Arabian Journal of Chemistry (2022) **15**, 104054

King Saud University

Arabian Journal of Chemistry

www.ksu.edu.sa
www.sciencedirect.com

ORIGINAL ARTICLE

On valency based topological properties of the starphene $St[n, m, l]$ and fenestrene $F[n, m]$

Peng Xu [a,b], Abdul Rauf [c,*], Muhammad Naeem [d], Adnan Aslam [e], Hafiz Muhammad Mueez Amin [f], Qammar Rubbab [g]

[a] *School of Computer Science of Information Technology, Qiannan Normal University for Nationalities, Duyun 558000, China*
[b] *Institute of Computational Science and Technology, Guangzhou University, Guangzhou, China*
[c] *Department of Mathematics, Air University Multan Campus, Multan, Pakistan*
[d] *Department of Mathematics, TIMES Institute, Multan, Pakistan*
[e] *Department of Computer Science, TIMES Institute, Multan, Pakistan*
[f] *University of Engineering and Technology, Lahore, Pakistan (RCET), Pakistan*
[g] *Department of Mathematics, Woman University Multan, Pakistan*

Received 28 March 2022; accepted 14 June 2022
Available online 18 June 2022

KEYWORDS

Valency based topological indices;
Starphene and fenestrene structures;
Algorithm for calculating valency based topological indices

Abstract In theoretical chemistry the quantitative parameters which are used to describe the atomic topology of graphs are termed as topological indices. Through these topological indices many physical and chemical characteristics such as melting point, entropy, energy generation and vaporisation enthalpy of chemical compounds can be predicted. The theory of graphs has a significant use in measuring the relationship of certain associated graphs with various topological indices. In this paper, we compute novel topological indices based on eV- and ve-degrees for starphene $St[n, m, l]$ and fenestrene $F[n, m]$. A Maple-based algorithm is proposed for the calculation of ve and eV-degree based topological indices from the graph adjacency matrix.

1. Introduction

Chemical graph theory is a branch of mathematical chemistry that applies graph theory to mathematical modeling of chemical phenomena. The topological index is a graph invariant that describes the molecular structure's topology and transforms it to a real number that predicts certain of its physico-chemical characteristics such as freezing point, infrared spectrum, boiling point, viscosity, melting point, electronic parameters, and density (Zhong et al., 2021; Süleyman, 2017; Rauf et al., 2021). The reader may access to some of the previously

* Corresponding author.
E-mail addresses: gdxupeng@gzhu.edu.cn (P. Xu), attari_ab092@yahoo.com (A. Rauf).
Peer review under responsibility of King Saud University.

Production and hosting by Elsevier

https://doi.org/10.1016/j.arabjc.2022.104054

published works on topological indices (Rauf et al., 2022; Sarkar et al., 2018; Sarkar and Pal, 2020; Naeem and Rauf, 2021; Rauf et al., 2021).

Starphene is a single ring of benzene that was surrounded by three identical substituents of arene (Rüdiger et al., 2019). The derivatives of benzene are manufactured on large scale for use in high-quality octane gasoline and production of polymer. Ortho-bromotetracene and ortho-dibromopentacene are suitable and undergoes the trimerization of Ni-catalyzed for the formation of starphene. The red starphene is made up of three hexacenes, with one centre ring shared with the orange star. Decastarphene-(3,3,3) is the largest unsubstituted derivatives of starphene which is formulated in 1968 by Clar and Mullen (1968). It is very complicated to prove that this is a complete aromatic conjugation that does not exist in starphene substituent. Starphene is an attractive compound due to its physicochemical properties. They inherited their character from arenes, which make them an interesting compound for the study of organic electronics and optics. It makes it very challenging for the synthesis of larger starphene due to their instability (Holec et al., 2021). The general fenestrenes uses the following formulas:

$$L\left(\left[\underbrace{2,\ldots,2}_{\frac{m-1}{2}-2},n,\underbrace{2,2,\ldots,2}_{m-1},n,\underbrace{2,\ldots,2}_{\frac{m-1}{2}-2}\right]\right).$$

This is the ZZ polynomial of fenestrenes. This formula is helpful to find the alternative formula for the ZZ polynomial of fenestrenes $F(n,m)$. The structure of fenestrenes contains zigzag chains that forms four disconnected parts (Chou and Witek, 2015). Generally, fenestrenes are used for the testing of pro-apoptotic activities on the two human cancer cell line (THP-1 and SW620) (Hulot et al., 2010).

Let $G=(V,E)$ be a simple graph, where $V=V(G)$ is a non-empty set of elements referred to as vertices or points and $E=E(G)$ is a set of unordered pairings of different members of $V(G)$ referred to as edges or lines. The sets $V(G)$ and $E(G)$ are referred to as the vertex set and edge set respectively. The degree of a vertex $v\in V(G)$, represented by the symbol d_v, is the number of edges that are incident to v. Two vertices u and v of G are adjacent if they are connected by an edge $e=uv$. The open neighbourhood of v is defined as the collection of vertices that are connected to u and is represented by the symbol $N(u)$. The closed neighbourhood of u denoted by $N[u]$ is obtained by adding the vertex u to $N(u)$.

Topological indices (TI) plays an important role in explaining and quantifying the molecular structure of hydrocarbons. The first topological index was defined by Wiener (1947) while he was working on the boiling point of paraffin. Randic index was introduced by Randic (1975) and for any graph G, it is defined as

$$R_{\frac{-1}{2}}(G)=\sum_{uv\in E}\frac{1}{\sqrt{d_v d_u}}.$$

Gutman and Trinajstic (1972) proposed the first and second Zagreb index in 1972 and applied them to the branching problem (Gutman et al., 1975). The first and second Zagreb indices are defined as

$$M_1(G)=\sum_{uv\in E(G)}(d_v+d_u)$$

$$M_2(G)=\sum_{uv\in E(G)}(d_v\times d_u).$$

The sum connectivity index was proposed by Zhou and Trinajstic (2009). It is denoted and defined as:

$$SCI(G)=\sum_{xy\in E}\frac{1}{\sqrt{d_v+d_u}}.$$

Zhong (2012) proposed the harmonic index which is defined as follows:

$$H(G)=\sum_{uv\in E}\left(\frac{2}{d_v+d_u}\right).$$

Estrada et al. (1998) introduced the notion of Atom Bond Connectivity (ABC) index which is defined as

$$ABC(G)=\sum_{uv\in E}\sqrt{\frac{d_v+d_u-2}{d_v d_u}}.$$

Graovac and Pisanski (1991) proposed Geometric Arithmetic (GA) index which is defined as

$$GA(G)=\sum_{uv\in E}\frac{2\sqrt{d_v d_u}}{d_v+d_u}.$$

For more details on the study and computation of topological indices, the reader may refer to (Aslam et al., 2018; Aslam et al., 2017; Bashir et al., 2017; Chu et al., 2021).

Recently, two variants of degree based topological indices were proposed by Randic (1975). These indices are based on ve-degree and eV degree. Some mathematical properties of these indices were discussed by Bollobs and Erdos (1998). Ediz (Amic et al., 1998; Graovac and Pisanski, 1991; Estrada et al., 1998) translated the classical degree based topological indices into eV-degree and ve-degree based topological indices. It was observed that ve-degree based zagreb index has strong predictability power than the classical Zagreb index. The eV-degree of any edge $uv=e\in E(G)$ is the total number of the vertices of closed neighbourhoods of the end vertices of an edge e. The eV degree of an edge e is denoted by $\Psi_{ev}(e)$. The ve-degree of any vertex $v\in V(G)$ is the total number of different edges which are adjacent to v and the first neighbor of v, and is denoted by $\Psi_{ve}(v)$. The Mathematical formulas for some of the eV-degree and ve-degree based indices are presented in Table 1.

2. Structure of starphene $St[n,m,l]$

In this section, we discuss a class of benzenoid system named starphene. Starphene is colorless and its melting point is 198°C. If three hexagons are attached by a common vertex, the benzenoid structure is called peri-condensed, otherwise, we say catacondensed. We denote the structure of starphene by $St[n,m,l]$, where m,n,l denotes the number of hexagons

Table 1 Ev-degrees and ve-degree based indices.

Ev-degree based topological indices	Notation	Mathematical Formula
Randić index	$\mathbb{R}^{ev}$	$\sum_{e\in E}\Psi_{ev}(e)^{-\frac{1}{2}}$
Zagreb index	$\mathbb{M}^{ev}$	$\sum_{e\in E}\Psi_{ev}(e)^2$
Ve-degree based topological indices	**Notation**	**Mathematical Formula**
First Zagreb β-index	$\mathbb{M}_1^{\beta ve}$	$\sum_{uv\in E}[\Psi_{ve}(u)+\Psi_{ve}(v)]$
Second Zagreb β-index	$\mathbb{M}_2^{\beta ve}$	$\sum_{uv\in E}[\Psi_{ve}(u)\times\Psi_{ve}(v)]$
Harmonic index	H^{ve}	$\sum_{uv\in E}\frac{2}{\Psi_{ve}(u)+\Psi_{ve}(v)}$
Sum Connectivity index	χ^{ve}	$\sum_{uv\in E}[\Psi_{ve}(u)+\Psi_{ve}(v)]^{-\frac{1}{2}}$
Geometric Arithmetic index	GA^{ve}	$\sum_{uv\in E}\frac{2\sqrt{\Psi_{ve}(u)\times\Psi_{ve}(v)}}{(\Psi_{ve}(u)+\Psi_{ve}(v))}$
Atom Bond Connectivity index	ABC^{ve}	$\sum_{uv\in E}\sqrt{\frac{\Psi_{ve}(u)+\Psi_{ve}(v)-2}{(\Psi_{ve}(u)\times\Psi_{ve}(v))}}$
Randić index	R^{ve}	$\sum_{uv\in E}[\Psi_{ve}(u)\times\Psi_{ve}(v)]^{-\frac{1}{2}}$
First Zagreb α-index	$M_1^{\alpha ve}$	$\sum_{v\in V}\Psi_{ve}(v)^2$

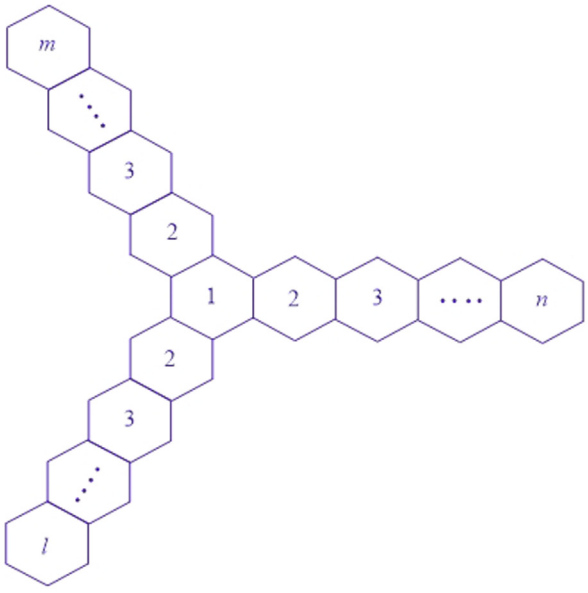


Fig. 1 Structure of starphene $St[n,m,l]$.

in each linear chain attached with the central hexagon respectively. The molecular structure of starphene is depicted in Fig. 1. The structure of $St[n,m,l]$ has total number of $2(2m+2n+2l-3)$ vertices and $5m+5n+5l-9$ edges. Let V_i denotes the vertex set of $St[n,m,l]$ containing the vertices of degree i. Then the vertex set $V(St[n,m,l])$ can be partitioned into two sets V_2 and V_3 with $|V_2| = 2m+2n+2l$ and $|V_3| = 2m+2n+2l-6$. Let $\varepsilon_{(i,\ j)}$ denotes the edge set containing the edges of $St[n,m,l]$ having degree of end vertices as i and j. The edge set of $St[n,m,l]$ can be partitioned as follows: $\varepsilon_{(2,\ 2)}$ containing 9 edge, $\varepsilon_{(2,\ 3)}$ containing $2(2m+2n+2l-9)$ edges and $\varepsilon_{(3,\ 3)}$ containing $m+n+l$ edges.

2.1. Main results

Theorem 1. *Let H denoted the graph of starphene $St[n,m,l]$. Let $m,n,l \geqslant 3$, then eV-degree Zagreb and Randic index are*

(a) $\mathrm{M}^{ev}(H) = 136m+136n+136l-306.$

(b) $\mathrm{R}^{ev}(H) = \left(\frac{4}{\sqrt{5}}+\frac{1}{\sqrt{6}}\right)m + \left(\frac{4}{\sqrt{5}}+\frac{1}{\sqrt{6}}\right)n + \left(\frac{4}{\sqrt{5}}+\frac{1}{\sqrt{6}}\right)l + \left(\frac{9}{2}-\frac{18}{\sqrt{5}}\right).$

Proof 1. By using the edge partition given in Table 2, we can compute the eV-degree Zagreb and Randić index as follows

Table 2 Edges partition for eV-degree of $St[n,m,l]$.

$(\Psi(u),\Psi(v))$	$\Psi_{ev}(e)$	Frequency
$\varepsilon_{(2,\ 2)}$	4	9
$\varepsilon_{(2,\ 3)}$	5	$2(2m+2n+2l-9)$
$\varepsilon_{(3,\ 3)}$	6	$m+n+l$

(a) Ev-degree Zagreb index

$$\mathrm{M}^{ev}(H) = \sum_{e\in E(H)} \Psi_{ev}(e)^2,$$

$$\mathrm{M}^{ev}(H) = (4)^2|\varepsilon_{(2,2)}| + (5)^2|\varepsilon_{(2,3)}| + (6)^2|\varepsilon_{(3,3)}|$$

$$= 136m+136n+136l-306.$$

(b) Ev-degree Randić index

$$\mathrm{R}^{ev}(H) = \sum_{e\in E(H)} \Psi_{ev}(e)^{-\frac{1}{2}},$$

$$\mathrm{R}^{ev}(H) = (4)^{-\frac{1}{2}}|\varepsilon_{(4,2)}| + (5)^{-\frac{1}{2}}|\varepsilon_{(2,3)}| + (6)^{-\frac{1}{2}}|\varepsilon_{(3,3)}|$$

$$= \left(\frac{4}{\sqrt{5}}+\frac{1}{\sqrt{6}}\right)m + \left(\frac{4}{\sqrt{5}}+\frac{1}{\sqrt{6}}\right)n + \left(\frac{4}{\sqrt{5}}+\frac{1}{\sqrt{6}}\right)l + \left(\frac{9}{2}-\frac{18}{\sqrt{5}}\right).$$

Fig. 2 and Numerical computation depicted in Table 5 and 6 shows an increasing behavior of eV-degree based indices with the increase in the value of n,m and l. Zhong et al. (2021) developed the quantitative structure–property relationship (QSPR) between physical properties (Docking Score, Binding Affinity, Molecular Weight and Topological Polar Surface) and ve- and eV-degree based topological indices. They examined that among eV-degree based indices, the first eV-degree Zagreb index (M^{ev}) predict the molecular weight better than eV-degree Randic index (R^{ev}). Hence, the above results of eV-degree based indices are helpful to measure the physical properties of starphene.

Theorem 2. *Let H be a structure of starphene, then*

$$\mathrm{M}_1^{\alpha ve}(H) = 170m+170n+170l-390$$

Proof 2. The partition of vertex set of starphene based on ve degree of each vertex is depicted in Table 3. By using Table 3, we have first ve-degree Zagreb α-index

$$\mathrm{M}_1^{\alpha ve}(H) = \sum_{v\in V(H)} \Psi_{ve}(v)^2,$$

$$\mathrm{M}_1^{\alpha ve}(H) = (4)^2(6) + (5)^2(6) + (6)^2(2m+2n+2l-12)$$

$$+ (7)^2(2m+2n+2l-12) + (8)^2(6)$$

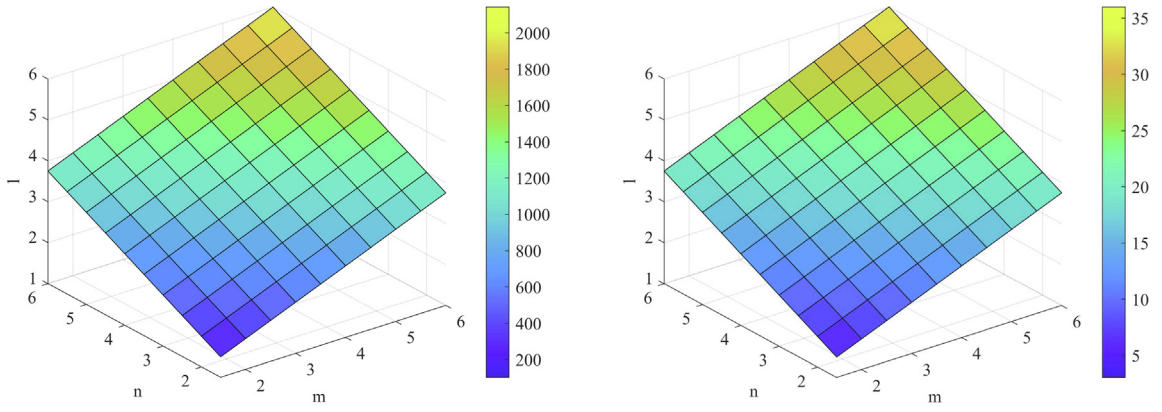
$$= 170m+170n+170l-390.$$

Fig. 3 shows an increasing behavior of first Zagreb alpha index ($M_1^{\alpha ve}$) with an increase in the values of n,m and l. Süleyman (2017) developed QSPR between physical properties (Enthalpy of vaporization (HVAP), Entropy, Standard enthalpy of vaporization (DHVAP), and Acentric factor) and ve and eV-degree based Zagreb and Randic type indices (Süleyman, 2017). He examines that $M_1^{\alpha ve}$ can be helpful to predict the physical property Acentric Factor. Zhong et al. (2021) analyzed that $M_1^{\alpha ve}$ can predict the molecular weight better than eV-degree Randic index (R^{ev}). Hence, the above result of ve-degree based index can be helpful to estimate the physical properties of starphene.

Theorem 3. *Let H be a structure of starphene $St[n,m,l]$ structure and $m,n,l \geqslant 3$, then*

(a) $\mathrm{M}_1^{\beta ve}(H) = 66m+66n+66l-144.$

(b) $\mathrm{M}_2^{\beta ve}(H) = 217m+217n+217l-504.$



(a) (b)

Fig. 2 Plots of the indices (a) M^{ev} and (b) R^{ev}.

Table 3 Vertices partition for ve-degrees of $St[n, m, l]$.

Ψ(u)	Ψ_{ve}(u)	Frequency
2	4	6
2	5	6
2	6	$2m + 2n + 2l - 12$
3	7	$2m + 2n + 2l - 12$
3	8	6

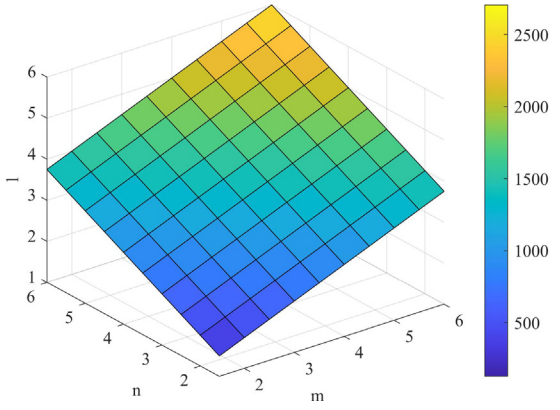


Fig. 3 Plot of $\mathsf{M}_1^{\chi ve}$.

(c) $\mathsf{ABC}^{ve}(H) = \left(\frac{4\sqrt{11}}{\sqrt{42}} + \frac{\sqrt{12}}{7}\right)m + \left(\frac{4\sqrt{11}}{\sqrt{42}} + \frac{\sqrt{12}}{7}\right)n + \left(\frac{4\sqrt{11}}{\sqrt{42}} + \frac{\sqrt{12}}{7}\right)l + \left(\frac{3\sqrt{6}}{4} + \frac{6\sqrt{7}}{\sqrt{20}} + \frac{6\sqrt{10}}{\sqrt{35}} - \frac{30\sqrt{11}}{\sqrt{42}} - \frac{6\sqrt{12}}{7} + \frac{3\sqrt{14}}{4} + 3\right).$

(d) $\mathsf{GA}^{ve}(H) = \left(\frac{8\sqrt{42}}{13} + 1\right)m + \left(\frac{8\sqrt{42}}{13} + 1\right)n + \left(\frac{8\sqrt{42}}{13} + 1\right)l + \left(\frac{8\sqrt{5}}{3} - \frac{60\sqrt{42}}{13} + \frac{24\sqrt{3}}{7} + \sqrt{35} + 3\right).$

(e) $\mathsf{H}^{ve}(H) = \frac{414}{546}m + \frac{414}{546}n + \frac{414}{546}l - \frac{427}{546}.$

(f) $\chi^{ve}(H) = \left(\frac{4}{\sqrt{13}} + \frac{1}{\sqrt{14}}\right)m + \left(\frac{4}{\sqrt{13}} + \frac{1}{\sqrt{14}}\right)n + \left(\frac{4}{\sqrt{13}} + \frac{1}{\sqrt{14}}\right)l + \left(\frac{3}{\sqrt{8}} + \frac{6}{\sqrt{12}} - \frac{30}{\sqrt{13}} + \frac{7}{2}\right).$

(g) $\mathsf{R}^{ve}(H) = \left(\frac{4}{\sqrt{42}} + \frac{1}{7}\right)m + \left(\frac{4}{\sqrt{42}} + \frac{1}{7}\right)n + \left(\frac{4}{\sqrt{42}} + \frac{1}{7}\right)l + \left(\frac{9}{14} + \frac{6}{\sqrt{20}} + \frac{6}{\sqrt{35}} - \frac{30}{\sqrt{42}} + \frac{6}{\sqrt{48}}\right).$

Proof 3. By using the edge partition given in Table 4, we can compute the topological indices based on the ve degree of end vertices of each edge as follows

(a) First Zagreb β-index

$$\mathsf{M}_1^{\beta ve}(H) = \sum_{uv \in E(H)} (\Psi_{ve}(u) + \Psi_{ve}(v)),$$

$$\mathsf{M}_1^{\beta ve}(H) = (8)|E_1^*| + (9)|E_2^*| + (12)|E_3^*| + (13)|E_4^*| + (14)|E_5^*| + (14)|E_6^*| + (16)|E_7^*| = 66m + 66n + 66l - 144.$$

(b) Second Zagreb β-index

$$\mathsf{M}_2^{\beta ve}(H) = \sum_{uv \in E(H)} (\Psi_{ve}(u) \times \Psi_{ve}(v)),$$

$$\mathsf{M}_2^{\beta ve}(H) = (16)|E_1^*| + (20)|E_2^*| + (35)|E_3^*| + (42)|E_4^*| + (48)|E_5^*| + (49)|E_6^*| + (64)|E_7^*| = 217m + 217n + 217l - 504.$$

(c) Atom-bond connectivity index

$$\mathsf{ABC}^{ve}(H) = \sum_{uv \in E(H)} \sqrt{\frac{\Psi_{ve}(u) + \Psi_{ve}(v) - 2}{(\Psi_{ve}(u) \times \Psi_{ve}(v))}},$$

$$\mathsf{ABC}^{ve}(H) = \left(\sqrt{\frac{6}{16}}\right)|E_1^*| + \left(\sqrt{\frac{7}{20}}\right)|E_2^*| + \left(\sqrt{\frac{10}{35}}\right)|E_3^*| + \left(\sqrt{\frac{11}{42}}\right)|E_4^*| + \left(\sqrt{\frac{12}{48}}\right)|E_5^*| + \left(\sqrt{\frac{12}{49}}\right)|E_6^*| + \left(\sqrt{\frac{14}{64}}\right)|E_7^*| = \left(\frac{4\sqrt{11}}{\sqrt{42}} + \frac{\sqrt{12}}{7}\right)(m + n + l) + \left(\frac{3\sqrt{6}}{4} + \frac{6\sqrt{7}}{\sqrt{20}} + \frac{6\sqrt{10}}{\sqrt{35}} - \frac{30\sqrt{11}}{\sqrt{42}} - \frac{6\sqrt{12}}{7} + \frac{3\sqrt{14}}{4} + 3\right).$$

Table 4 Edges Partition based on ve-degree of end vertices of each edge of $St[n,m,l]$.

Edge	$(\Psi_{ve}(u), \Psi_{ve}(v))$	Frequency
E_1^*	(4, 4)	3
E_2^*	(4, 5)	6
E_3^*	(5, 7)	6
E_4^*	(6, 7)	$2(2m+2n+2l-15)$
E_5^*	(6, 8)	6
E_6^*	(7, 7)	$m+n+l-6$
E_7^*	(8, 8)	6

(d) Geometric-arithmetic index

$$GA^{ve}(H) = \sum_{uv\in E(H)} \frac{2\sqrt{\Psi_{ve}(u)\times\Psi_{ve}(v)}}{(\Psi_{ve}(u)+\Psi_{ve}(v))},$$

$$\begin{aligned} GA^{ve}(H) &= \left(\tfrac{2\sqrt{16}}{8}\right)|E_1^*| + \left(\tfrac{2\sqrt{20}}{9}\right)|E_2^*| + \left(\tfrac{2\sqrt{35}}{12}\right)|E_3^*| \\ &\quad + \left(\tfrac{2\sqrt{42}}{13}\right)|E_4^*| + \left(\tfrac{2\sqrt{48}}{14}\right)|E_5^*| \\ &\quad + \left(\tfrac{2\sqrt{49}}{14}\right)|E_6^*| + \left(\tfrac{2\sqrt{64}}{16}\right)|E_7^*| \\ &= \left(\tfrac{8\sqrt{42}}{13}+1\right)m + \left(\tfrac{8\sqrt{42}}{13}+1\right)n + \left(\tfrac{8\sqrt{42}}{13}+1\right)l \\ &\quad + \left(\tfrac{8\sqrt{5}}{3} - \tfrac{60\sqrt{42}}{13} + \tfrac{24\sqrt{3}}{7} + \sqrt{35} + 3\right). \end{aligned}$$

(e) Harmonic index

$$H^{ve}(H) = \sum_{uv\in E(H)} \frac{2}{\Psi_{ve}(u)+\Psi_{ve}(v)},$$

$$\begin{aligned} H^{ve}(H) &= \left(\frac{2}{8}\right)|E_1^*| + \left(\frac{2}{9}\right)|E_2^*| + \left(\frac{2}{12}\right)|E_3^*| \\ &\quad + \left(\frac{2}{13}\right)|E_4^*| + \left(\frac{2}{14}\right)|E_5^*| + \left(\frac{2}{14}\right)|E_6^*| + \left(\frac{2}{16}\right)|E_7^*| \\ &= \frac{414}{546}m + \frac{414}{546}n + \frac{414}{546}l - \frac{427}{546}. \end{aligned}$$

(f) Sum-connectivity index

$$\chi^{ve}(H) = \sum_{uv\in E(H)} (\Psi_{ve}(u)+\Psi_{ve}(v))^{-\frac{1}{2}},$$

$$\begin{aligned} \chi^{ve}(H) &= (8)^{-\frac{1}{2}}|E_1^*| + (9)^{-\frac{1}{2}}|E_2^*| + (12)^{-\frac{1}{2}}|E_3^*| + (13)^{-\frac{1}{2}}|E_4^*| \\ &\quad + (14)^{-\frac{1}{2}}|E_5^*| + (14)^{-\frac{1}{2}}|E_6^*| + (16)^{-\frac{1}{2}}|E_7^*| \\ &= \left(\tfrac{4}{\sqrt{13}} + \tfrac{1}{\sqrt{14}}\right)m + \left(\tfrac{4}{\sqrt{13}} + \tfrac{1}{\sqrt{14}}\right)n + \left(\tfrac{4}{\sqrt{13}} + \tfrac{1}{\sqrt{14}}\right)l \\ &\quad + \left(\tfrac{3}{\sqrt{8}} + \tfrac{6}{\sqrt{12}} - \tfrac{30}{\sqrt{13}} + \tfrac{7}{2}\right). \end{aligned}$$

(g) Randic index

$$R^{ve}(H) = \sum_{uv\in E(H)} (\Psi_{ve}(u)\times\Psi_{ve}(v))^{-\frac{1}{2}},$$

$$\begin{aligned} R^{ve}(H) &= (16)^{-\frac{1}{2}}|E_1^*| + (20)^{-\frac{1}{2}}|E_2^*| + (35)^{-\frac{1}{2}}|E_3^*| \\ &\quad + (42)^{-\frac{1}{2}}|E_4^*| + (48)^{-\frac{1}{2}}|E_5^*| \\ &\quad + (49)^{-\frac{1}{2}}|E_6^*| + (64)^{-\frac{1}{2}}|E_7^*| \\ &= \left(\tfrac{4}{\sqrt{42}} + \tfrac{1}{7}\right)m + \left(\tfrac{4}{\sqrt{42}} + \tfrac{1}{7}\right)n \\ &\quad + \left(\tfrac{4}{\sqrt{42}} + \tfrac{1}{7}\right)l + \left(\tfrac{9}{14} + \tfrac{6}{\sqrt{20}} + \tfrac{6}{\sqrt{35}} - \tfrac{30}{\sqrt{42}} + \tfrac{6}{\sqrt{48}}\right). \end{aligned}$$

Table 5 Numerical results of topological indices for different values of $[n,m,l]$.

$[n,m,l]$	$M^{ev}(H)$	$R^{ev}(H)$	$M_1^{\alpha ve}(H)$	$M_1^{\beta ve}(H)$	$M_2^{\beta ve}(H)$
[1, 1, 1]	102	3.0415	126	54	147
[2, 2, 2]	510	9.6328	642	252	798
[3, 3, 3]	918	16.2241	1158	450	1449
[4, 4, 4]	1326	22.8154	1674	648	2100
[5, 5, 5]	1734	29.4067	2190	846	2751
[6, 6, 6]	2142	35.9980	2706	1044	3402
[7, 7, 7]	2550	42.5893	3222	1242	4053
[8, 8, 8]	2958	49.1806	3738	1440	4704
[9, 9, 9]	3366	55.7719	4254	1638	5355
[10, 10, 10]	3774	62.3632	4770	1836	6006

Figs. 4–7 shows the behavior of the computed topological indices based on ve degree. The values of all these topological indices increases with the increase in the value of m,n and l. Süleyman (2017) examines that the second Zagreb beta index can be used to predicts the entropy and the Randic index can be helpful to predicts the Enthalpy of vaporization and Standard enthalpy of vaporization. Zhong et al. (2021) investigated that the first Zagreb beta index ($M_1^{\beta ve}$) predicts the molecular weight and Topological Polar Surface better than other ve-degree based topological indices. Overall, $M_1^{\beta ve}$ is the best predictor of the molecular weight and Topological Polar Surface in all ve- and eV-degree based indices. Hence, the above results are helpful to measure the physical properties of starphene.

3. Structure of fenestrene $F[n,m]$

In this section, we discuss about the fenestrene structure which belongs to the class of benzenoid systems. Acenes are benzene rings fused linearly. We denote the structure of fenestrene by $F[n,m]$, where m and n denoted the number of hexagons in each row and column respectively. The molecular structure of fenestrene is depicted in Fig. 8. The structure of $F[n,m]$ has $8(m+n)$ vertices. For $n=1,2$ the graph of $F[n,m]$ has $6mn+7m+5n+1$ edges and for $n\geqslant 3$ it has $20m+10n-10$ edges. Let $\varepsilon_{(i,\ j)}$ denotes the edge set containing the edges of $F[n,m]$ with end vertices of degree i and j respectively. The edge set of $F[n,m]$ can be partitioned based on the degree of end vertices as follows: $\varepsilon_{(2,\ 2)}$ containing $4m+2$ edge, $\varepsilon_{(2,\ 3)}$ containing $8m+8n-12$ edges and $\varepsilon_{(3,\ 3)}$ containing $8m+2n$ edges.

3.1. Main results

Theorem 4. *Let H denotes the structure of fenestrene $F[n,m]$. Let $m\geqslant 2$ and $n\geqslant 3$, then eV-degree Zagreb and Randic index of fenestrene are*

(a) $M^{ev}(H) = 552m+272n-268.$

(b) $R^{ev}(H) = \left(\frac{8}{\sqrt{5}} + \frac{8}{\sqrt{6}} + 2\right)m + \left(\frac{8}{\sqrt{5}} + \frac{2}{\sqrt{6}}\right)n - \frac{12}{\sqrt{5}} + 1.$

Proof 4. By using the edge partition given in Table 7, we can compute the eV-degree Zagreb and Randic index as follows

(a) Ev-degree Zagreb index

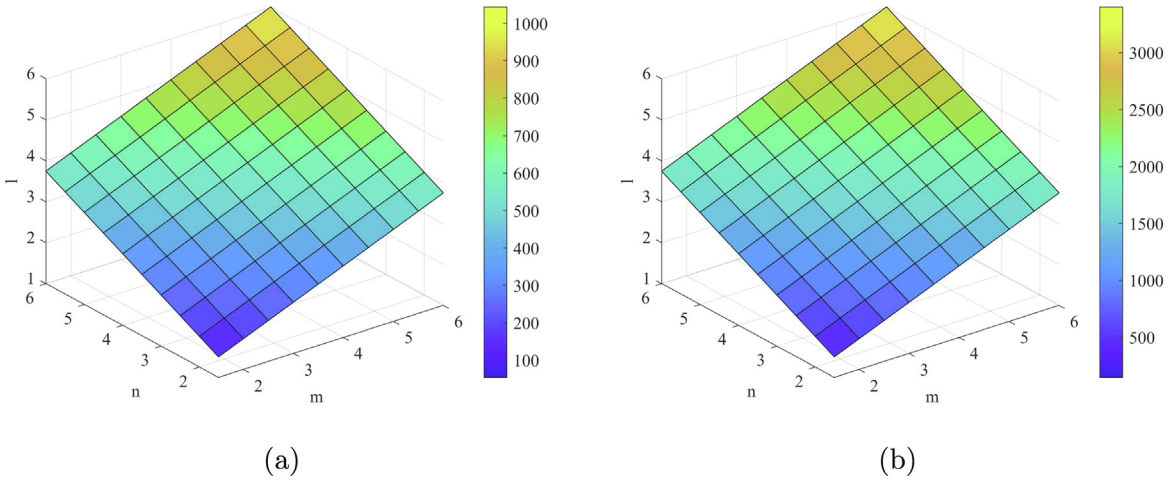


Fig. 4 plots of the indices (a) $M_1^{\beta ve}$ and (b) $M_2^{\beta ve}$.

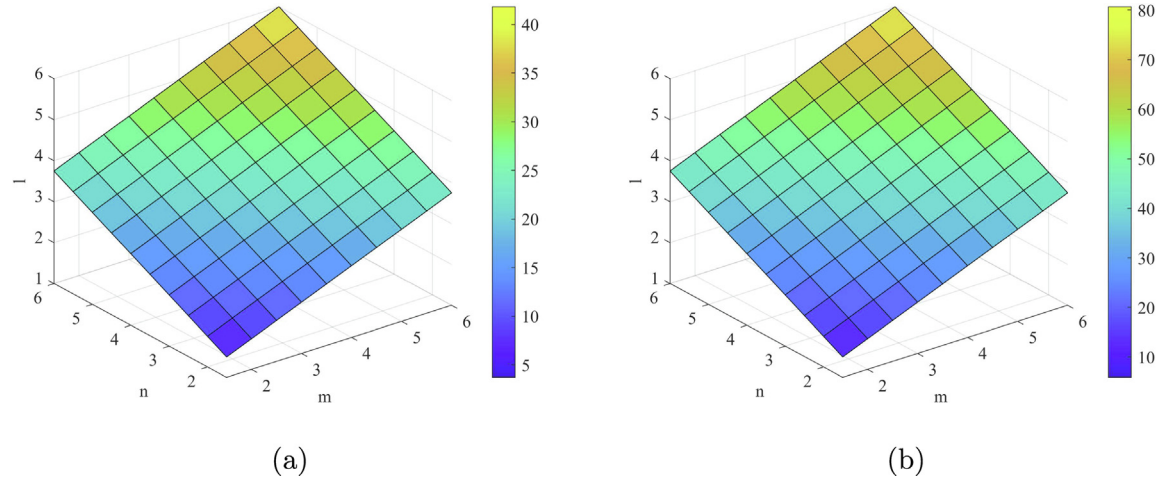


Fig. 5 plots of the indices (a) ABC^{ve} and (b) GA^{ve}.

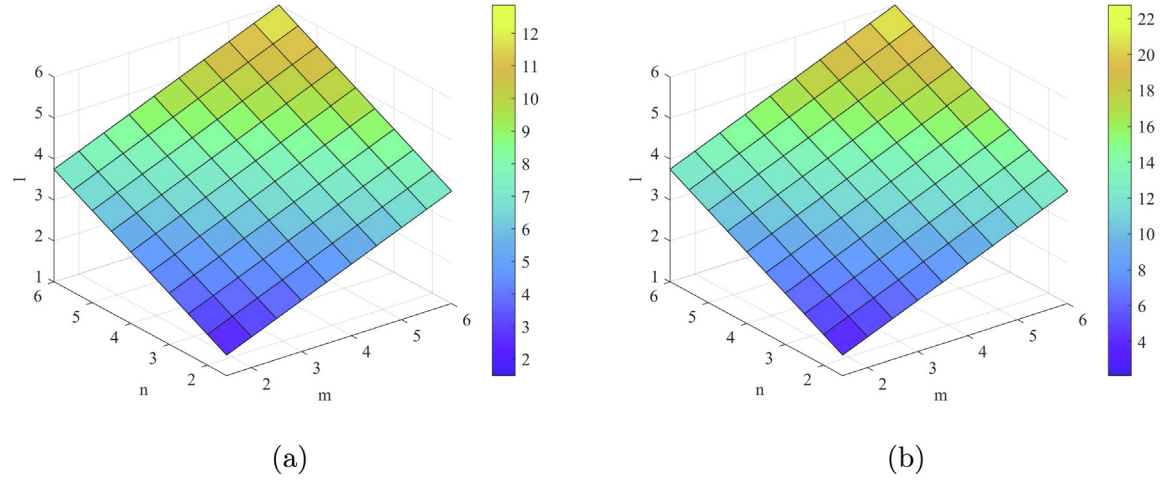


Fig. 6 Plots of the indices (a) H^{ve} and (b) χ^{ve}.

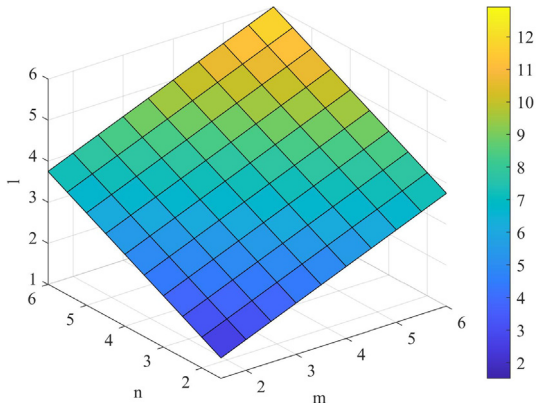


Fig. 7 Plot of the indices R^{ve}.

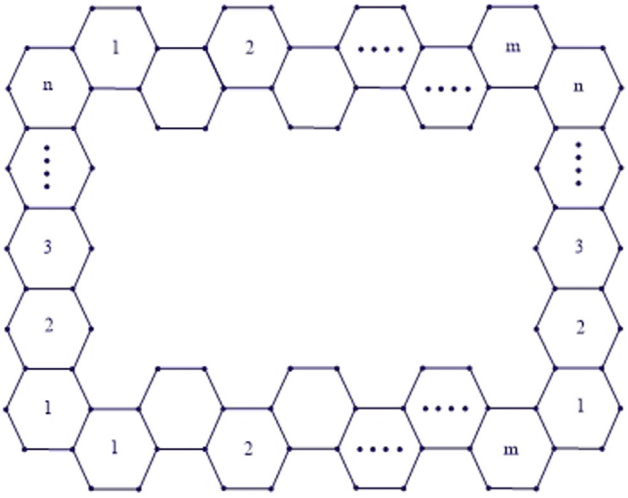


Fig. 8 Fenestrene structure $F[n,m]$.

Table 6 Numerical results of the indices for different values of $[n,m,l]$.

$[n,m,l]$	$\mathsf{ABC}^{ve}(H)$	$\mathsf{GA}^{ve}(H)$	$\mathsf{H}^{ve}(H)$	$\chi^{ve}(H)$	$\mathsf{R}^{ve}(H)$
[1, 1, 1]	3.7037	5.8707	−0.0073	2.1022	1.5158
[2, 2, 2]	11.3295	20.8352	2.2674	6.2322	3.7960
[3, 3, 3]	18.9554	35.7996	4.5421	10.3622	6.0762
[4, 4, 4]	26.5812	50.7641	6.8168	14.4921	8.3565
[5, 5, 5]	34.2070	65.7285	9.0916	18.6221	10.6367
[6, 6, 6]	41.8328	80.6929	11.3663	22.7521	12.9169
[7, 7, 7]	49.4586	95.6574	13.6410	26.8821	15.1971
[8, 8, 8]	57.0844	110.6218	15.9158	31.0121	17.4773
[9, 9, 9]	64.7102	125.5863	18.1905	35.1421	19.7575
[10, 10, 10]	72.3360	140.5507	20.4652	39.2721	22.0377

$$\mathsf{M}^{ev}(H) = \sum_{e\in E(H)} \Psi_{ev}(e)^2,$$
$$\mathsf{M}^{ev}(H) = (4)^2|\varepsilon_{(2,2)}| + (5)^2|\varepsilon_{(2,3)}| + (6)^2|\varepsilon_{(3,3)}|$$
$$= 552m + 272n - 268.$$

Table 7 Edges partitions for eV-degree of $F[n,m]$.

$(\Psi(u),\Psi(v))$	$\Psi_{ev}(e)$	Frequency
$\varepsilon_{(2,\ 2)}$	4	$4m+2$
$\varepsilon_{(2,\ 3)}$	5	$8m+8n-12$
$\varepsilon_{(3,\ 3)}$	6	$8m+2n$

(b) Ev-degree Randić index

$$\mathsf{R}^{ev}(H) = \sum_{e\in E(H)} \Psi_{ev}(e)^{-\frac{1}{2}},$$
$$\mathsf{R}^{ev}(H) = (4)^{-\frac{1}{2}}|\varepsilon_{(4,2)}| + (5)^{-\frac{1}{2}}|\varepsilon_{(2,3)}| + (6)^{-\frac{1}{2}}|\varepsilon_{(3,3)}|$$
$$= \left(\tfrac{8}{\sqrt{5}} + \tfrac{8}{\sqrt{6}} + 2\right)m + \left(\tfrac{8}{\sqrt{5}} + \tfrac{2}{\sqrt{6}}\right)n - \tfrac{12}{\sqrt{5}} + 1.$$

Theorem 5. *Let H denotes the structure of fenestrene $F[n,m]$, then*

$$\mathsf{M}_1^{\alpha ve}(H) = 712m + 340n - 316$$

Proof 5. The vertex partition of H based on ve degree is depicted in Table 8. Using the definition of the topological index we get

$$\mathsf{M}_1^{\alpha ve}(H) = \sum_{v\in V(H)} \Psi_{ve}(v)^2,$$
$$\mathsf{M}_1^{\alpha ve}(H) = (5)^2(8m+4) + (6)^2(4n-8) + (7)^2(4n-4)$$
$$+ (8)^2(8m-4) + (9)^2(4)$$
$$= 712m + 340n - 316.$$

Theorem 6. *Let H be a structure of fenestrene $F[n,m]$ structure and $m \geqslant 2$ and $n \geqslant 3$, then*

(a) $\mathsf{M}_1^{\beta ve}(H) = 272m + 134n - 134.$

(b) $\mathsf{M}_2^{\beta ve}(H) = 932m + 448n - 422.$

(c) $\mathsf{ABC}^{ve}(H) = \left(\frac{8\sqrt{2}}{5} + \frac{4\sqrt{11}}{\sqrt{10}} + \sqrt{14}\right)m + \left(\frac{8\sqrt{11}}{\sqrt{42}} + \frac{\sqrt{13}}{\sqrt{14}}\right)n +$
$\left(\frac{4\sqrt{2}}{5} + \frac{12\sqrt{2}}{\sqrt{7}}. -\frac{4\sqrt{11}}{\sqrt{10}} - \frac{20\sqrt{11}}{\sqrt{42}} - \frac{\sqrt{13}}{\sqrt{14}}c + \frac{4\sqrt{14}}{\sqrt{63}} + \frac{4\sqrt{15}}{3\sqrt{2}} - \frac{4}{5}\right).$

(d) $\mathsf{GA}^{ve}(H) = \left(\frac{32\sqrt{10}}{13} + 12\right)m + \left(\frac{16\sqrt{42}}{13} + \frac{8\sqrt{14}}{15}\right)n + \left(\frac{16\sqrt{3}}{7} -\right.$
$\left.\frac{40\sqrt{42}}{13} - \frac{32\sqrt{10}}{13}. + 2\sqrt{35} - \frac{8\sqrt{14}}{15} + \frac{3\sqrt{7}}{2} + \frac{16\sqrt{72}}{17} - 8\right).$

(e) $\mathsf{H}^{ve}(H) = \frac{197}{65}m + \frac{52}{45}n + \frac{42991}{21420}.$

Table 8 Vertex partition of $F[n,m]$ based on ve degree.

$\Psi(u)$	$\Psi_{ve}(u)$	Frequency
2	5	$8m+4$
2	6	$4n-8$
3	7	$4n-4$
3	8	$8m-4$
3	9	4

Table 9 Edges Partition based on ve-degree of end vertices of each edge of $F[n,m]$.

Edge	$(\Psi_{ve}(u), \Psi_{ve}(v))$	Frequency
E_1^*	(5, 5)	$4m+2$
E_2^*	(5, 7)	12
E_3^*	(5, 8)	$8m-8$
E_4^*	(6, 7)	$4(2n-5)$
E_5^*	(6, 8)	4
E_6^*	(7, 8)	$2n-2$
E_7^*	(7, 9)	4
E_8^*	(8, 8)	$8m-10$
E_9^*	(8, 9)	8

(f) $\chi^{ve}(H) = \left(\frac{4}{\sqrt{10}}+\frac{8}{\sqrt{13}}+2\right)m+\left(\frac{8}{\sqrt{13}}+\frac{2}{\sqrt{15}}\right)n+\left(\frac{2}{\sqrt{10}}+\frac{9}{\sqrt{3}}-\frac{8}{\sqrt{13}}-\frac{20}{\sqrt{13}}+\frac{4}{\sqrt{14}}.-\frac{2}{\sqrt{15}}-\frac{5}{2}+\frac{8}{\sqrt{17}}+1\right).$

(g) $\mathsf{R}^{ve}(H) = \left(\frac{4}{5}+\frac{5}{\sqrt{10}}+1\right)m+\left(\frac{8}{\sqrt{42}}+\frac{1}{\sqrt{14}}\right)n+(\frac{2}{5}+\frac{12}{\sqrt{35}}-\frac{4}{\sqrt{13}}-\frac{20}{\sqrt{42}}+\frac{1}{\sqrt{9}}.-\frac{1}{\sqrt{14}}+\frac{4}{3\sqrt{7}}-\frac{5}{4}+\frac{4}{3\sqrt{2}}).$

Proof 6. By using the edge partition given in Table 9, we can compute the indices based on the ve degree of end vertices of each edge as follows

(a) First Zagreb β-index

$$\mathsf{M}_1^{\beta ve}(H) = \sum_{uv\in E(H)} (\Psi_{ve}(u)+\Psi_{ve}(v)),$$

$$\begin{aligned}\mathsf{M}_1^{\beta ve}(H) &= (10)|E_1^*|+(12)|E_2^*|+(13)|E_3^*|+(13)|E_4^*|\\ &\quad+(14)|E_5^*|+(15)|E_6^*|+(16)|E_7^*|\\ &\quad+(16)|E_8^*|+(17)|E_9^*|\\ &= 272m+134n-134.\end{aligned}$$

(b) Second Zagreb β-index

$$\mathsf{M}_2^{\beta ve}(H) = \sum_{uv\in E(H)} (\Psi_{ve}(u)\times\Psi_{ve}(v)),$$

$$\begin{aligned}\mathsf{M}_2^{\beta ve}(H) &= (25)|E_1^*|+(35)|E_2^*|+(40)|E_3^*|+(42)|E_4^*|\\ &\quad+(48)|E_5^*|+(56)|E_6^*|+(63)|E_7^*|\\ &\quad+(64)|E_8^*|+(72)|E_9^*|\\ &= 932m+448n-422.\end{aligned}$$

(c) Atom-bond connectivity index

$$\mathsf{ABC}^{ve}(H) = \sum_{uv\in E(H)} \sqrt{\frac{\Psi_{ve}(u)+\Psi_{ve}(v)-2}{(\Psi_{ve}(u)\times\Psi_{ve}(v))}}, \mathsf{ABC}^{ve}(H) = \left(\sqrt{\frac{8}{25}}\right)|E_1^*|$$

$$+\left(\sqrt{\frac{10}{35}}\right)|E_2^*|+\left(\sqrt{\frac{11}{40}}\right)|E_3^*|+\left(\sqrt{\frac{11}{42}}\right)|E_4^*|+\left(\sqrt{\frac{12}{48}}\right)|E_5^*|+\left(\sqrt{\frac{13}{56}}\right)|$$

$$E_6^*|+\left(\sqrt{\frac{14}{63}}\right)|E_7^*|+\left(\sqrt{\frac{14}{64}}\right)|E_8^*|+\left(\sqrt{\frac{15}{72}}\right)|E_9^*|$$

$$=\left(\frac{8\sqrt{2}}{5}+\frac{4\sqrt{11}}{\sqrt{10}}+\sqrt{14}\right)m+\left(\frac{8\sqrt{11}}{\sqrt{42}}+\frac{\sqrt{13}}{\sqrt{14}}\right)n$$

$$+\left(\frac{4\sqrt{2}}{5}+\frac{12\sqrt{2}}{\sqrt{7}}-\frac{4\sqrt{11}}{\sqrt{10}}-\frac{20\sqrt{11}}{\sqrt{42}}-\frac{\sqrt{13}}{\sqrt{14}}+\frac{4\sqrt{14}}{\sqrt{63}}+\frac{4\sqrt{15}}{3\sqrt{2}}-\frac{4}{5}\right).$$

(d) Geometric-arithmetic index

$$\mathsf{GA}^{ve}(H) = \sum_{uv\in E(H)} \frac{2\sqrt{\Psi_{ve}(u)\times\Psi_{ve}(v)}}{(\Psi_{ve}(u)+\Psi_{ve}(v))}, \mathsf{GA}^{ve}(H) = \left(\frac{2\sqrt{25}}{10}\right)|E_1^*|$$

$$+\left(\frac{2\sqrt{35}}{12}\right)|E_2^*|+\left(\frac{2\sqrt{40}}{13}\right)|E_3^*|+\left(\frac{2\sqrt{42}}{13}\right)|E_4^*|+\left(\frac{2\sqrt{48}}{14}\right)|E_5^*|$$

$$+\left(\frac{2\sqrt{56}}{15}\right)|E_6^*|+\left(\frac{2\sqrt{63}}{16}\right)|E_7^*|+\left(\frac{2\sqrt{64}}{16}\right)|E_8^*|+\left(\frac{2\sqrt{72}}{17}\right)|E_9^*|$$

$$=\left(\frac{32\sqrt{10}}{13}+12\right)m+\left(\frac{16\sqrt{42}}{13}+\frac{8\sqrt{14}}{15}\right)n$$

$$+\left(\frac{16\sqrt{3}}{7}-\frac{40\sqrt{42}}{13}-\frac{32\sqrt{10}}{13}+2\sqrt{35}-\frac{8\sqrt{14}}{15}+\frac{3\sqrt{7}}{2}+\frac{16\sqrt{72}}{17}-8\right).$$

(e) Harmonic index

$$\mathsf{H}^{ve}(H) = \sum_{uv\in E(H)} \frac{2}{\Psi_{ve}(u)+\Psi_{ve}(v)}, \mathsf{H}^{ve}(H) = \left(\frac{2}{10}\right)|E_1^*|+\left(\frac{2}{12}\right)|E_2^*|$$

$$+\left(\frac{2}{13}\right)|E_3^*|+\left(\frac{2}{13}\right)|E_4^*|+\left(\frac{2}{14}\right)|E_5^*|+\left(\frac{2}{15}\right)|E_6^*|+\left(\frac{2}{16}\right)|E_7^*|+\left(\frac{2}{16}\right)|E_8^*|$$

$$+\left(\frac{2}{17}\right)|E_9^*| = \frac{197}{65}m+\frac{52}{45}n+\frac{42991}{21420}.$$

(f) Sum-connectivity index

$$\chi^{ve}(H) = \sum_{uv\in E(H)} (\Psi_{ve}(u)+\Psi_{ve}(v))^{-\frac{1}{2}}, \chi^{ve}(H) = (10)^{-\frac{1}{2}}|E_1^*|$$

$$+(12)^{-\frac{1}{2}}|E_2^*|+(13)^{-\frac{1}{2}}|E_3^*|+(13)^{-\frac{1}{2}}|E_4^*|+(14)^{-\frac{1}{2}}|E_5^*|+(15)^{-\frac{1}{2}}|E_6^*|$$

$$+(16)^{-\frac{1}{2}}|E_7^*|+(16)^{-\frac{1}{2}}|E_8^*|+(17)^{-\frac{1}{2}}|E_9^*| = \left(\frac{4}{\sqrt{10}}+\frac{8}{\sqrt{13}}+2\right)m$$

$$+\left(\frac{8}{\sqrt{13}}+\frac{2}{\sqrt{15}}\right)n+\left(\frac{2}{\sqrt{10}}+\frac{9}{\sqrt{3}}-\frac{8}{\sqrt{13}}-\frac{20}{\sqrt{13}}+\frac{4}{\sqrt{14}}-\frac{2}{\sqrt{15}}-\frac{5}{2}+\frac{8}{\sqrt{17}}+1\right).$$

(g) Randić index

$$\mathsf{R}^{ve}(H) = \sum_{uv\in E(H)} (\Psi_{ve}(u)\times\Psi_{ve}(v))^{-\frac{1}{2}},$$

$$\mathsf{R}^{ve}(H) = (25)^{-\frac{1}{2}}|E_1^*|+(35)^{-\frac{1}{2}}|E_2^*|+(40)^{-\frac{1}{2}}|E_3^*|+(42)^{-\frac{1}{2}}|E_4^*|$$

$$+(48)^{-\frac{1}{2}}|E_5^*|+(56)^{-\frac{1}{2}}|E_6^*|$$

$$+(63)^{-\frac{1}{2}}|E_7^*|+(64)^{-\frac{1}{2}}|E_8^*|+(72)^{-\frac{1}{2}}|E_9^*|$$

$$=\left(\frac{4}{5}+\frac{5}{\sqrt{10}}+1\right)m+\left(\frac{8}{\sqrt{42}}+\frac{1}{\sqrt{14}}\right)n$$

$$+\left(\frac{2}{5}+\frac{12}{\sqrt{35}}-\frac{4}{\sqrt{13}}-\frac{20}{\sqrt{42}}+\frac{1}{\sqrt{9}}-\frac{1}{\sqrt{14}}+\frac{4}{3\sqrt{7}}-\frac{5}{4}+\frac{4}{3\sqrt{2}}\right).$$

Figs. 9–14 and Numerical computations depicted in Tables 10 and 11 shows that an increase in the value of n and m increases the value of these topological indices. Zhong et al. (2021) examined that the first eV-degree Zagreb index (M^{ev}) predict the molecular weight better than eV-degree Randic index (R^{ev}). The first ve-degree Zagreb beta index ($M_1^{\beta ve}$) predicts the molecular weight and Topological Polar Surface better than other ve-degree of end vertices based indices. Overall, $M_1^{\beta ve}$ is the best predictor of the molecular weight and Topological Polar Surface in all ve- and eV-degree based indices. Süleyman (2017) examines that the $M_1^{\chi ve}$ can be helpful to predicts the physical property Acentric Factor. Also, the second Zagreb beta index predicts the entropy and the Randic index predicts the Enthalpy of vaporization and Standard enthalpy of vaporization, respectively. Hence, the above results are helpful to measure the physical properties of fenestrene.

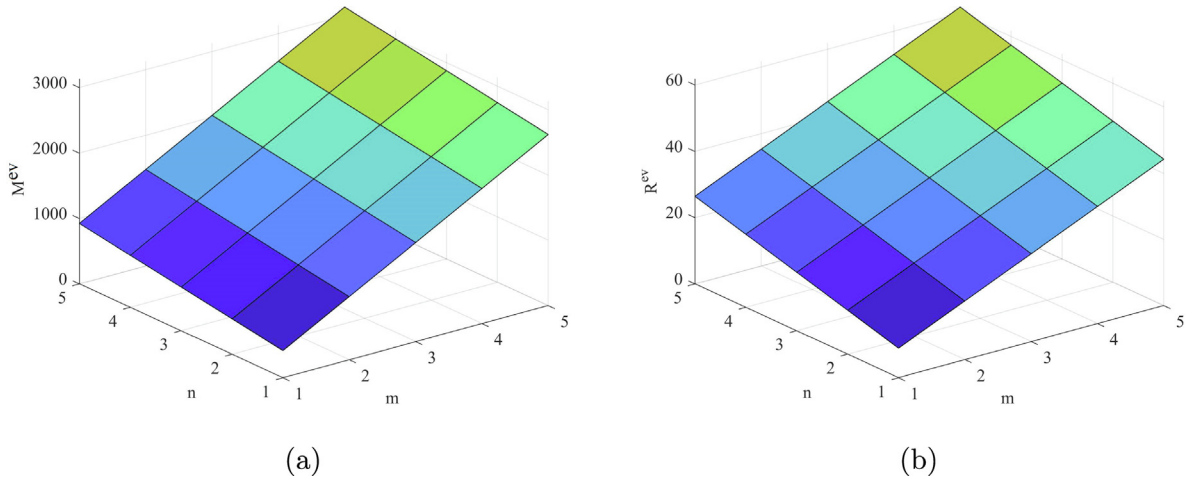


Fig. 9 Plots of the indices, (a) M^{ev} and (b) R^{ev}.

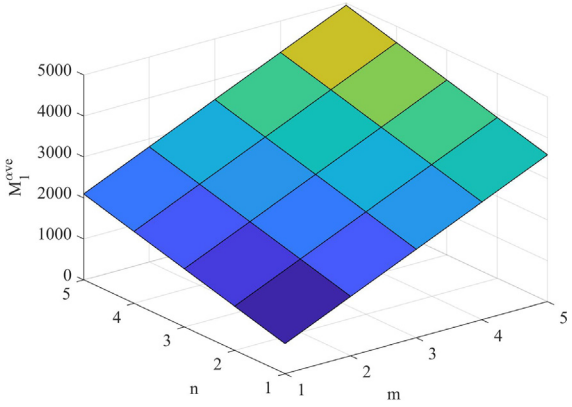


Fig. 10 Plot of M_1^{ave}.

4. Numerical results and discussions

There are numerous applications of experimental research in chem-informatics and biomedicine, where different graph topological evaluations are utilized to handle many complex schemes. In the book "Methods of Chemometrics", Xu and Shao (2004) incorporated the QSAR/QSPR applications systematically. We have calculated the numerical results based on the topological indices of starphene $St[n, m, l]$ and fenestrene $F[n, m]$. Graphs and tables assist visualize the physical meaning of computed indices. The results are shown in the Tables 5 and 6 for the molecular structure of starphene $St[n, m, l]$ and in Tables 10 and 11 for the molecular structure of fenestrene $F[n, m]$. It can been seen from Figs. 2,3,4,5,6,7,9 ,10,11,12,13,14 that all the computed topological indices increase with the increase in the values of m, n, and l respectively. Rauf et al. (2021) developed the QSPR between ve and eV-degree based indices and physical properties of benzene derivatives. They examined that enthalpy, boiling point,

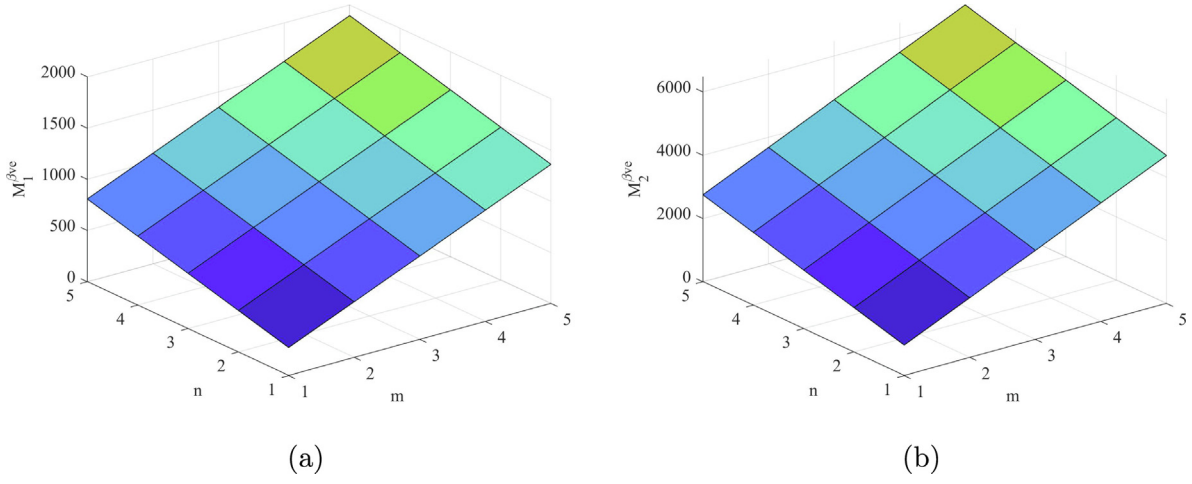


Fig. 11 plots of the indices (a) $M_1^{\beta ve}$ and (b) $M_2^{\beta ve}$.

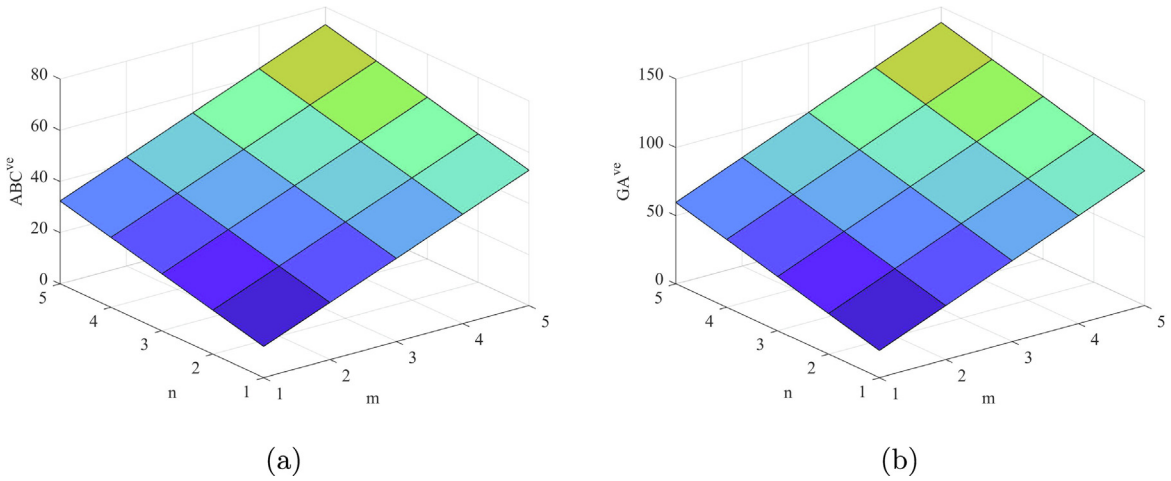


Fig. 12 plots of the indices (a) ABC^{ve} and (b) GA^{ve}.

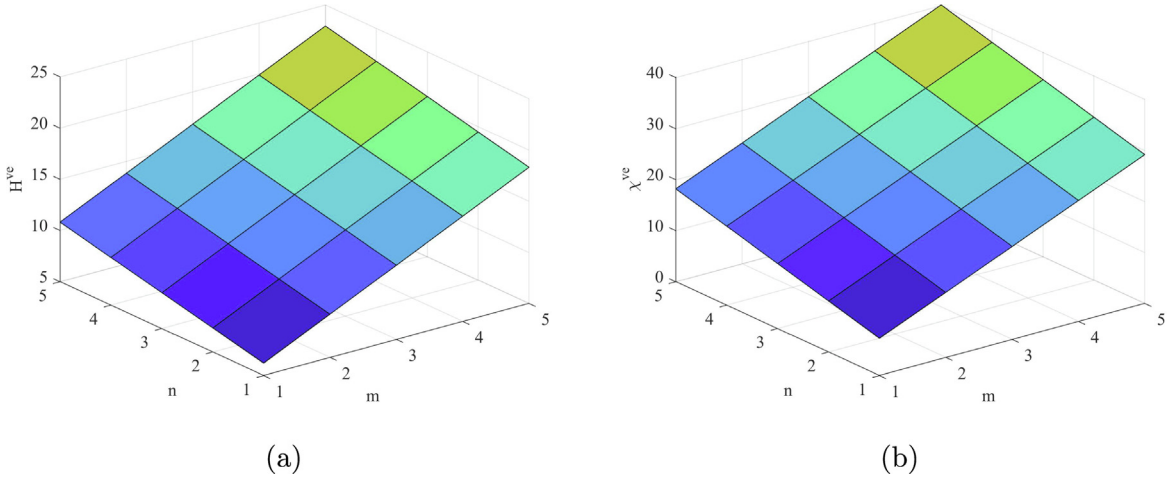


Fig. 13 Plots of the indices (a) H^{ve} and (b) χ^{ve}.

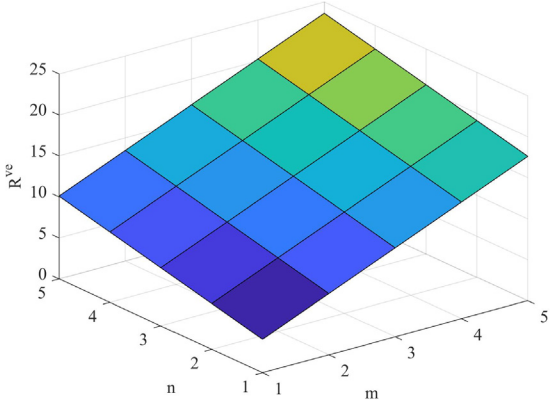


Fig. 14 Plot of the indices R^{ve}.

molecular weight and π-electron energy can be predicted by $\mathsf{R}^{ve}, \mathsf{ABC}^{ve}, \chi^{ve}$ and R^{ev}, respectively. Hence, the computed results can be helpful to predict certain physical/chemical properties of the considered structures.

5. Special case for calculations in starphene molecular structure: Application of maple algorithm

We can compute the degree matrix, eV-degree and ve-degree for the given graph through Maple software. Consider the molecular graph of starphene with $n = 3, m = 3$ and $l = 3$ having 30 vertices and 36 edges. First we get an adjacency matrix M of a graph whose size is 30-by-30. The resultant adjacency matrix M is obtained by using newGraph software whose calculation procedure is given in Hayat and Khan (2021).

Now, from the adjacency matrix we calculated ve-degree and eV-degree of vertices using Maple software. For the degree of vertices, we add the row entries of M. After adding the row entries we get a matrix MI of order 30-by-1.

MI =[2, 2, 2, 3, 2, 3, 3, 2, 3, 2, 2, 2, 2, 3, 2, 3, 3, 2, 3, 2, 2, 2, 2, 3, 2, 3, 3, 2, 3, 2].

The above matrix gives the degree of vertices according to vertices labelled in Fig. 15. For ve-degree of vertices, we will multiply the adjacency matrix M and MI. We get the required column matrix KI for ve-degree of vertices.

Table 10 Numerical results of the indices for different values of $[n,m]$.

$[n,m]$	$M^{ev}(H)$	$R^{ev}(H)$	$M_1^{\chi ve}(H)$	$M_1^{\beta ve}(H)$	$M_2^{\beta ve}(H)$
[**1**, **1**]	556	14.2379	736	272	958
[**2**, **2**]	1380	27.4758	1788	678	2338
[**3**, **3**]	2204	40.7137	2840	1084	3718
[**4**, **4**]	3028	53.9516	3892	1490	5098
[**5**, **5**]	3852	67.1895	4944	1896	6478
[**6**, **6**]	4676	80.4274	5996	2302	7858
[**7**, **7**]	5500	93.6653	7048	2708	9238
[**8**, **8**]	6324	106.9032	8100	3114	10618
[**9**, **9**]	7148	120.1411	9152	3520	11998
[**10**, **10**]	7972	133.3790	10204	3926	13378

Table 11 Numerical results of the indices for different values of $[n,m]$.

$[n,m]$	$ABC^{ve}(H)$	$GA^{ve}(H)$	$H^{ve}(H)$	$\chi^{ve}(H)$	$R^{ve}(H)$
[1, 1]	12.1459	19.7815	6.1934	7.2746	4.0880
[2, 2]	27.4033	49.5374	10.3797	15.4936	8.9708
[3, 3]	42.6607	79.2933	14.5660	23.7125	13.8536
[4, 4]	57.9181	109.0492	18.7523	31.9314	18.7364
[5, 5]	73.1755	138.8051	22.9387	40.1503	23.6193
[6, 6]	88.4329	168.5610	27.1250	48.3692	28.5021
[7, 7]	103.6903	198.3170	31.3113	56.5881	33.3849
[8, 8]	118.9477	228.0729	35.4976	64.8070	38.2678
[9, 9]	134.2051	257.8288	39.6840	73.0259	43.1506
[10, 10]	149.4624	287.5847	43.8703	81.2448	48.0334

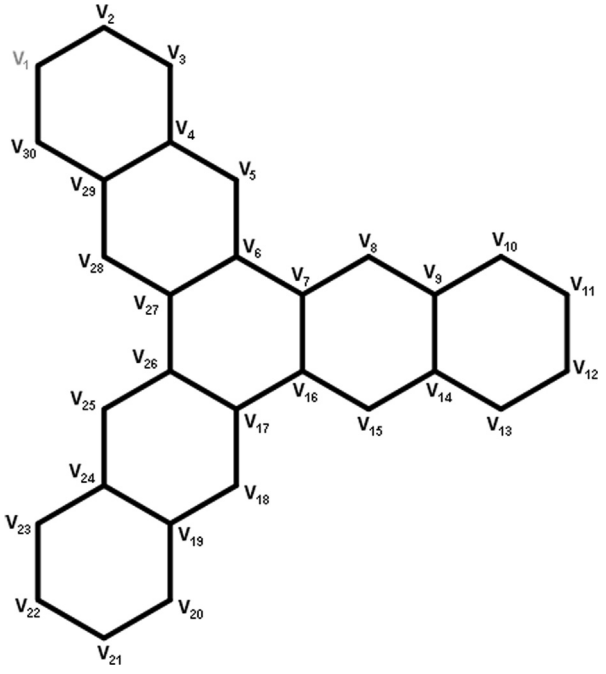


Fig. 15 Starphene structure for $n = 3, m = 3$ and $l = 3$.

KI= [4, 4, 5, 7, 6, 8, 8, 6, 7, 5, 4, 4, 5, 7, 6, 8, 8, 6, 7, 5, 4, 4, 5, 7, 6, 8, 8, 6, 7, 5] Let i and j denotes the rows and columns of adjacency matrix. For eV-degree we will multiply the (i,j)th entry of the adjacency matrix with the sum of $MI(M)_i$ and $MI(M)_j$. We get a matrix (namely N) of order 30-by-30. Finally we consider the upper triangular matrix and use the commands to compute each topological index. The values of the computed indices are presented below

$$M^{ev}(G) = 918.$$
$$M^{ev}(G) = \tfrac{3\sqrt{6}}{2} + \tfrac{18\sqrt{5}}{5} + \tfrac{9}{2}.$$
$$M_1^{\chi ve}(G) = 1140.$$
$$M_1^{\beta ve}(G) = 450.$$
$$M_2^{\beta ve}(G) = 1449.$$
$$ABC^{ve}(G) = 3 + \tfrac{45\sqrt{14}}{28} + \tfrac{\sqrt{462}}{7} + \tfrac{3\sqrt{6}}{4} + \tfrac{3\sqrt{35}}{5} + \tfrac{6\sqrt{3}}{7}.$$
$$GA^{ve}(G) = 12 + \tfrac{8\sqrt{5}}{3} + \sqrt{35} + \tfrac{12\sqrt{42}}{13} + \tfrac{24\sqrt{3}}{7}.$$
$$H^{ve}(G) = \tfrac{3299}{546}.$$
$$\chi^{ve}(G) = \tfrac{7}{2}$$
$$+ \tfrac{3\sqrt{2}}{4} + \sqrt{(3) + \tfrac{6\sqrt{13}}{13} + \tfrac{9\sqrt{14}}{14}}.R^{ve}(G) = \tfrac{27}{14} + \tfrac{3\sqrt{5}}{5} + \tfrac{6\sqrt{35}}{35} + \tfrac{\sqrt{42}}{7} + \tfrac{\sqrt{3}}{2}.$$

Similarly, we can calculate all the above indices through an adjacency matrix for fenestrene. Our results can be verified of fenestrene for case $m \geqslant 2$ and $n \geqslant 3$.

6. Conclusion

In this paper, we assessed the eV and ve degree indices and their graphical representations for the molecular structures of starphene $St[n,m,l]$ and fenestrene $F[n,m]$. These indices may be helpful to predict the physicochemical characteristics of starphene and fenestrene (Süleyman, 2017; Rauf et al., 2021). Moreover, a special case for starphene is presented in Section 6 by using software (Maple) to calculate the eV and ve-degree based topological indices. All the results obtained here can be verified by using our proposed algorithm.

Funding

This work was funded in part by the National Natural Science Foundation of China (grant no. 62002079).

Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

References

Amic, Dragan, Bešlo, Drago, Lucic, Bono, Nikolic, Sonja, Trinajstic, Nenad, 1998. The vertex-connectivity index revisited. J. Chem. Informat. Comput. Sci. 38 (5), 819–822.

Aslam, A., Bashir, Y., Ahmed, S., Gao, W., 2017. On topological indices of certain dendrimer structures. Z. Naturforsch. 72, 559–566.

Aslam, A., Jamil, M.K., Gao, W., Nazeer, W., 2018. On topological aspects of some dendrimer structures. Nanotechnol. Rev. 7, 123–129.

Bashir, Y., Aslam, A., Kamran, M., Qureshi, I., Jahangir, A., Rafiq, M., Bibi, N., Muhammad, N., 2017. On forgotten topological indices of some dendrimers structure. Molecules 22, 867–874.

Bollobs, Bela, Erdos, Paul, 1998. Graphs of extremal weights. Ars Combinatoria 50, 225–233.

Chou, Chien-Pin, Witek, Henryk A. 2015. Two examples for the application of the ZZDecomposer: Zigzag-edge coronoids and fenestrenes. MATCH Commun. Mathe. Comput. Chem. 73(2).

Chu, Yu-Ming, Muhammad, Abid, Qureshi, Muhammad Imran, Fahad, Asfand, Aslam, Adnan, 2021. Irregular topological indices of certain metal organic frameworks. Main Group Metal Chem. 44 (1), 73–81.

Clar, E., Mullen, A., 1968. The non-existence of a threefold aromatic conjugation in linear benzologues of triphenylene (starphenes). Tetrahedron 24 (23), 6719–6724.

Estrada, Ernesto, Torres, Luis, Rodriguez, Lissette, Gutman, Ivan, 1998. An atom-bond connectivity index: Modelling the enthalpy of formation of alkanes. Indian J. Chem. 37A (10), 849–855.

Graovac, Ante, Pisanski, Tomaž, 1991. On the Wiener index of a graph. J. Mathe. Chem. 8 (1), 53–62.

Gutman, I., Trinajstic, N., 1972. Chem. Phys. Lett. 17, 535–538.

Gutman, I., Ruscic, B., Trinajstic, N., Wilcox, C.F., 1975. J. Chem. Phys. 62 (9), 3399–3405.

Hayat, S., Khan, S., 2021. Quality testing of spectrum-based valency descriptors for polycyclic aromatic hydrocarbons with applications. J. Mol. Struct. 1228, 129789.

Holec, Jan, Beatrice Cogliati, James Lawrence, Alejandro Berdonces-Layunta, Pablo Herrero, Yuuya Nagata, Marzena Banasiewicz et al. 2021. A Large Starphene Comprising Pentacene Branches. Angew. Chem. Int. Ed. 60(14), 7752–7758.

Hulot, Catherine, Peluso, Jean, Blond, Gaëlle, Muller, Christian D., Suffert, Jean, 2010. Synthesis of exotic polycycles such as cyclooctatrienes and fenestrenes with differential pro-apoptotic activities on human TRAIL-resistant metastatic cell lines. Bioorganic Medicinal Chem. Lett. 20 (22), 6836–6839.

Naeem, Muhammad, Rauf, Abdul, 2021. Degree Based Weighted Entropy Indices of Hyaluronic Acid-Curcumin Conjugates: an Anti-Tumor Drug. Polycyclic Aromat. Compd., 1–18

Randic, Milan, 1975. Characterization of molecular branching. J. Am. Chem. Soc. 97 (23), 6609–6615.

Rauf, Abdul, Naeem, Muhammad, Bukhari, Saira Usman, 2021. Quantitative structure–property relationship of Ev-degree and Ve-degree based topological indices with physico-chemical properties of benzene derivatives and application. Int. J. Quantum Chem., e26851

Rauf, Abdul, Naeem, Muhammad, Maqbool, Saba, Siddiqui, Muhammad Kamran, 2021. Irregularity indices for certain anti-tumor and anti-covid drugs. Polycyclic Aromat. Compd., 1–14

Rauf, Abdul, Naeem, Muhammad, Aslam, Adnan, 2022. Quantitative structure–property relationship of edge weighted and degree-based entropy of benzene derivatives. Int. J. Quantum Chem. 122 (3), e26839.

Rüdiger, Elias C., Müller, Matthias, Freudenberg, Jan, Bunz, Uwe HF, 2019. Starphenes and Phenes: Structures and Properties. Organic Mater. 1 (01), 001–018.

Sarkar, Prosanta, Pal, Anita, 2020. General fifth M-Zagreb polynomials of benzene ring implanted in the p-type-surface in 2D network. Biointerface Res. Appl. Chem. 10 (6), 6881–6892.

Sarkar, Prosanta, De, Nilanjan, Pal, Anita, 2018. The (a, b)-Zagreb index of nanostar dendrimers. U.P.B. Sci. Bull. Series B 80 (4), 67–82.

Süleyman, Ediz, 2017. Predicting some physicochemical properties of octane isomers: A topological approach using ev-degree and ve-degree Zagreb indices. Int. J. Syst. Sci. Appl. Mathe. 2 (5), 87–92.

Wiener, Harry, 1947. Structural determination of paraffin boiling points. J. Am. Chem. Soc. 69 (1), 17–20.

Xu, Lu, Shao, X.G. 2004. Methods of chemometrics. Academic Press, Beijing.

Zhong, L., 2012. The harmonic index for graphs. Appl. Mathe. Lett. 25, 561–566.

Zhong, Jian-Feng, Rauf, Abdul, Naeem, Muhammad, Rahman, Jafer, Aslam, Adnan, 2021. Quantitative Structure-Property Relationships (QSPR) of Valency Based Topological Indices with Covid-19 drugs and Application. Arabian J. Chem., 103240

Zhou, B., Trinajstic, N., 2009. On a novel connectivity index. J. Math. Chem. 46, 1252–1270.