \mathfrak{d}_\mathfrak{v}) \\
&\quad \cdot (\log F(\mathfrak{d}_u, \mathfrak{d}_\mathfrak{v})) - (\log\mathscr{X}(\Gamma)) \\
&= \log\mathscr{X}(\Gamma) - \frac{1}{\mathscr{X}(\Gamma)}\sum_{\mathfrak{u}\mathfrak{v} \in E(\Gamma)}F(\mathfrak{d}_u, \mathfrak{d}_\mathfrak{v})\log F(\mathfrak{d}_u, \mathfrak{d}_\mathfrak{v}),
\end{aligned}
\tag{15}
$$

where $TI(\Gamma) = \mathscr{X}$.

Theorem 4. *If Γ is a superphenalene, then the VDB entropy measures are computed as*

(1) $ENT_{M_1}(\Gamma) = \log(486n^2 - 768n + 306) - 1/486n^2 - 768n + 306[(48n - 24)\log(4) + (120n - 120)\log(5) + (486n^2 - 936n + 450)\log(6)],$

(2) $ENT_{M_2}(\Gamma) = \log(729n^2 - 1212n + 507) - 1/729n^2 - 1212n + 507[(48n - 24)\log(4) + (144n - 144)\log(6) + (729n^2 - 1404n + 675)\log(9)],$

(3) $ENT_{M_2^m}(\Gamma) = \log(9n^2 - (31/3)n + 17/6) - 1/(9n^2 - (31/3)n + 17/6)[(3n - 3/2)\log(1/4) + (4n - 4)\log(1/6) + (9n^2 - (52/3)n + 25/3)\log(1/9)],$

(4) $ENT_{RM_2}(\Gamma) = \log(324n^2 - 564n + 246) - 1/324n^2 - 564n + 246[(12n - 6)\log(1) + (48n - 48)\log(2) + (324n^2 - 624n + 300)\log(4)],$

(5) $ENT_{HM}(\Gamma) = \log(2916n^2 - 4824n + 2004) - (1/2916n^2 - 4824n + 2004)[(192n - 96)\log(16) + (600n - 600)\log(25) + (2916n^2 - 5616n + 2700)\log(36)],$

(6) $ENT_A(\Gamma) = \log((59049/64)n^2 - (23823/16)n + 39315/64) - (1/(59049/64)n^2 - (23823/16)n + 39315/64)[(96n - 48)\log(8) + (192n - 192)\log(8) + ((59049/64)n^2 - (28431/16)n + 54675/64)\log(9/4)^3],$

(7) $ENT_{ABC}(\Gamma) = \log(54n^2 + 18\sqrt{2}n - 15\sqrt{2} - 104n + 50) - 1/54n^2 + 18\sqrt{2}n - 15\sqrt{2} - 104n + 50[(\sqrt{2}(6n - 3))\log(\sqrt{1/2}) + \sqrt{2}(12n - 12)\log(\sqrt{1/2}) + (54n^2 - 104n + 50)\log(\sqrt{4/9})],$

(8) $ENT_{GA}(\Gamma) = \log(81n^2 - 144n + 69 + (48/5)\sqrt{6}n - (48/5)\sqrt{6}) - (1/81n^2 - 144n + 69 + (48/5)\sqrt{6}n - (48/5)\sqrt{6})[(12n - 6)\log(1) + ((2/5)\sqrt{6}(24n - 24))\log(2\sqrt{6}/5) + (81n^2 - 156n + 75)\log(1)],$

(9) $ENT_{S\,DD}(\Gamma) = \log(162n^2 - 236n + 86) - (1/162n^2 - 236n + 86)[(24n - 12)\log(2) + (52n - 52)\log(13/6) + (162n^2 - 312n + 150)\log(2)],$

(10) $ENT_R(\Gamma) = \log(27n^2 + 4\sqrt{6}n - 4\sqrt{6} - 46n + 22) - 1/27n^2 + 4\sqrt{6}n - 4\sqrt{6} - 46n + 22[(6n - 3)\log(1/2) + (\sqrt{6}(4n - 4))\log(1/\sqrt{6}) + ((81/2)n^2 - 78n + 75/2)\log(1/3)],$

(11) $ENT_F(\Gamma) = \log(1458n^2 - 2400n + 990) - (1/1458n^2 - 2400n + 990)[(96n - 48)\log(8) + (312n - 312)\log(13) + (1458n^2 - 2808n + 1350)\log(18)],$

(12) $ENT_{\chi}(\Gamma) = \log(6n - 3 + (24/5)\sqrt{5}n - (24/5)\sqrt{5} + (27/2)\sqrt{6}n^2 - 26\sqrt{6}n + (25/2)\sqrt{6}) - (1/6n - 3 + (24/5)\sqrt{5}n - (24/5)\sqrt{5} + (27/2)\sqrt{6}n^2 - 26\sqrt{6}n + (25/2)\sqrt{6})[(6n - 3)\log(1/2) + ((1/5)\sqrt{5}(24n - 24))\log(1/\sqrt{5}) + ((1/6)\sqrt{6}(81n^2 - 156n + 75))\log(1/\sqrt{6})].$

Proof. Let $\Gamma = SP(n)$ be the molecular graph of a superphenalene. The cardinality of superphenalene is $V(\Gamma) = 54n^2 - 72n + 24$ and $E(\Gamma) = 81n^2 - 120n + 45$. This theorem is proved in a similar way to that of in [38]. In order to prove the above results, the definitions of VDB indices, VDB entropy measures and the edge partition Table 1 have been used. □

7. Irregularity Indices for QSPR Studies

Irregularity indices are numerical parameters that quantify the degree to which a molecular graph possesses an irregular structure. The irregularity of a molecular structure can be applied to a number of unresolved problems, including those in the fields of material engineering and chemistry [38]. Many physical and chemical properties can be predicted by studying the irregularity of graphs in QSPR and QSAR studies. These properties include a wide range of
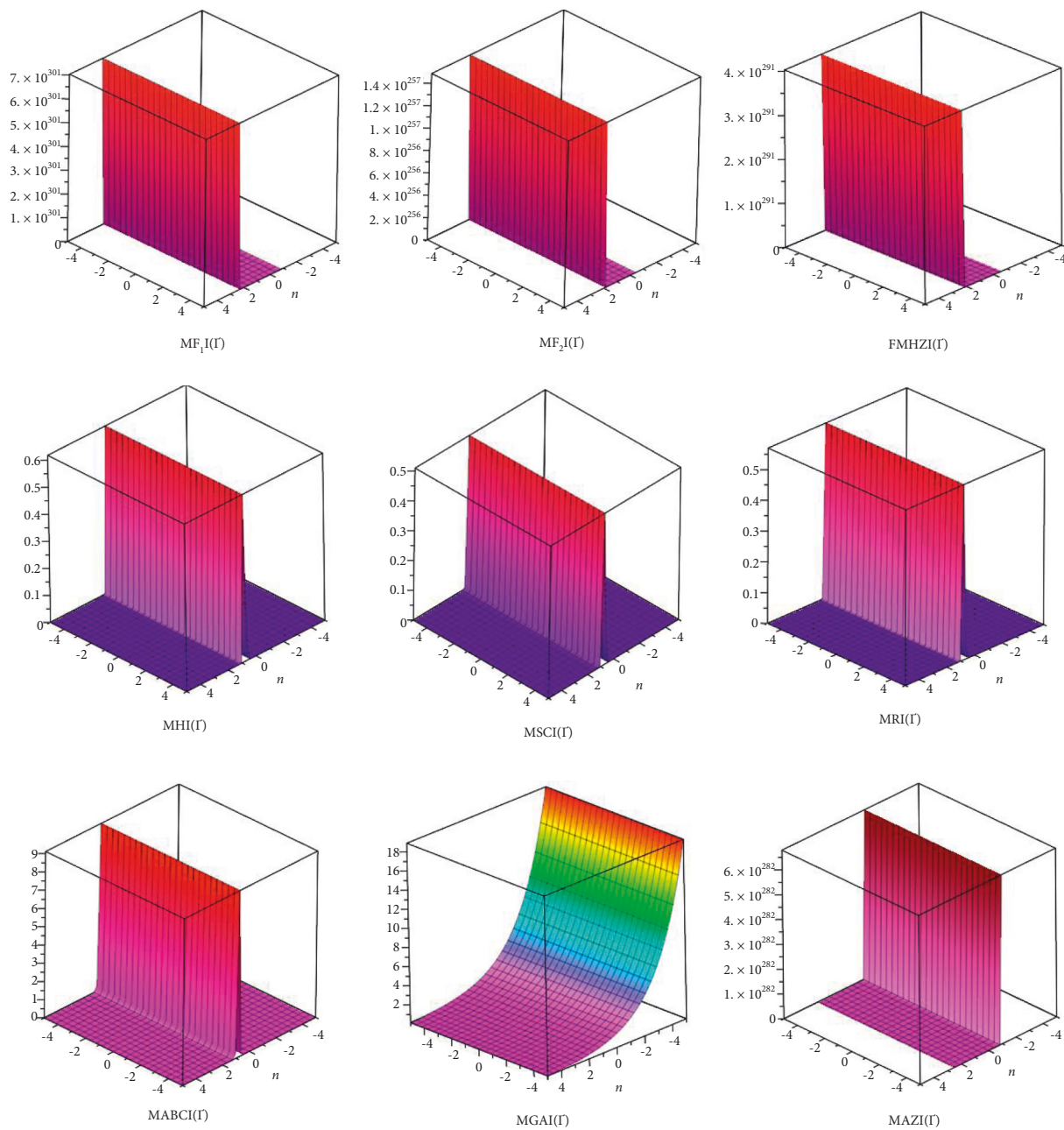
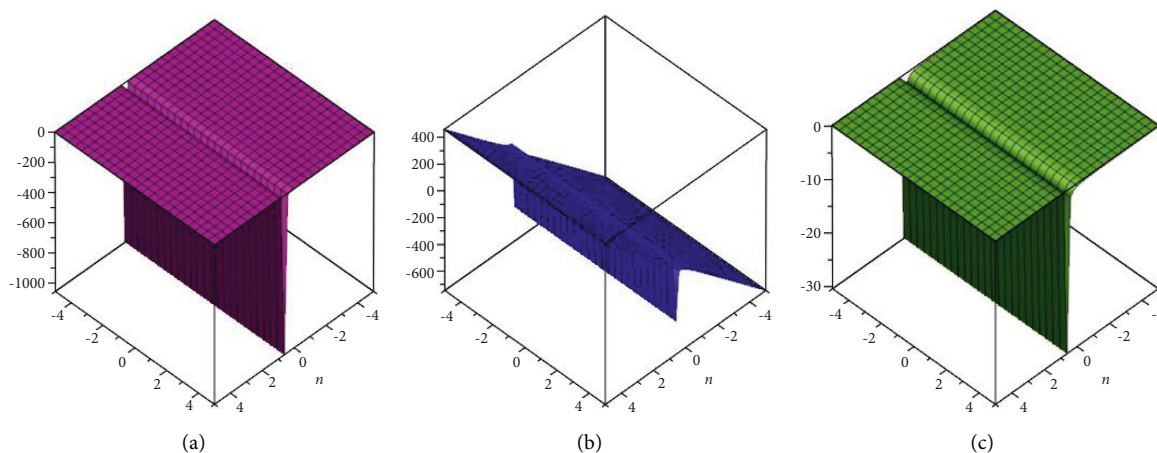FIGURE 2: 3D graphical representations for Theorem 1.

FIGURE 3: 3D plots for $VAR(\Gamma)$, $IR1(\Gamma)$, $IR2(\Gamma)$ in Theorem 5.

TABLE 3: Numerical comparison for Theorem 3.

n	$ABC(\Gamma)$	$GA(\Gamma)$	$B_1(\Gamma)$	$B_2(\Gamma)$	$HB_1(\Gamma)$	$HB_2(\Gamma)$	$MB_1(\Gamma)$	$MB_2(\Gamma)$	$H_b(\Gamma)$
1	4.2426	6	48	48	192	192	3	3	6
2	87.698	128.52	1626	2592	10566	28440	42.657	30.167	85.314
3	279.15	413.03	5472	9024	36816	103344	128.60	84.333	257.20
4	578.61	859.55	11586	19344	78942	224904	260.83	165.50	521.66
5	986.06	1468.1	19968	33552	136944	393120	439.34	273.67	878.69

TABLE 4: Numerical comparison for Theorem 4.

n	$ENT_{M_1}(\Gamma)$	$ENT_{M_2}(\Gamma)$	$ENT_{M_2^m}(\Gamma)$	$ENT_{RM_2}(\Gamma)$	$ENT_{HM}(\Gamma)$	$ENT_A(\Gamma)$
1	1.792	1.792	1.792	1.792	1.792	1.792
2	4.851	4.826	4.807	4.780	4.828	6.266
3	6.020	6.006	5.988	5.980	6.007	7.651
4	6.754	6.744	6.729	6.726	6.746	8.468
5	7.290	7.282	7.270	7.269	7.283	9.047

TABLE 5: Numerical comparison for Theorem 4.

n	$ENT_{ABC}(\Gamma)$	$ENT_{GA}(\Gamma)$	$ENT_{SDD}(\Gamma)$	$ENT_R(\Gamma)$	$ENT_F(\Gamma)$	$ENT_\chi(\Gamma)$
1	1.792	1.792	1.792	1.792	1.792	1.792
2	4.859	4.860	4.859	5.181	4.829	1.769
3	6.026	6.026	6.026	6.437	6.008	2.617
4	6.758	6.758	6.758	7.209	6.746	3.230
5	7.293	7.293	7.293	7.766	7.284	3.703

thermodynamics, such as melting and boiling points and vapour enthalpies, as well as resistance and toxicity [39, 40].

Theorem 5. *If Γ is the superphenalene, then the VDB irregularity indices are derived as*

(1) $VAR(\Gamma) = (36n^3 - 91n^2 + 76n - 21/(9n^2 - 12n + 4)^2)$

(2) $IR1(\Gamma) = (30(36n^3 - 91n^2 + 76n - 21)/9n^2 - 12n + 4)$

(3) $IR2(\Gamma) = (9\sqrt{243n^2 - 404n + 169/27n^2 - 40n + 15} - n^2 - 12\sqrt{243n^2 - 404n + 169/27n^2 - 40n + 15}\, n - 27n^2 + 4\sqrt{243n^2 - 404n + 169/27n^2 - 40n + 15} + 40n - 15)/(9n^2 - 12n + 4)$

(4) $IRDIF(\Gamma) = 1/3 \cdot (24n - 24),$

(5) $AL(\Gamma) = 24n - 24$

(6) $IRL(\Gamma) = 0.40545 \cdot (24n - 24)$

(7) $IRLU(\Gamma) = 1/2 \cdot (24n - 24)$

(8) $IRLF(\Gamma) = 1/\sqrt{6} \cdot (24n - 24)$

(9) $IRF(\Gamma) = 24n - 24$

(10) $IRLA(\Gamma) = 2/5 \cdot (24n - 24)$

(11) $IRA(\Gamma) = 0.16832 \cdot (24n - 24)$

(12) $IRB(\Gamma) = 0.10106 \cdot (24n - 24)$

Proof. Let $\Gamma = SP(n)$ be the molecular graph of a superphenalene, then $V(\Gamma) = 54n^2 - 72n + 24$ and

$E(\Gamma) = 81n^2 - 120n + 45$. The above results are generated using the partition Table 1 and the definitions of VDB irregularity-based indices. □

8. 3D Graphical Comparisons and Numerical Analysis

In Theorem 1, Theorem 3, Theorem 4, and Theorem 5, the mathematical expressions of VDB multiplicative TIs and VDB irregularity indices are derived using the edge partition approach and the M-polynomial. A few of these indices have been selected, and their values are plotted against the parameters that define the structural topology of a molecule. The 3D graphical plots of the selected indices will help the reader identify and understand the relationship between the indices of a substance and its molecular structure underneath. The graphs also help in identifying the differences and similarities in the behavioural tendencies of the indices. It is depicted in Figures 2 and 3.

In this section, the magnitudes of the VDB and its related indices are determined using the mathematical expressions of $SP(n)$, by altering the values of the variables n from 1 to 9. These numerical values are listed in Tables 3–5. The results corroborate the dependency between the structural topology of a molecule and the expressions of the corresponding VDB Tis. It is also evident from the numerical values that while some indices show a similar change in magnitude with respect to the varying structural variable, some other indices exhibit vastly different behaviours. The numerical results
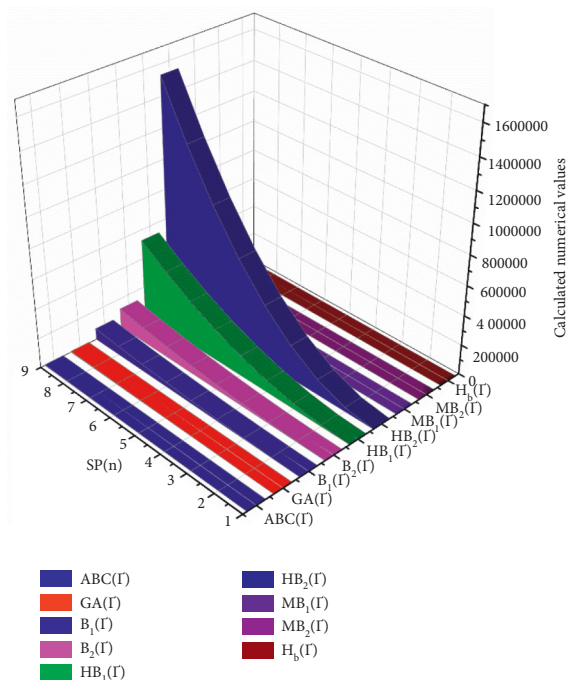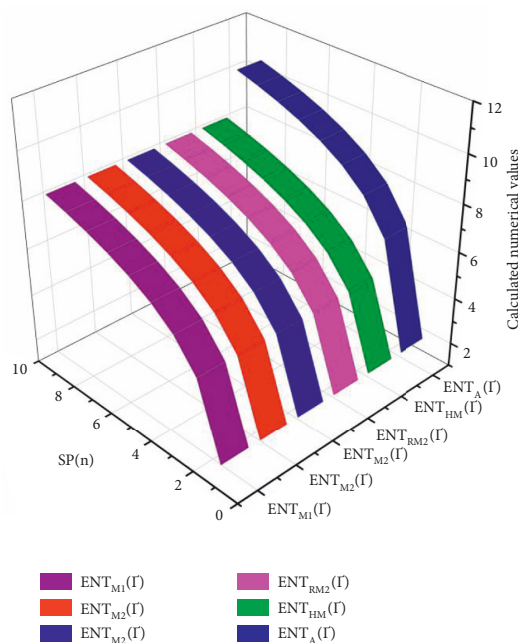
FIGURE 4: 3D visualisation of Table 3.

FIGURE 5: 3D visualisation of Table 4.

enable theoretical chemists to analyse these patterns for the design and synthesis of new compounds. It is represented graphically in Figures 4–6.
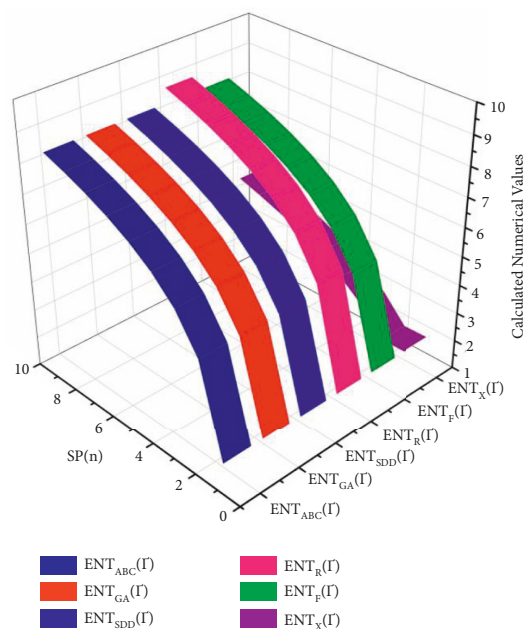

FIGURE 6: 3D visualisation of Table 5.

9. Conclusion

In this article, VDB multiplicative TIs, M-Polynomial and the corresponding VDB indices, VDB irregularity indices, and VDB entropy measures have been computed for superphenalene. The approach of studying superphenalene using four kinds of VDB indices has never been attempted before. Hence, the obtained results are unique and significant, as they offer an easy and convenient approach to studying the compound theoretically. Furthermore, the 3D visualisations of the computed expressions provide a visual understanding of the relation between the VDb TIs and the underlying molecular topology. This structure can also be explored using eccentricity-based indices, as the eccentricity TIs have not been computed for these structures before. This is a potential open problem for future research.

Data Availability

No data were used to support this study.

Conflicts of Interest

The authors declare no conflicts of interest.

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