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Retraction

Retracted: Computation of Vertex Degree-Based Molecular Descriptors of Hydrocarbon Structure

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This article has been retracted by Hindawi following an investigation undertaken by the publisher [1]. This investigation has uncovered evidence of one or more of the following indicators of systematic manipulation of the publication process:

(1) Discrepancies in scope
(2) Discrepancies in the description of the research reported
(3) Discrepancies between the availability of data and the research described
(4) Inappropriate citations
(5) Incoherent, meaningless and/or irrelevant content included in the article
(6) Peer-review manipulation

The presence of these indicators undermines our confidence in the integrity of the article's content and we cannot, therefore, vouch for its reliability. Please note that this notice is intended solely to alert readers that the content of this article is unreliable. We have not investigated whether authors were aware of or involved in the systematic manipulation of the publication process.

Wiley and Hindawi regrets that the usual quality checks did not identify these issues before publication and have since put additional measures in place to safeguard research integrity.

We wish to credit our own Research Integrity and Research Publishing teams and anonymous and named external researchers and research integrity experts for contributing to this investigation.

The corresponding author, as the representative of all authors, has been given the opportunity to register their agreement or disagreement to this retraction. We have kept a record of any response received.

References

[1] Z. S. Mufti, R. Anjum, A. Abbas, S. Ali, M. Afzal, and A. Alam, "Computation of Vertex Degree-Based Molecular Descriptors of Hydrocarbon Structure," *Journal of Chemistry*, vol. 2022, Article ID 3621403, 15 pages, 2022.

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Research Article

Computation of Vertex Degree-Based Molecular Descriptors of Hydrocarbon Structure

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Topological indices are such numbers or set of numbers that describe topology of structures. Nearly 400 topological indices are calculated so far. The prognostication of physical, chemical, and biological attributes of organic compounds is an important and still unsolved problem of computational chemistry. Topological index is the tool to predict the physicochemical properties such as boiling point, melting point, density, viscosity, and polarity of organic compounds. In this study, some degree-based molecular descriptors of hydrocarbon structure are calculated.

1. Introduction

The invention of graph theory in 18th century was a biggest game changer in the field of mathematics by a Swiss Mathematician Leonard Euler (1702–1782). He used graphs to tackle the famous problem of Konigsberg bridge [1, 2]. In this study, $G = (\mathbb{V}, \mathbb{E})$ is a simple undirected graph containing a set of vertices $\mathbb{V}$ and an edges set $\mathbb{E}$ [3]. The number of lines connected to a vertex is called a degree of a vertex and is denoted by Deg_u.

Topological indices investigate the features of graphs that persist constant after continual changing in graph. They describe symmetry of chemical structures with a number and then work for the improvement of QSAR and QSPR which both are employed to build a connection among the molecular structure and mathematical tools. These indices are useful to associate physiochemical properties of compounds (such as entropy, boiling and melting point, flammability, and many more).

Topological indices are invariants of structures, so they are independent of pictorial representation [4]. Among three categories of molecular descriptors, vertex degree-based indices are considerably significant. Medicine industries are producing new and advanced medicines which are effective for mankind and ecology. Graph theory and molecular descriptors are playing a significant role in analysing the physiochemical properties of organic compounds.

Hydrocarbon structure is an aromatic hydrocarbon and a unique structure composed of benzene through covalent bond. There are six sigma and six pi bonds in each benzene ring present in this compound. It is a nonpolar structure, and each benzene has a bond angle of 120°. It can be used in making of plastic, nylon, and dyes. It cannot be dissolved in water but in organic solvents. It has a sharp melting point because of the presence of benzene but does not have high boiling point. The structure is flammable and also show resonance.

1.1. Derivation of Degree-Based Topological Indices

1.1.1. First General Zagreb Index. The 1st general Zagreb index was introduced by Li and Zhao and is given as [5]

$$M_\alpha(G^*) = \sum_{p\in V(G^*)} \left(\mathrm{Deg}_p\right)^\alpha. \tag{1}$$

Classes of Zagreb Indices. We have two Zagreb groups of indices, first Zagreb index and second Zagreb index denoted by M_1 and M_2 [6–8]. They are proposed in late seventies by Gutman and Tranjistic.

1.1.2. First Zagreb Index. The first Zagreb index can be written as [9, 10]

$$M_1(G^*) = \sum_{pq\in \mathbb{E}(G^*)} \left(\mathrm{Deg}_p + \mathrm{Deg}_q\right). \tag{2}$$

1.1.3. Second Zagreb Index. The mathematical form is [9]

$$M_2(G^*) = \sum_{pq\in \mathbb{E}(G^*)} \left(\mathrm{Deg}_p \times \mathrm{Deg}_q\right). \tag{3}$$

Multiple and Polynomial Zagreb Indices. In 2012, advanced forms of Zagreb descriptors were suggested, with names 1st and 2nd multiple Zagreb descriptors given as $PM_1(G^*)$ and $PM_2(G^*)$ [8]. The polynomials are helpful to calculate Zageb index. 1st and 2nd Zagreb polynomial descriptors are denoted as $M_1(G^*, j)$ and $M_2(G^*, j)$.

1.1.4. First and Second Multiple Zagreb Indices. The 1st and 2nd multiple Zagreb indices are

$$PM_1(G^*) = \prod_{pq\in \mathbb{E}(G^*)} \left(\mathrm{Deg}_p + \mathrm{Deg}_q\right), \tag{4}$$

$$PM_2(G^*) = \prod_{pq\in \mathbb{E}(G^*)} \left(\mathrm{Deg}_p \times \mathrm{Deg}_q\right). \tag{5}$$

1.1.5. First and Second Polynomial Zagreb Indices. The 1st and 2nd polynomial Zagreb indices are

$$M_1(G^*, j) = \sum_{pq\in \mathbb{E}(G^*)} j^{\left(\mathrm{Deg}_p+\mathrm{Deg}_q\right)}, \tag{6}$$

$$M_2(G^*, j) = \sum_{pq\in \mathbb{E}(G^*)} j^{\left(\mathrm{Deg}_p\times\mathrm{Deg}_q\right)}. \tag{7}$$

1.1.6. Modified Zagreb Index. The modified form of Zagreb index was put forward in 2013 by G. H Shirdil, H. Rezapour, and A.M.Sayadi.

$$HM(G^*) = \sum_{pq\in \mathbb{E}(G^*)} \left(\mathrm{Deg}_p + \mathrm{Deg}_q\right)^2. \tag{8}$$

1.1.7. Second Modified Zagreb Index. The 2nd modified Zagreb index is

$$M_2(G^*) = \sum_{pq\in \mathbb{E}(G^*)} \frac{1}{\left(\mathrm{Deg}_p \times \mathrm{Deg}_q\right)}. \tag{9}$$

1.1.8. Reduced 2nd Zagreb Index. It was written by Furtula, and its formula is

$$RM_2(G^*) = \sum_{pq\in \mathbb{E}(G^*)} \left(\mathrm{Deg}_p - 1 \times \mathrm{Deg}_q - 1\right). \tag{10}$$

1.1.9. Atom Bond Connectivity Index. Ernesto Estrada and Torres defined the abovementioned index [8, 11]. It is helpful in modeling thermodynamic properties of hydrocarbons.

$$ABC(G^*) = \sum_{pq\in \mathbb{E}(G^*)} \sqrt{\frac{\mathrm{Deg}_p + \mathrm{Deg}_q - 2}{\mathrm{Deg}_p\mathrm{Deg}_q}}. \tag{11}$$

1.1.10. Atom Bond Connectivity Index of 4th Order. Ghorbani and Ghazi suggested this index [7].

$$ABC_4(G^*) = \sum_{pq\in \mathbb{E}(G^*)} \sqrt{\frac{S_p + S_q - 2}{S_pS_q}}. \tag{12}$$

1.1.11. General Randić Connectivity Index. Millan Randić introduced molecular descriptors for the first time based on degree of vertices. Initially, it was coined as branching index [10] and familiar to find the branching of hydrocarbons. In 1998, Eddrös and Bollobás suggested the general form of this index by switching the factor $(-1/2)$ with $\alpha\varepsilon$I R [12].

$$R_\alpha(G^*) = \sum_{pq\in \mathbb{E}(G^*)} \left(\mathrm{Deg}_p\mathrm{Deg}_q\right)^\alpha. \tag{13}$$

1.1.12. Randić Index. We may call this index as first-degree-based topological index [8].

$$R(G^*) = \sum_{pq\in \mathbb{E}(G^*)} \frac{1}{\sqrt{\mathrm{Deg}_p\mathrm{Deg}_q}}. \tag{14}$$

1.1.13. Reciprocal Randić Index (RRI). Favaron, Mahéo, and Saclé invented a new index RRI [13].

$$RR(G^*) = \sum_{pq\in\mathbb{E}(G^*)} \sqrt{\mathrm{Deg}_p\mathrm{Deg}_q}. \quad (15)$$

1.1.14. RRR Index. It is equivalent of RR index [13]. It can be written as

$$RRR(G^*) = \sum_{pq\in\mathbb{E}(G^*)} \sqrt{\left(\mathrm{Deg}_p - 1\right)\left(\mathrm{Deg}_q - 1\right)}. \quad (16)$$

1.1.15. GA Index. Vukicevic̀ and Furtula proposed the GA index [4, 7, 8].

$$GA(G^*) = \sum_{pq\in\mathbb{E}(G^*)} \frac{2\sqrt{\mathrm{Deg}_p\mathrm{Deg}_q}}{\mathrm{Deg}_p + \mathrm{Deg}_q}. \quad (17)$$

1.1.16. GA_5 Index. Grovac et al. suggested the GA_5 index in 2011.

$$GA_5(G^*) = \sum_{pq\in\mathbb{E}(G^*)} \frac{2\sqrt{S_pS_q}}{S_p + S_q}. \quad (18)$$

1.1.17. Forgotten Index. Gutman and Futula suggested an index [14]. It is represented by $F(G^*)$.

$$F(G^*) = \sum_{pq\in\mathbb{E}(G^*)} \left(\mathrm{Deg}_p^2 + \mathrm{Deg}_q^2\right). \quad (19)$$

1.1.18. General Sum Connectivity Index. Zhou and Trinajstić proposed new index [8, 15]. It is defined as

$$\chi_\alpha(G^*) = \sum_{pq\in\mathbb{E}(G^*)} \left(\mathrm{Deg}_p + \mathrm{Deg}_q\right)^\alpha, \quad (20)$$

where $\alpha\epsilon$I R.

1.1.19. SD Index. In 2010, D.vukicevic and Furtula proposed this useful index denoted by SD (*G*) [17–21].

$$\mathrm{SD}(G^*) = \sum_{pq\in\mathbb{E}(G^*)} \frac{\mathrm{Deg}_p^2 + \mathrm{Deg}_q^2}{\left(\mathrm{Deg}_p \times \mathrm{Deg}_q\right)}. \quad (21)$$

1.1.20. Harmonic Index. Siemion Fajtlowicz prepared a computer program that is helpful in automatic generation of conjectures [8] and also suggested a degree-based element; then, Zhang unwrapped this element and named harmonic index [22–25].

$$H(G^*) = \sum_{pq\in\mathbb{E}(G^*)} \frac{2}{\left(\mathrm{Deg}_p + \mathrm{Deg}_q\right)}. \quad (22)$$

2. Topological Indices of Hydrocarbon Structure

In this study, numbers of molecular descriptors of the hydrocarbon structure are computed (Figure 1).

2.1. Description of Graph of Hydrocarbon Structure. Chemical properties of graph shown in Figure 2 are given (Tables 1–4).

Our concerned graph is shown in Figure 2, and it is denoted by G^*.

Theorem 1. *G^* is a graph of hydrocarbon structure, and its first general Zagreb index is given as follows:*

$$M_\alpha(G^*) = 48pq(2^\alpha) + 18pq(3^\alpha) - q(3^\alpha) - p(3^\alpha) \quad (23)$$

Proof. Consider graph G^*, i.e., shown in Figure 2. G^* has $54pq$ points in which $30pq + 2p + 2q$ of degree 2 vertices and $24pq - 2p - 2q$ of degree 3.

By applying the definition of $M_\alpha(G^*)$ (1),

$$M_\alpha(G^*) = \sum_{p\in\mathbb{V}(G^*)} \left(Deg_p\right)^\alpha, \quad (24)$$

we have the required results:

$$M_\alpha(G^*) = 48pq(2^\alpha) + 18pq(3^\alpha) - q(3^\alpha) - p(3^\alpha) \quad (25)$$

□

Theorem 2. *First Zagreb index of graph G^* is given as follows:*

$$\begin{aligned} M_1(G^*) = {} & 12pq(4) + 4p(4) + 4q(4) + 36pq(5) - 4p(5) \\ & - 4q(5) + 18pq(6) - p(6) - q(6). \end{aligned} \quad (26)$$

Proof. $\mathbb{E}(G^*)$ of G^* is divided into 3 groups.

$\mathbb{E}_1(G^*)$ holds $12pq + 4p + 4q$ arcs pq, here $\mathrm{Deg}_p = \mathrm{Deg}_q = 2$

$\mathbb{E}_2(G^*)$ has $36pq - 4p - 4q$ arcs pq, here $\mathrm{Deg}_p = 2$, $\mathrm{Deg}_q = 3$

$\mathbb{E}_3(G^*)$ contains $18pq - q - p$ arcs pq, here $\mathrm{Deg}_p = 3$, $\mathrm{Deg}_q = 3$

Consider

$|\mathbb{E}_1(G^*)| = e_{2,2}$
$|\mathbb{E}_2(G^*)| = e_{2,3}$
$|\mathbb{E}_2(G^*)| = e_{3,3}$

From equation (6), we get

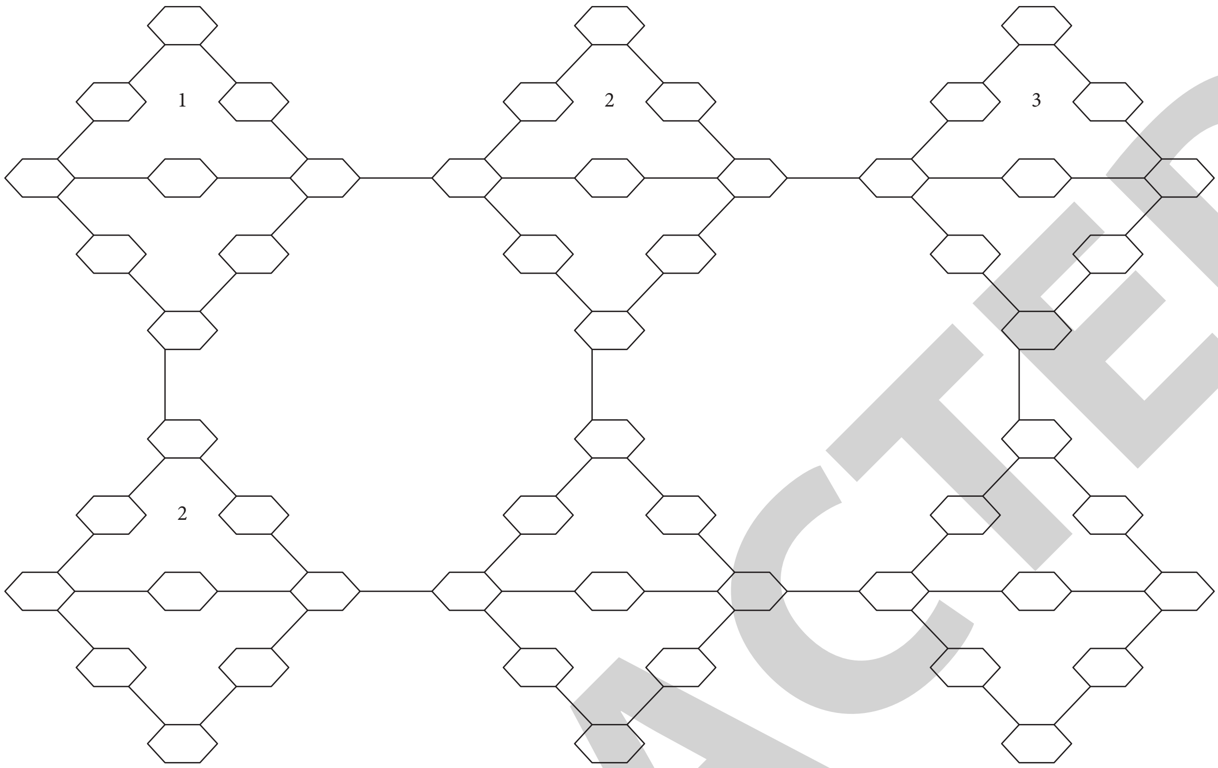

Figure 1: Unit (2, 3) of hydrocarbon structure.

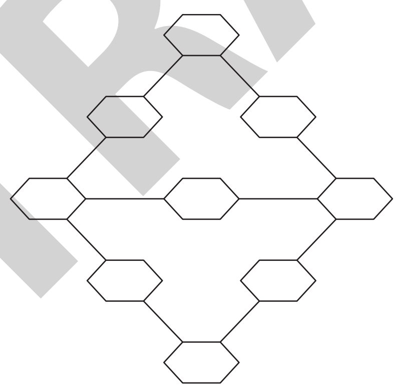

Figure 2: Unit (1, 1) of hydrocarbon structure.

$$
\begin{aligned}
M_1(G^*) &= \sum_{pq\in\mathbb{E}(G^*)} \left(\mathrm{Deg}_p + \mathrm{Deg}_q\right),\\
M_1(G^*) &= \sum_{pq\in\mathbb{E}_1(G^*)} \left(\mathrm{Deg}_p + \mathrm{Deg}_q\right) + \sum_{pq\in\mathbb{E}_2(G^*)} \left(\mathrm{Deg}_p + \mathrm{Deg}_q\right) + \sum_{pq\in\mathbb{E}_3(G^*)} \left(\mathrm{Deg}_p + \mathrm{Deg}_q\right)\\
&= \left|\mathbb{E}_1(G^*)\right|4 + \left|\mathbb{E}_2(G^*)\right|5 + \left|\mathbb{E}_3(G^*)\right|6\\
&= (12pq + 4p + 4q)(4) + (36pq - 4p - 4q)(5) + (18pq - q - p)(6)\\
&= 12pq(4) + 4p(4) + 4q(4) + 36pq(5) - 4p(5) - 4q(5) + 18pq(6)\\
&\quad - q(6) - p(6).
\end{aligned}
\tag{27}
$$

□

Table 1: Chemical properties of graph G^*.

Chemical formula	$C_{54}H_{34}$
Exact mass	682.27
Molecular weight	682.85
Elemental analysis	C, 94.98; H, 5.02

Table 2: Partition of graph G^* on the basis of degrees.

Degree of vertex	Number of vertices
2	$30pq+2p+2q$
3	$24pq-2p-2q$
Sum	$66pq-q-p$

Theorem 3. *First and second polynomial and multiple Zagreb indices of (hydrocarbon structure) G^* are given as follows:*

(1) $PM_1(G^*) = 4^{12pq+4p+4q} \times 5^{36pq-4p-4q} \times 6^{18pq-q-p}$;

(2) $PM_2(G^*) = 4^{12pq+4p+4q} \times 6^{36pq-4p-4q} \times 9^{18pq-q-p}$;

(3) $M_1(G^*, j) = (12pq+4p+4q)j^4 + (36pq-4p-4q)j^5 + (18pq-p-q)j^6$;

(4) $M_2(G^*, j) = (12pq+4p+4q)j^4 + (36pq-4p-4q)j^6 + (18pq-p-q)j^9$;

Proof. $\mathbb{E}(G^*)$ is grouped in 3 edge partitions depending on end vertices degrees. $\mathbb{E}_1(G^*)$ contains $12pq+4p+4q$ edges, where $\mathrm{Deg}_p = \mathrm{Deg}_q = 2$. $\mathbb{E}_2(G^*)$ has $36pq-4p-4q$ edges pq, where $\mathrm{Deg}_p = 2$ and $\mathrm{Deg}_q = 3$. $\mathbb{E}_3(G^*)$ has $18pq-p-q$ lines pq, where $\mathrm{Deg}_p = 3$ and $\mathrm{Deg}_q = 3$. Consider $|\mathbb{E}_1(G^*)| = e_{2,2}$, $|\mathbb{E}_2(G^*)| = e_{2,3}$, and $|\mathbb{E}_2(G^*)| = e_{3,3}$.

By utilizing the definition of $PM_1(G^*)$,

$$\begin{aligned} PM_1(G^*) &= \prod_{pq\in\mathbb{E}(G^*)} \left(\mathrm{Deg}_p + \mathrm{Deg}_q\right),\\ PM_1(G^*) &= \prod_{pq\in\mathbb{E}_1(G^*)} \left(\mathrm{Deg}_p + \mathrm{Deg}_q\right) \times \prod_{pq\in\mathbb{E}_2(G^*)} \left(\mathrm{Deg}_p + \mathrm{Deg}_q\right) \times \prod_{pq\in\mathbb{E}_3(G^*)} \left(\mathrm{Deg}_p + \mathrm{Deg}_q\right)\\ &= 4^{|\mathbb{E}_1(G^*)|} \times 5^{|\mathbb{E}_2(G^*)|} \times 6^{|\mathbb{E}_3(G^*)|}\\ &= 4^{12pq+4p+4q} \times 5^{36pq-4p-4q} \times 6^{18pq-q-p}. \end{aligned} \tag{28}$$

Now,

$$\begin{aligned} PM_2(G^*) &= \prod_{pq\in\mathbb{E}(G^*)} \left(\mathrm{Deg}_p \times \mathrm{Deg}_q\right),\\ PM_2(G^*) &= \prod_{pq\in\mathbb{E}_1(G^*)} \left(\mathrm{Deg}_p \times \mathrm{Deg}_q\right) \times \prod_{pq\in\mathbb{E}_2(G^*)} \left(\mathrm{Deg}_p \times \mathrm{Deg}_q\right) \times \prod_{pq\in\mathbb{E}_3(G^*)} \left(\mathrm{Deg}_p \times \mathrm{Deg}_q\right)\\ &= 4^{|\mathbb{E}_1(G^*)|} \times 5^{|\mathbb{E}_2(G^*)|} \times 6^{|\mathbb{E}_3(G^*)|}\\ &= 4^{12pq+4p+4q} \times 5^{36pq-4p-4q} \times 6^{18pq-p-q}. \end{aligned} \tag{29}$$

By utilizing $M_1(G^*, j)$ from (6),

$$\begin{aligned} M_1(G^*, j) &= \sum_{pq\in\mathbb{E}(G^*)} j^{\left(\mathrm{Deg}_p+\mathrm{Deg}_q\right)},\\ M_1(G^*, j) &= \sum_{pq\in\mathbb{E}_1(G^*)} j^{\left(\mathrm{Deg}_p+\mathrm{Deg}_q\right)} + \sum_{pq\in\mathbb{E}_2(G^*)} j^{\left(\mathrm{Deg}_p+\mathrm{Deg}_q\right)} + \sum_{pq\in\mathbb{E}_3(G^*)} j^{\left(\mathrm{Deg}_p+\mathrm{Deg}_q\right)}\\ &= \sum_{pq\in\mathbb{E}_1(G^*)} j^4 + \sum_{pq\in\mathbb{E}_1(G^*)} j^5 + \sum_{pq\in\mathbb{E}_1(G^*)} j^6\\ &= \left|\mathbb{E}_1(G^*)\right| j^4 + \left|\mathbb{E}_2(G^*)\right| j^5 + \left|\mathbb{E}_3(G^*)\right| j^6\\ &= (12pq+4p+4q)j^4 + (36pq-4p-4q)j^5 + (18pq-q-p)j^6. \end{aligned} \tag{30}$$

Table 3: Edge partition of graph G^* with respect to starting and ending vertices of each edge.

$(\mathrm{Deg}_p, \mathrm{Deg}_q)$ where p, q εE (G)	Number of vertices
(2,2)	$112pq + 4p + 4q$
(2,3)	$36pq - 4p - 4q$
(3,3)	$18pq - p - q$
Sum	$66pq - p - q$

From equation (7), we have

$$\begin{aligned}
M_2(G^*, j) &= \sum_{pq\in\mathbb{E}(G^*)} j^{\left(\mathrm{Deg}_p+\mathrm{Deg}_q\right)},\\
M_2(G^*, j) &= \sum_{pq\in\mathbb{E}_1(G^*)} j^{\left(\mathrm{Deg}_p+\mathrm{Deg}_q\right)} + \sum_{pq\in\mathbb{E}_2(G^*)} j^{\left(\mathrm{Deg}_p+\mathrm{Deg}_q\right)} + \sum_{pq\in\mathbb{E}_3(G^*)} j^{\left(\mathrm{Deg}_p+\mathrm{Deg}_q\right)}\\
&= \sum_{pq\in\mathbb{E}_1(G^*)} j^4 + \sum_{pq\in\mathbb{E}_1(G^*)} j^6 + \sum_{pq\in\mathbb{E}_1(G^*)} j^9\\
&= \left|\mathbb{E}_1(G^*)\right| j^4 + \left|\mathbb{E}_2(G^*)\right| j^6 + \left|\mathbb{E}_3(G^*)\right| j^9\\
&= (12pq + 4p + 4q)\, j^4 + (36pq - 4p - 4q)\, j^6 + (18pq - q - p)\, j^9.
\end{aligned} \tag{31}$$

This completes the proof. □

Theorem 4. *Harmonic index, second Zagreb index, and reduced second Zagreb index of G^* are as follows:*

(1) Hyper-Zagreb index of graph G^* is

$$\begin{aligned}
HM(G^*) &= 12pq(16) + 4p(16) + 4q(16) + 36pq(25)\\
&\quad - 4p(25) - 4q(25) + 18pq(36) - q(36) - p(36).
\end{aligned} \tag{32}$$

(2) Second Zagreb index is

$$M_2(G^*) = 11pq + \frac{2}{9}p + \frac{2}{9}q. \tag{33}$$

(3) Reduced 2^{nd} Zagreb index is

$$RM_2(G^*) = -20p - 24q + 144pq. \tag{34}$$

Proof. $\mathbb{E}(G^*)$ is grouped in 3 partitions. $\mathbb{E}_1(G^*)$ holds $12pq + 4p + 4q$ edges, where $\mathrm{Deg}_p = \mathrm{Deg}_q = 2$. $\mathbb{E}_2(G^*)$ supports $36pq - 4p - 4q$ edges pq, where $\mathrm{Deg}_p = 2$ and $\mathrm{Deg}_q = 3$. $\mathbb{E}_3(G^*)$ keeps $18pq - q - p$ edges, where $\mathrm{Deg}_p = 3$ and $\mathrm{Deg}_q = 3$. Consider $|\mathbb{E}_1(G^*)| = e_{2,2}$, $|\mathbb{E}_2(G^*)| = e_{2,3}$, and $|\mathbb{E}_2(G^*)| = e_{3,3}$.

From (8), we define $HM(G^*)$ as

$$\begin{aligned}
HM(G^*) &= \sum_{pq\in\mathbb{E}(G^*)} \left(\mathrm{Deg}_p + \mathrm{Deg}_q\right)^2,\\
HM(G^*) &= \sum_{pq\in\mathbb{E}_1(G^*)} \left[\mathrm{Deg}_p + \mathrm{Deg}_q\right]^2 + \sum_{pq\in\mathbb{E}_2(G^*)} \left[\mathrm{Deg}_p + \mathrm{Deg}_q\right]^2 + \sum_{pq\in\mathbb{E}_3(G^*)} \left[\mathrm{Deg}_p + \mathrm{Deg}_q\right]^2\\
&= 16\left|\mathbb{E}_1(G^*)\right| + 25\left|\mathbb{E}_2(G^*)\right| + 36\left|\mathbb{E}_3(G^*)\right|\\
&= 16(12pq + 4p + 4q) + 25(36pq - 4p - 4q) + 36(18pq - q - p)\\
&= 1740pq - 72p - 72q.
\end{aligned} \tag{35}$$

Table 4: Edge grouping of a graph G^* of hydrocarbon structure with accordance of degree summation of adjoining end vertices of every edges.

Degree of vertices	Number of vertices
(4, 4)	$2p$
(4, 5)	$4p+4q$
(5, 5)	$12pq-2p$
(5, 7)	$22pq-2p$
(5, 8)	$2pq+2p+4q$
(6, 7)	$6pq-2p-4q$
(6, 8)	$6pq-2p-4q$
(7, 7)	$2pq-p-q$
(7, 8)	$8pq$
(7, 9)	$2pq$
(8, 8)	$2pq$
(8, 9)	$4pq$
Sum	$66pq-p-q$

By using the definition of $M_2(G^*)$,

$$M_2(G^*) = \sum_{pq\in\mathbb{E}(G^*)} \frac{1}{(\mathrm{Deg}_p + \mathrm{Deg}_q)},$$

$$\begin{aligned} M_2(G^*) &= |\mathbb{E}_1(G^*)|\left(\frac{1}{4}\right) + |\mathbb{E}_2(G^*)|\left(\frac{1}{6}\right) + |\mathbb{E}_3(G^*)|\left(\frac{1}{9}\right) \\ &= \frac{(12pq+4p+4q)}{4} + \frac{(36pq-4p-4q)}{6} + \frac{(18pq-q-p)}{9} \\ &= 11pq + \frac{2}{9}p + \frac{2}{9}q. \end{aligned} \tag{36}$$

By substituting the values in equation (10),

$$RM_2(G^*) = \sum_{pq\in\mathbb{E}(G^*)} \left(\mathrm{Deg}_p - 1 \times \mathrm{Deg}_q - 1\right). \tag{37}$$

With the help of (3) and (4), we have

$$\begin{aligned} RM_2(G^*) &= |\mathbb{E}_1(G^*)|(1)(1) + |\mathbb{E}_2(G^*)|(1)(2) + |\mathbb{E}_3(G^*)|(2)(2) \\ &= (12pq+4p+4q) + (36pq-4p-4q)(2) + (18pq-q-p)(4) \\ &= 12pq + 4p + 4q + 36pq(2) - 4p(2) - 4q(2) + 18pq(4) - q(4) \\ &\quad - p(4). \end{aligned} \tag{38}$$

□

Theorem 5. *ABC index of graph hydrocarbon structure is given as follows:*

$$ABC(G^*) = 48pq\frac{1}{2\sqrt{2}} + 18pq\left(\frac{2}{3}\right) - q\left(\frac{2}{3}\right) - p\left(\frac{2}{3}\right). \tag{39}$$

Proof. G^* encounters $66pq-p-q$ number of edges and $54pq$ vertices. Vertex count of degree 2 is $30pq+2p+2q$ and of degree 3 is $24pq-2p-2q$. The cardinality arc group E of G^* is $66pq-p-q$. $\mathbb{E}(G^*)$ grouped into 3 disjoint arc groups, i.e., $\mathbb{E}(G^*) = \mathbb{E}_1(G^*) \cup \mathbb{E}_2(G^*) \cup \mathbb{E}_3(G^*)$. $\mathbb{E}_1(G^*)$ has $12mn+4n+4m$ edges pq, where $\mathrm{Deg}_p = \mathrm{Deg}_q = 2$. $\mathbb{E}_2(G^*)$ supports $36pq-4p-4q$ edges pq, where $\mathrm{Deg}_p = 2$ and $\mathrm{Deg}_q = 3$. $\mathbb{E}_3(G^*)$ has $18pq-p-q$ arcs pq, where $\mathrm{Deg}_p = \mathrm{Deg}_q = 3$.

We use $ABC(G^*)$ in (11) as

$$ABC(G^*) = \sum_{pq\in\mathbb{E}(G^*)} \sqrt{\frac{\mathrm{Deg}_p + \mathrm{Deg}_q - 2}{\mathrm{Deg}_p\mathrm{Deg}_q}},$$

$$\begin{aligned} ABC(G^*) &= |\mathbb{E}_1(G^*)|\frac{1}{2\sqrt{2}} + |\mathbb{E}_2(G^*)|\frac{1}{2\sqrt{2}} + |\mathbb{E}_3(G^*)|\frac{2}{3} \\ &= (12pq+4p+4q)\frac{1}{2\sqrt{2}} + (3pq-4p-4q)\frac{1}{2\sqrt{2}} + (18pq-q-p)\frac{2}{3} \\ &= \left(12pq\left(\frac{1}{2}\right) + 4p\left(\frac{1}{2}\right) + 4q\left(\frac{1}{2}\right)\right)\sqrt{2} + \left(36pq\left(\frac{1}{2}\right) - 4q\left(\frac{1}{2}\right) - 4p\left(\frac{1}{2}\right)\right)\sqrt{2} \\ &\quad + 18pq\left(\frac{2}{3}\right) - q\left(\frac{2}{3}\right) - p\left(\frac{2}{3}\right). \end{aligned} \tag{40}$$

□

Theorem 6. *(1) $ABC_4(G^*)$ of G^* is*

$$\begin{aligned}ABC_4(G^*) &= 2p\left(\frac{1}{4\sqrt{6}}\right) + 4p\left(\frac{1}{10\sqrt{35}}\right) + 4q\left(\frac{1}{10\sqrt{35}}\right) + 12pq\left(\frac{2}{5\sqrt{2}}\right)\\
&\quad - 2p\left(\frac{2}{5\sqrt{2}}\right) + 22pq\left(\frac{1}{7\sqrt{14}}\right) - 2p\left(\frac{1}{7\sqrt{14}}\right) + 2pq\left(\frac{1}{20\sqrt{110}}\right)\\
&\quad + 2p\left(\frac{1}{20\sqrt{110}}\right) + 4q\left(\frac{1}{20\sqrt{110}}\right) + 6q\left(\frac{1}{42\sqrt{462}}\right)\\
&\quad - 2p\left(\frac{1}{42\sqrt{462}}\right) - 4q\left(\frac{1}{42\sqrt{462}}\right) + 6pq\left(\frac{1}{2}\right) - 2p\left(\frac{1}{2}\right) - 4q\left(\frac{1}{2}\right)\\
&\quad + 2pq\left(\frac{2}{7\sqrt{3}}\right) - p\left(\frac{2}{7\sqrt{3}}\right) - q\left(\frac{2}{7\sqrt{3}}\right) + 8pq\left(\frac{1}{28\sqrt{182}}\right)\\
&\quad + 2pq\left(\frac{1}{3\sqrt{2}}\right) + 2pq\left(\frac{1}{8\sqrt{14}}\right) + 4pq\left(\frac{1}{12\sqrt{30}}\right).\end{aligned} \tag{41}$$

(2) $GA_5(G^*)$ is

$$\begin{aligned}GA_5(G^*) &= 2p + 4n\left(\frac{4}{9\sqrt{5}}\right) + 4q\left(\frac{4}{9\sqrt{5}}\right) + 14pq(1) - 3p(1) + 22pq\left(\frac{1}{6\sqrt{35}}\right)\\
&\quad - 2p\left(\frac{1}{6\sqrt{35}}\right) + 2pq\left(\frac{4}{13\sqrt{10}}\right) + 2p\left(\frac{4}{13\sqrt{10}}\right) + 4q\left(\frac{4}{13\sqrt{10}}\right)\\
&\quad + 6pq\left(\frac{2}{13\sqrt{42}}\right) - 2p\left(\frac{2}{13\sqrt{42}}\right) - 4q\left(\frac{2}{13\sqrt{42}}\right) + 6pq\left(\frac{4}{7\sqrt{3}}\right)\\
&\quad - 2p\left(\frac{4}{7\sqrt{3}}\right) - 4q\left(\frac{4}{7\sqrt{3}}\right) - q(1) + 8pq\left(\frac{4}{15\sqrt{14}}\right) + pq\left(\frac{3}{4\sqrt{7}}\right)\\
&\quad + pq(2) + 4pq\left(\frac{12}{17\sqrt{2}}\right).\end{aligned} \tag{42}$$

Proof. The graph G^* has $66pq - q - p$ number of edges. $\mathbb{E}(G^*)$ can be distributed into twelve disunite groups of edges.

$\mathbb{E}_i(G^*)$, $i = 4, 5, 6 \ldots, 15$. $\mathbb{E}(G^*) = \cup_{i=4}^{15}\mathbb{E}_i(G^*)$.

$\mathbb{E}_4(G^*)$ has $2n$ lines pq, where $S_p = S_q = 4$. $\mathbb{E}_5(G^*)$ supports $4p + 4q$ lines pq, where $S_p = 4$ and $S_q = 5$. $\mathbb{E}_6(G^*)$ contains $12pq - 2p$ edges, where $S_p = S_q = 5$. $\mathbb{E}_7(G^*)$ contains $22pq - 2p$ edges, where $S_p = 5$ and $S_q = 7$. $\mathbb{E}_8(G^*)$ keeps $2pq + 2p + 4q$ edges, where $S_p = 5$ and $S_q = 8$. $E_9(G^*)$ contains $6pq - 2p - 4q$ edges, where $S_p = 6$ and $S_q = 7$. $\mathbb{E}_{10}(G^*)$ contains $6pq - 2p - 4q$ edges, where $S_p = 6$ and $S_q = 8$. $\mathbb{E}_{11}(G^*)$ contains $2pq - p - q$ edges, where $S_p = S_q = 7$. $\mathbb{E}_{12}(G^*)$ holds $8pq$ edges, where $S_p = 7$ and $S_q = 8$. $\mathbb{E}_{13}(G^*)$ holds $2pq$ edges, where $S_p = 7$ and $S_q = 9$. The edge set $\mathbb{E}_{14}(G^*)$ keep $2mn$ edges, where $S_p = S_q = 8$. $\mathbb{E}_{15}(G^*)$ holds $4mn$ edges, here pq, where $S_p = 8$ and $S_q = 9$.

The index is defined in equation (12):

$$ABC_4(G^*) = \sum_{pq \in \mathbb{E}(G^*)} \sqrt{\frac{S_p + S_q - 2}{S_p S_q}}, \tag{43}$$

$$\begin{aligned}
ABC_4(G^*) &= \sqrt{\frac{4+4-2}{4\times 4}}\left|\mathbb{E}_4(G^*)\right| + \sqrt{\frac{4+5-2}{4\times 5}}\left|\mathbb{E}_5(G^*)\right| + \sqrt{\frac{5+5-2}{5\times 5}}\left|\mathbb{E}_6(G^*)\right| \\
&\quad + \sqrt{\frac{5+7-2}{5\times 7}}\left|\mathbb{E}_7(G^*)\right| + \sqrt{\frac{5+8-2}{5\times 8}}\left|\mathbb{E}_8(G^*)\right| + \sqrt{\frac{6+7-2}{6\times 7}}\left|\mathbb{E}_9(G^*)\right| \\
&\quad + \sqrt{\frac{6+8-2}{6\times 8}}\left|\mathbb{E}_{10}(G^*)\right| + \sqrt{\frac{7+7-2}{7\times 7}}\left|\mathbb{E}_{11}(G^*)\right| + \sqrt{\frac{7+8-2}{7\times 8}}\left|\mathbb{E}_{12}(G^*)\right| \\
&\quad + \sqrt{\frac{7+9-2}{7\times 9}}\left|\mathbb{E}_{13}(G^*)\right| + \sqrt{\frac{8+8-2}{8\times 8}}\left|\mathbb{E}_{14}(G^*)\right| + \sqrt{\frac{8+9-2}{8\times 9}}\left|\mathbb{E}_{15}(G^*)\right| \\
&= \sqrt{\frac{6}{16}}\left|\mathbb{E}_4(G^*)\right| + \sqrt{\frac{7}{20}}\left|\mathbb{E}_5(G^*)\right| + \sqrt{\frac{8}{25}}\left|\mathbb{E}_6(G^*)\right| + \sqrt{\frac{10}{35}}\left|\mathbb{E}_7(G^*)\right| \\
&\quad + \sqrt{\frac{11}{40}}\left|\mathbb{E}_8(G^*)\right| + \sqrt{\frac{11}{42}}\left|\mathbb{E}_9(G^*)\right| + \sqrt{\frac{12}{48}}\left|\mathbb{E}_{10}(G^*)\right| + \sqrt{\frac{12}{49}}\left|\mathbb{E}_{11}(G^*)\right| \\
&\quad + \sqrt{\frac{13}{56}}\left|\mathbb{E}_{12}(G^*)\right| + \sqrt{\frac{14}{63}}\left|\mathbb{E}_{13}(G^*)\right| + \sqrt{\frac{14}{64}}\left|\mathbb{E}_{14}(G^*)\right| + \sqrt{\frac{15}{72}}\left|\mathbb{E}_{15}(G^*)\right|.
\end{aligned} \tag{44}$$

After substituting the values $E(G^*) = \cup_{i=5}^{13} E_i(G^*)$, we get

$$\begin{aligned}
&= \sqrt{\frac{6}{16}}(2p) + \sqrt{\frac{7}{20}}(4p+4q) + \sqrt{\frac{8}{25}}(12pq-2q) + \sqrt{\frac{10}{35}}(22pq-2p) \\
&\quad + \sqrt{\frac{11}{40}}(2pq+2p+4q) + \sqrt{\frac{11}{42}}(6pq-2p-4q) + \sqrt{\frac{12}{48}}(6pq-2p-4q) \\
&\quad + \sqrt{\frac{12}{49}}(2pq-p-q) + \sqrt{\frac{13}{56}}(8mn) + \sqrt{\frac{14}{63}}(2pq) + \sqrt{\frac{15}{72}}(4pq).
\end{aligned} \tag{45}$$

After simplification, we get

$$\begin{aligned}
&= \frac{1}{2\sqrt{6}}p + \frac{1}{10\sqrt{35}}(4p+4q) + \frac{2}{5\sqrt{2}}(12pq-2p) + \frac{1}{7\sqrt{14}}(22pq-2p) \\
&\quad + \frac{1}{20\sqrt{110}}(2pq+2p+4q) + \frac{1}{42\sqrt{462}}(6pq-2p-4q) + 3pq - p - 2q \\
&\quad + \frac{2}{7\sqrt{3}}(2pq-q-p) + \frac{2}{7\sqrt{182}}pq + \frac{2}{3\sqrt{2}}pq + \frac{1}{3\sqrt{30}}pq.
\end{aligned} \tag{46}$$

By utilizing the definition of $GA_5(G^*)$ from equation (18),

$$GA_5(G^*) = \sum_{pq \in \mathbb{E}(G^*)} \frac{2\sqrt{S_p S_q}}{S_p + S_q}, \tag{47}$$

$$\begin{aligned}
GA_5(G^*) &= \frac{2\sqrt{4\times 4}}{4+4}\left|\mathbb{E}_4(G^*)\right| + \frac{2\sqrt{4\times 5}}{4+5}\left|\mathbb{E}_5(G^*)\right| + \frac{2\sqrt{5\times 5}}{5+5}\left|\mathbb{E}_6(G^*)\right| \\
&\quad + \frac{2\sqrt{5\times 7}}{5+7}\left|\mathbb{E}_7(G^*)\right| + \frac{2\sqrt{5\times 8}}{5+8}\left|\mathbb{E}_8(G^*)\right| + \frac{2\sqrt{6\times 7}}{6+7}\left|\mathbb{E}_9(G^*)\right| \\
&\quad + \frac{2\sqrt{6\times 8}}{6+8}\left|\mathbb{E}_{10}(G^*)\right| + \frac{2\sqrt{7\times 7}}{7+7}\left|\mathbb{E}_{11}(G^*)\right| + \frac{2\sqrt{7\times 8}}{7+8}\left|\mathbb{E}_{12}(G^*)\right| \\
&\quad + \frac{2\sqrt{7\times 9}}{7+9}\left|\mathbb{E}_{13}(G^*)\right| + \frac{2\sqrt{8\times 8}}{8+8}\left|\mathbb{E}_{14}(G^*)\right| + \frac{2\sqrt{8\times 9}}{8+9}\left|\mathbb{E}_{15}(G^*)\right|.
\end{aligned} \tag{48}$$

After substituting the values $\mathbb{E}(G^*) = \cup_{i=5}^{13}\mathbb{E}_i(G^*)$, we get

$$
\begin{aligned}
&= \frac{2\sqrt{16}}{8}(2p) + \frac{2\sqrt{20}}{9}(4p+4q) + \frac{2\sqrt{25}}{10}(12pq-2p) + \frac{2\sqrt{35}}{12}(22pq-2p) \\
&+ \frac{2\sqrt{40}}{13}(2pq+2p+4q) + \frac{2\sqrt{42}}{13}(6pq-2p-4q) + \frac{2\sqrt{48}}{14}(6pq-2p-4q) \\
&+ \frac{2\sqrt{49}}{14}(2pq-q-p) + \frac{2\sqrt{56}}{15}(8pq) + \frac{2\sqrt{63}}{16}(2pq) + +\frac{2\sqrt{64}}{16}(2pq) \\
&+ \frac{2\sqrt{72}}{17}(4pq).
\end{aligned}
\tag{49}
$$

After simplification,

$$
\begin{aligned}
&= -p + \frac{4}{9\sqrt{5}}(4p+4q) + 16pq + \frac{1}{6\sqrt{35}}(22pq-2p) + \frac{4}{13}\sqrt{10}(2pq+2p+4q) \\
&+ \frac{2}{13\sqrt{42}}(6pq-2p-4q) + \frac{4}{7\sqrt{3}}(6pq-2p-4q) - q + \frac{32}{15}\sqrt{14}pq + \frac{3}{4\sqrt{7}}pq \\
&+ \frac{48}{17}\sqrt{2}pq.
\end{aligned}
\tag{50}
$$

□

Theorem 7. *Consider the following:*

(1) The general Randić index of graph G^* is given as follows:

$$R_\alpha(G^*) = 12pq(4^\alpha) + 4p(4^\alpha) + 4q(4^\alpha) + 36pq(6^\alpha) - 4p(6^\alpha) - 4q(6^\alpha) + 18pq(9^\alpha) - q(9^\alpha) - p(9^\alpha). \tag{51}$$

(2) Randić index of graph G^* is

$$R(G^*) = 12pq + \frac{5}{3}p + \frac{5}{3}q + \frac{1}{6\sqrt{6}}(36pq-4p-4q). \tag{52}$$

(3) Reduced reciprocal Randić index of graph G^* is

$$RRR(G^*) = 48pq + 2p + 2q + \sqrt{2}(36pq-4p-4q). \tag{53}$$

(4) Reciprocal Randić index of graph G^* is

$$RR(G^*) = 78pq + 5p + 5q + \sqrt{6}(36pq-4p-4q). \tag{54}$$

Proof. G^* encounters $66pq-p-q$ lines and $54pq$ vertices. Vertices of degree 2 are $30pq+2p+2q$ and of degree 3 are $24pq-2p-2q$. The cardinality of $\mathbb{E}$ of G^* is $66pq-p-q$. $\mathbb{E}(G^*)$ is divided into 3 dissociate edge groups that rely on the degrees of the end points, i.e., $\mathbb{E}(G^*) = \mathbb{E}_1(G^*) \cup \mathbb{E}_2(G^*) \cup \mathbb{E}_3(G^*)$. $\mathbb{E}_1(G^*)$ has $12pq+4p+4q$ edges pq, where $\mathrm{Deg}_p = \mathrm{Deg}_q = 2$. $\mathbb{E}_2(G^*)$ has $36pq-4p-4q$ edges pq, where $\mathrm{Deg}_p = 2$ and $\mathrm{Deg}_q = 3$. $\mathbb{E}_3(G^*)$ has $18pq-p-q$ arcs pq, where $\mathrm{Deg}_p = \mathrm{Deg}_q = 3$.

We use general Randic index in (13) as

$$R_\alpha(G^*) = \sum_{pq\in\mathbb{E}(G^*)} \left(\mathrm{Deg}_p \mathrm{Deg}_q\right)^\alpha. \tag{55}$$

Now, we have

$$
\begin{aligned}
R_\alpha(G^*) &= \sum_{pq\in\mathbb{E}_1(G^*)} \left(\mathrm{Deg}_p \mathrm{Deg}_q\right)^\alpha + \sum_{pq\in\mathbb{E}_2(G^*)} \left(\mathrm{Deg}_p \mathrm{Deg}_q\right)^\alpha + \sum_{xy\in\mathbb{E}_3(G^*)} \left(\mathrm{Deg}_p \mathrm{Deg}_q\right)^\alpha \\
&= 4\left|\mathbb{E}_1(G^*)\right| + 6\left|\mathbb{E}_2(G^*)\right| + 9\left|\mathbb{E}_3(G^*)\right| \\
&= 4(12pq + 4p + 4q) + 6(36pq - 4q - 4p) + 9(18pq - p - q).
\end{aligned}
\tag{56}
$$

After simplification, we get

$$
= 426pq - 17p - 17q. \tag{57}
$$

By the use of Randić index (14),

$$
\begin{aligned}
R(G^*) &= \sum_{pq\in\mathbb{E}(G^*)} \frac{1}{\sqrt{\mathrm{Deg}_p \mathrm{Deg}_q}}, \\
R(G^*) &= \sum_{pq\in\mathbb{E}_1(G^*)} \frac{1}{\sqrt{\mathrm{Deg}_p \mathrm{Deg}_q}} + \sum_{pq\in\mathbb{E}_2(G^*)} \frac{1}{\sqrt{\mathrm{Deg}_p \mathrm{Deg}_q}} + \sum_{pq\in\mathbb{E}_3(G^*)} \frac{1}{\sqrt{\mathrm{Deg}_p \mathrm{Deg}_q}} \\
&= \frac{1}{2}\left|\mathbb{E}_1(G^*)\right| + \frac{1}{\sqrt{6}}\left|\mathbb{E}_2(G^*)\right| + \frac{1}{3}\left|\mathbb{E}_3(G^*)\right| \\
&= \frac{1}{2}(12pq + 4p + 4q) + \frac{1}{\sqrt{6}}(36pq - 4q - 4p) + \frac{1}{3}(18pq - p - q).
\end{aligned}
\tag{58}
$$

After simplification,

$$
R(G^*) = 12pq + \frac{5}{3}n + \frac{5}{3}q + \frac{1}{6\sqrt{6}}(36pq - 4p - 4q). \tag{59}
$$

Definition of $RRR(G^*)$ index from equation (16) is

$$
\begin{aligned}
RRR(G^*) &= \sum_{pq\in\mathbb{E}(G^*)} \sqrt{\left(\mathrm{Deg}_p - 1\right)\left(\mathrm{Deg}_q - 1\right)}, \\
RRR(G^*) &= \sum_{pq\in\mathbb{E}_1(G^*)} \sqrt{\left(\mathrm{Deg}_p - 1\right)\left(\mathrm{Deg}_q - 1\right)} + \sum_{pq\in\mathbb{E}_2(G^*)} \sqrt{\left(\mathrm{Deg}_p - 1\right)\left(\mathrm{Deg}_q - 1\right)} \\
&\quad + \sum_{pq\in\mathbb{E}_3(G^*)} \sqrt{\left(\mathrm{Deg}_p - 1\right)\left(\mathrm{Deg}_q - 1\right)} \\
&= 1\left|\mathbb{E}_1(G^*)\right| + \sqrt{2}\left|\mathbb{E}_2(G^*)\right| + 2\left|\mathbb{E}_3(G^*)\right| \\
&= (12pq + 4p + 4q) + \sqrt{2}(36pq - 4q - 4p) + 2(18pq - p - q) \\
&= 48pq + 2p + 2q + \sqrt{2}(36pq - 4q - 4p).
\end{aligned}
\tag{60}
$$

Now, by utilizing the definition of reduced Randić index from equation (15),

$$\begin{aligned}RR(G^*) &= \sum_{pq\in\mathbb{E}(G^*)} \sqrt{\mathrm{Deg}_p\mathrm{Deg}_q},\\ &= \sum_{pq\in\mathbb{E}_1(G^*)} \sqrt{\mathrm{Deg}_p\mathrm{Deg}_q} + \sum_{pq\in\mathbb{E}_2(G^*)} \sqrt{\mathrm{Deg}_p\mathrm{Deg}_q} + \sum_{pq\in\mathbb{E}_3(G^*)} \sqrt{\mathrm{Deg}_p\mathrm{Deg}_q}\\ &= 2\left|\mathbb{E}_1(G^*)\right| + \sqrt{6}\left|\mathbb{E}_2(G^*)\right| + 3\left|\mathbb{E}_3(G^*)\right|\\ &= 2(12pq + 4p + 4q) + \sqrt{6}(36pq - 4q - 4p) + 3(18pq - p - q).\end{aligned} \tag{61}$$

Theorem 8. *We have graph G^* and its different indices are explained here.*

(1) GA index is as follows:

$$GA(G^*) = 30pq + 3p + 3q + 36pq\left(\frac{2}{5\sqrt{6}}\right) - 4p\left(\frac{2}{5\sqrt{6}}\right) - 4q\left(\frac{2}{5\sqrt{6}}\right). \tag{62}$$

(2) Sum connectivity index is given as follows:

$$\begin{aligned}X_\alpha(G^*) = {} & 12pq(4^\alpha) + 4p(4^\alpha) + 4q(4^\alpha) + 36pq(5^\alpha)\\ & - 4p(5^\alpha) - 4q(5^\alpha) + 18pq(6^\alpha) - q(6^\alpha) - p(6^\alpha).\end{aligned} \tag{63}$$

(3) Forgotten index of G^* is

$$\begin{aligned}F(G^*) = {} & 12pq(8) + 4p(8) + 4q(8) + 36pq(13)\\ & - 4p(13) - 4q(13) + 18pq(18) - q(18) - p(18).\end{aligned} \tag{64}$$

□

Proof. G^* encounters $66pq - p - q$ edges and $54pq$ vertices. Vertex count of degree 2 are $30pq + 2p + 2q$ and of degree 3 are $24pq - 2p - 2q$. The cardinality line group $\mathbb{E}$ of G^* is $66pq - p - q$. $E(G^*)$ is classified into three disjoint edge groups, i.e., $\mathbb{E}(G^*) = \mathbb{E}_1(G^*) \cup \mathbb{E}_2(G^*) \cup \mathbb{E}_3(G^*)$. $\mathbb{E}_1(G^*)$ has $12pq + 4p + 4q$ edges pq, where $\mathrm{Deg}_p = \mathrm{Deg}_q = 2$. $\mathbb{E}_2(G^*)$ has $36pq - 4p - 4q$ edges pq, where $\mathrm{Deg}_p = 2$ and $\mathrm{Deg}_q = 3$. $\mathbb{E}_3(G^*)$ has $18pq - p - q$ edges pq, where $\mathrm{Deg}_p = \mathrm{Deg}_q = 3$.

We use geometric arithmetic index in (17) as

$$GA(G^*) = \sum_{pq\in\mathbb{E}(G^*)} \frac{2\sqrt{\mathrm{Deg}_p\mathrm{Deg}_q}}{\mathrm{Deg}_p+\mathrm{Deg}_q},$$

$$\begin{aligned}GA(G^*) &= \sum_{pq\in\mathbb{E}_1(G^*)} \frac{2\sqrt{\mathrm{Deg}_p\mathrm{Deg}_q}}{\mathrm{Deg}_p+\mathrm{Deg}_q} + \sum_{pq\in\mathbb{E}_2(G^*)} \frac{2\sqrt{\mathrm{Deg}_p\mathrm{Deg}_q}}{\mathrm{Deg}_p+\mathrm{Deg}_q} + \sum_{pq\in\mathbb{E}_3(G^*)} \frac{2\sqrt{\mathrm{Deg}_p\mathrm{Deg}_q}}{\mathrm{Deg}_p+\mathrm{Deg}_q}\\ &= 1\left|\mathbb{E}_1(G^*)\right| + \left(\frac{2}{5\sqrt{6}}\right)\left|\mathbb{E}_2(G^*)\right| + 1\left|\mathbb{E}_3(G^*)\right|\\ &= (12pq + 4p + 4q) + \sqrt{6}(36pq - 4q - 4p) + (18pq - p - q).\end{aligned} \tag{65}$$

After simplification, we obtain

$$= 30pq + 3p + 3q + \sqrt{6}(36pq - 4q - 4p). \tag{66}$$

From equation (20), we get

$$\begin{aligned}
\chi_\alpha(G^*) &= \sum_{pq\in\mathbb{E}(G^*)} \left(\mathrm{Deg}_p + \mathrm{Deg}_q\right)^\alpha,\\
\chi_\alpha(G^*) &= \sum_{pq\in\mathbb{E}_1(G^*)} \left(\mathrm{Deg}_p + \mathrm{Deg}_q\right)^\alpha + \sum_{pq\in\mathbb{E}_2(G^*)} \left(\mathrm{Deg}_p + \mathrm{Deg}_q\right)^\alpha + \sum_{pq\in\mathbb{E}_3(G^*)} \left(\mathrm{Deg}_p + \mathrm{Deg}_q\right)^\alpha\\
&= (4)^\alpha\left|\mathbb{E}_1(G^*)\right| + (5)^\alpha\left|\mathbb{E}_2(G^*)\right| + (6)^\alpha\left|\mathbb{E}_3(G^*)\right|\\
&= (4)^\alpha(12pq + 4p + 4q) + (5)^\alpha(36pq - 4q - 4p) + (6)^\alpha(18pq - p - q).
\end{aligned} \tag{67}$$

We use forgotten index in (19) as

$$\begin{aligned}
F(G^*) &= \sum_{pq\in\mathbb{E}(G^*)} \left(\mathrm{Deg}_p^2 + \mathrm{Deg}_q^2\right),\\
F(G^*) &= \sum_{pq\in\mathbb{E}_1(G^*)} \left(\mathrm{Deg}_p^2 + \mathrm{Deg}_q^2\right) + \sum_{pq\in\mathbb{E}_2(G^*)} \left(\mathrm{Deg}_p^2 + \mathrm{Deg}_q^2\right) + \sum_{pq\in\mathbb{E}_3(G^*)} \left(\mathrm{Deg}_p^2 + \mathrm{Deg}_q^2\right)\\
&= 8\left|\mathbb{E}_1(G^*)\right| + 13\left|\mathbb{E}_2(G^*)\right| + 18\left|\mathbb{E}_3(G^*)\right|\\
&= 8(12pq + 4p + 4q) + 13(36pq - 4q - 4p) + 18(18pq - p - q)\\
&= 888pq - 38p - 38q.
\end{aligned} \tag{68}$$

□

Theorem 9. *Let G^* be graph:*

(1) Symmetric division index is

$$SD(G^*) = 138pq - \frac{8}{3}p - \frac{8}{3}q. \tag{69}$$

(2) Harmonic index is

$$H(G^*) = \frac{132}{5}pq + \frac{1}{15}p + \frac{1}{15}q. \tag{70}$$

Proof. G^* encounters $66pq - p - q$ edge and $54pq$ points. Vertex counts of degree 2 are $30pq + 2p + 2q$ and of degree 3 are $24pq - 2p - 2q$. The edge set $E(G^*)$ splits into three distinct line groups.

$\mathbb{E}(G^*) = \mathbb{E}_1(G^*) \cup \mathbb{E}_2(G^*) \cup \mathbb{E}_3(G^*)\mathbb{E}_1(G^*)$ has $12pq + 4p + 4q$ lines pq, where $\mathrm{Deg}_p = \mathrm{Deg}_q = 2$. $\mathbb{E}_2(G^*)$ has $36pq - 4p - 4q$ lines pq, where $\mathrm{Deg}_p = 2$ and $\mathrm{Deg}_q = 3$. $\mathbb{E}_3(G^*)$ has $18pq - p - q$ lines pq, where $\mathrm{Deg}_p = \mathrm{Deg}_q = 3$.

From equation (21), we obtain

$$\begin{aligned}
SD(G^*) &= \sum_{pq\in\mathbb{E}(G^*)} \frac{\mathrm{Deg}_p^2 + \mathrm{Deg}_q^2}{\left(\mathrm{Deg}_p \times \mathrm{Deg}_q\right)}\\
SD(G^*) &= \sum_{pq\in\mathbb{E}_1(G^*)} \frac{\mathrm{Deg}_p^2 + \mathrm{Deg}_q^2}{\left(\mathrm{Deg}_p \times \mathrm{Deg}_q\right)} + \sum_{pq\in\mathbb{E}_2(G^*)} \frac{\mathrm{Deg}_p^2 + \mathrm{Deg}_q^2}{\left(\mathrm{Deg}_p \times \mathrm{Deg}_q\right)} + \sum_{pq\in\mathbb{E}_3(G^*)} \frac{\mathrm{Deg}_p^2 + \mathrm{Deg}_q^2}{\left(\mathrm{Deg}_p \times \mathrm{Deg}_q\right)}\\
&= 2\left|\mathbb{E}_1(G^*)\right| + \frac{13}{5}\left|\mathbb{E}_2(G^*)\right| + 2\left|\mathbb{E}_3(G^*)\right|\\
&= 2(12pq + 4p + 4q) + \frac{13}{5}(36pq - 4q - 4p) + 2(18pq - p - q).
\end{aligned} \tag{71}$$

From equation (22),

$$
\begin{aligned}
H(G^{*}) &= \sum_{pq\in\mathbb{E}(G^{*})} \frac{2}{\left(\mathrm{Deg}_p \times \mathrm{Deg}_q\right)}\\
H(G^{*}) &= \sum_{pq\in\mathbb{E}_1(G^{*})} \frac{2}{\left(\mathrm{Deg}_p \times \mathrm{Deg}_q\right)} + \sum_{pq\in\mathbb{E}_2(G^{*})} \frac{2}{\left(\mathrm{Deg}_p \times \mathrm{Deg}_q\right)} + \sum_{pq\in\mathbb{E}_3(G^{*})} \frac{2}{\left(\mathrm{Deg}_p \times \mathrm{Deg}_q\right)}\\
&= \frac{2}{4}\left|\mathbb{E}_1(G^{*})\right| + \frac{2}{5}\left|\mathbb{E}_2(G^{*})\right| + \frac{2}{6}\left|\mathbb{E}_3(G^{*})\right|\\
&= \frac{1}{2}(12pq + 4p + 4q) + \frac{2}{5}(36pq - 4q - 4p) + \frac{1}{3}(18pq - p - q)\\
&= \frac{132}{5}pq + \frac{19}{15}p + \frac{19}{15}q.
\end{aligned}
\tag{72}
$$

□

3. Conclusion

We find some topological descriptors of hydrocarbon structure. Randić index has well known applications in the study of physicochemical characteristics of alkane, for example, surface area, enthalpy of formation, boiling point, and melting point. The index has the most functional role in pharmacology. Similarly, forgotten index is helpful to figure out the strength of organic structures. Symmetric division index has productive applications to find heat formation of chemical structures. GA index can forecast biological activities of compounds. ABC index has an outstanding role in finding strain energy and stability of isoparaffins. Our results will be helpful to estimate the physicochemical properties of hydrocarbon structures.

4. Future Work

In future, we will find the distance-based and spectrum-based topological indices of hydrocarbon structures.

Data Availability

No data were used to support this study.

Conflicts of Interest

The authors declares that there are no conflicts of interest.

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References

[1] D. Chassapis and M. Kotsakosta, "Crossing the bridges of Konigsberg in a primary mathematics classroom," *Mathematics in School*, vol. 32, no. 1, pp. 11–13, 2003.

[2] F. Harary, Ed., *A Seminar on Graph Theory*, Courier Dover Publications, Mineola, NY, USA, 2015.

[3] J. A. Bondy and U. S. R. Murty, *Graph Theory with Applications*, Vol. 290, Macmillan, , London, UK, 1976.

[4] J. M. Rodriguez and J. M. Sigarreta, "On the geometric-arithmetic index," *MATCH Communications in Mathematical and in Computer Chemistry*, vol. 74, pp. 103–120, 2015.

[5] S. Zhang and H. Zhang, "Unicyclic graphs with the first three smallest and largest first general Zagreb index," *MATCH Communications in Mathematical and in Computer Chemistry*, vol. 55, no. 20, p. 6, 2006.

[6] G. H. Fath-Tabar, "Old and new Zagreb indices of graphs," *MATCH Communications in Mathematical and in Computer Chemistry*, vol. 65, pp. 79–84, 2011.

[7] M. Ghorbani and M. Ghazi, "Computing some topological indices of triangular Benzenoid," *Digest Journal of Nanomaterials and Biostructures*, vol. 5, no. 4, pp. 1107–1111, 2010.

[8] I. Gutman, "Degree-based topological indices," *Croatica Chemica Acta*, vol. 86, no. 4, pp. 351–361, 2013.

[9] K. C. Das and I. Gutman, "Some properties of the second Zagreb index," *MATCH Communications in Mathematical and in Computer Chemistry*, vol. 52, no. 1, pp. 3–1, 2004.

[10] E. Deutsch and S. Klavžar, "M-polynomial and degree-based topological indices," 2014, https://arxiv.org/abs/1407.1592.

[11] K. C. Das, I. Gutman, and B. Furtula, "On atom-bond connectivity index," *Chemical Physics Letters*, vol. 511, no. 4–6, pp. 452–454, 2011.

[12] X. Li and Y. Shi, "A survey on the Randic index," *MATCH Communications in Mathematical and in Computer Chemistry*, vol. 59, no. 1, pp. 127–156, 2008.

[13] I. Gutman, B. Furtula, and C. Elphick, "Three new/old vertex-degree-based topological indices," *MATCH Communications in Mathematical and in Computer Chemistry*, vol. 72, no. 3, pp. 617–632, 2014.

[14] H. A. J. R. A. Siddiqui and M. R. Farahani, "Forgotten polynomial and forgotten index of certain interconnection networks," *Open Journal of Mathematical Analysis*, vol. 1, no. 1, pp. 45–60, 2017.

[15] B. Zhou and N. Trinajstić, "On general sum-connectivity index," *Journal of Mathematical Chemistry*, vol. 47, no. 1, pp. 210–218, 2010.

[16] A. Ali, S. Elumalai, and T. Mansour, "On the symmetric division deg index of molecular graphs," *MATCH Communications in Mathematical and in Computer Chemistry*, vol. 83, pp. 205–220, 2020.

[17] M. Baca, J. Horváthová, M. Mokrišová, and A. Suhányiová, “On topological indices of fullerenes,” *Applied Mathematics and Computation*, vol. 251, pp. 154–161, 2015.
[18] S. C. Basak, A. T. Balaban, G. D. Grunwald, and B. D. Gute, “Topological indices: their nature and mutual relatedness,” *Journal of Chemical Information and Computer Sciences*, vol. 40, no. 4, pp. 891–898, 2000.
[19] K. C. Das, I. Gutman, and B. Furtula, “Survey on geometric-arithmetic indices of graphs,” *MATCH Communications in Mathematical and in Computer Chemistry*, vol. 65, no. 3, pp. 595–644, 2011.
[20] K. C. Das, “On geometric-arithmetic index of graph,” *MATCH Communications in Mathematical and in Computer Chemistry*, vol. 64, no. 3, pp. 619–630, 2010.
[21] R. Gozalbes, J. Doucet, and F. Derouin, “Application of topological descriptors in QSAR and drug design: history and new trends,” *Current Drug Targets - Infectious Disorders*, vol. 2, no. 1, pp. 93–102, 2002.
[22] M. Imran, S. Hayat, and M. Y. H. Mailk, “On topological indices of certain interconnection networks,” *Applied Mathematics and Computation*, vol. 244, pp. 936–951, 2014.
[23] V. R. Kulli, “Reduced second hyper-Zagreb index and its polynomial of certain silicate networks,” *Journal of Mathematics and Informatics*, vol. 14, pp. 11–16, 2018.
[24] B. Mondal and K. De, “An overview applications of graph theory in real field,” *International Journal of Scientific Research in Computer Science, Engineering and Information Technology*, vol. 2, no. 5, pp. 751–759, 2017.
[25] S. Nikoliç, G. Kovaçeviç, A. Miliçeviç, and N. Trinajstiç, “The Zagreb indices 30 years after,” *Croatica Chemica Acta*, vol. 76, no. 2, pp. 113–124, 2003.