A STUDY OF TOPOLOGICAL ASSESSMENT OF HEXANE PARA-LINE GRAPHS WITH THE ANALYSIS OF THE CHEMICAL COMPOSITION

Mukhtar Ahmad[1], Ather Qayyum[2], Muhammad Maaz[3], Muhammad Muawwaz[3] and Siti Suzlin Supadi[2]

[1] Department of Mathematics, Khawja Fareed University of Engineering and Information Technology Rahim Yar Khan, Pakistan.

[2] Institute of Mathematical Sciences, Universiti Malaya, Malaysia .

[3] Institute of Southern Punjab Multan, Pakistan.

Correspondence Author: dratherqayyum@um.edu.my

Correspondence Author: itxmemuktar@gmail.com

Abstract: Topological indices (TIs) are widely utilized as molecular descriptors in the development of quantitative structure-activity relationships (QSAR), quantitative structure-property relationships (QSPR) and quantitative structure-toxicity relationships (QSTR). Molecular descriptors play a crucial role in mathematical chemistry, particularly in investigations involving quantitative structure-property relationships (QSPR) and quantitative structure-activity relationships (QSAR). A topological index represents a numerical mapping of a molecule's structure. It is employed to characterize the physicochemical properties of specific substances and remains unchanged under graph transformations. The focus of our study is to analyze the chemical composition of pentacene. Our research developed into various indices, including the general randic connectivity index, the first and second multiple zagreb indices, the first general zagreb index, the atomic bond connectivity index, the hyper zagreb index, the geometric arithmetic index, the general sum-connectivity index, the fifth class of geometric arithmetic indices for hexane para-line graphs of multi-pentacene, linear pentacene and linear [n]-pentacene.

Keywords: Graphs of hexane para-line, topological indices, pentacene, nanostructures, linear pentacene.

1. Introduction and Preliminaries

All substances molecule possesses qualities, both chemical and physical and certain may also exhibit physiologically active characteristics. Several pharmaceutical companies are really hunting for novel antibacterial chemicals. For this reason, hundreds of compounds are examined, however costly examinations for biology. In order to circumvent such issue, additional methods for investigating potential antibiotics employ the relationship between structural features and biological activity or features of chemical and physical nature. Topological indices or molecular descriptors, provide insights into the physicochemical properties of molecules. They are valuable tools for understanding and explaining the characteristics of chemical compounds. Several graph invariants have been created in recent years and have been used in many academic fields such as structural chemistry, environmental chemistry, theoretical chemistry, pharmacology and toxicology. Because of the substantial industrial need, researchers are urged to study topological indices. More than 400 topological indexes have been opened a consequence of research. Chemical compounds topological structures and chemical characteristics are tightly related, since each compound's shape is critical to

determining its functionality. Topological indices are often used in multilinear regression modelling, chemical documentation, drug design, QSAR/QSPR modelling and database selection. Molecular descriptors are utilized to describe the physicochemical properties of molecular structures. These descriptors can be classified into three main types degree-based indices [1-5], distance-based indices [6-11] and spectrum-based indices [12-15]. Studies that have been documented in the literature (see [16-18]) use indicators that are based on both distances and degrees.

Due to pentacene's important functions in both electrical devices and organic solar cells, a popular hydrocarbon semiconductor, it is necessary to optimise organic solar cells for less expensive energy sources[19]. The georgia institute of technology researchers have developed method to produce portable artificial solar cells. Pentacene has been shown to be a very efficient means of converting sunlight into energy. In contrast to other materials, pentacene functions well as a semiconductor due to its crystalline properties. Pentacene's relevance motivated us to do topological study on it and as a result, we have made several important discoveries that could be helpful for analysing pentacene's physical and chemical characteristics See [20, 21] for further topological research on pentacene.

Hexane is an organic compound classified as a straight-chain alkane containing six carbon atoms, represented by the molecular formula C_6H_{14}. It is characterized as a colorless and odorless liquid in its pure form, with a boiling point of approximately 69 celsius (156 farhenheit). Hexane is commonly employed as a non-polar solvent due to its relative safety, low reactivity, afford ability and ease of evaporation. Additionally, hexane plays a significant role as a constituent in gasoline. Sometimes, the term "hexane" refers to a mixture consisting primarily ($>$ 60 percent) of hexane, along with varying amounts of isomeric compounds such as 2-methyl pentane, 3-methyl pentane and possibly smaller quantities of non-isomeric alkanes (cyclo) of C_5, C_6 and C_7. Hexane is preferred in large-scale operations where a single isomer is not required, such as in the context of cleaning solvents or chromatography procedures. Hexane is a refined crude oil used in various industrial applications, including adhesives, roofing materials, leather products, cooking oil extraction, degreasing, cleaning, and textile manufacturing. It is commonly used in the US for soybean oil extraction, causing controversy due to FDA lack of regulation. In laboratories, it is used to extract grease and oil contaminants for analysis. Hexane is also used in reactions involving strong foundations, like the creation of organolithium compounds like butyllithium. Hexane serves as a non-polar solvent in chromatography, where it finds widespread use. However, it's important to note that hexane may contain impurities in the form of higher alkanes, which have similar retention times as the solvent itself. Consequently, fractions containing hexane may also contain these impurities, which can lead to the presence of alkanes in solid compounds obtained from chromatographic analysis, potentially interfering with the accuracy of the analysis.

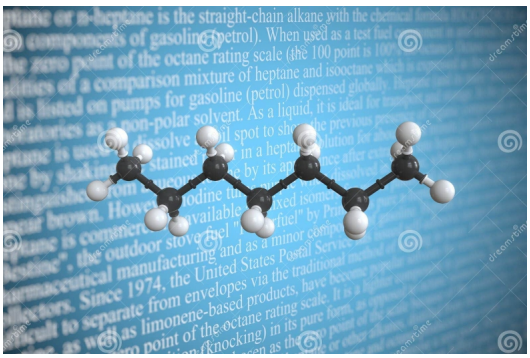


FIGURE 1. fig

Hexane's acute toxicity is relatively low. In halation of n-hexane or hexane n at a concentration of 5000 parts per million (ppm) for a duration of just 10 minutes can result in significant vertigo. Exposure to concentrations ranging from 2500 to 1000 ppm for 12 hours can lead to symptoms such as fatigue, loss of appetite, drowsiness and tingling or numbness in the extremities. In the range of 2500 to 5000 ppm, it can cause cold pulsation in the extremities, muscle weakness, headache, loss of appetite and blurred vision. Prolonged occupational exposure to elevated levels of n-hexane or hexane n has been associated with neurotoxicity among workers in printing presses, as well as peripheral neuropathy in auto mechanics in the United States, Europe, Asia and North America, particularly in furniture and shoe factories. In certain circumstances, n-hexane is permitted for various applications such as serving as a denaturant for alcohol and as a cleaning agent in the textile, furniture and leather industries. Similar to gasoline, hexane is highly volatile and poses a risk of explosion. Figure 1(a) depicts the molecular graph and its structure of hexane . Further more, figure 2(b) and (c) exhibit the hexane para-line graphs derived from the molecular plot of hexane. now figure are;

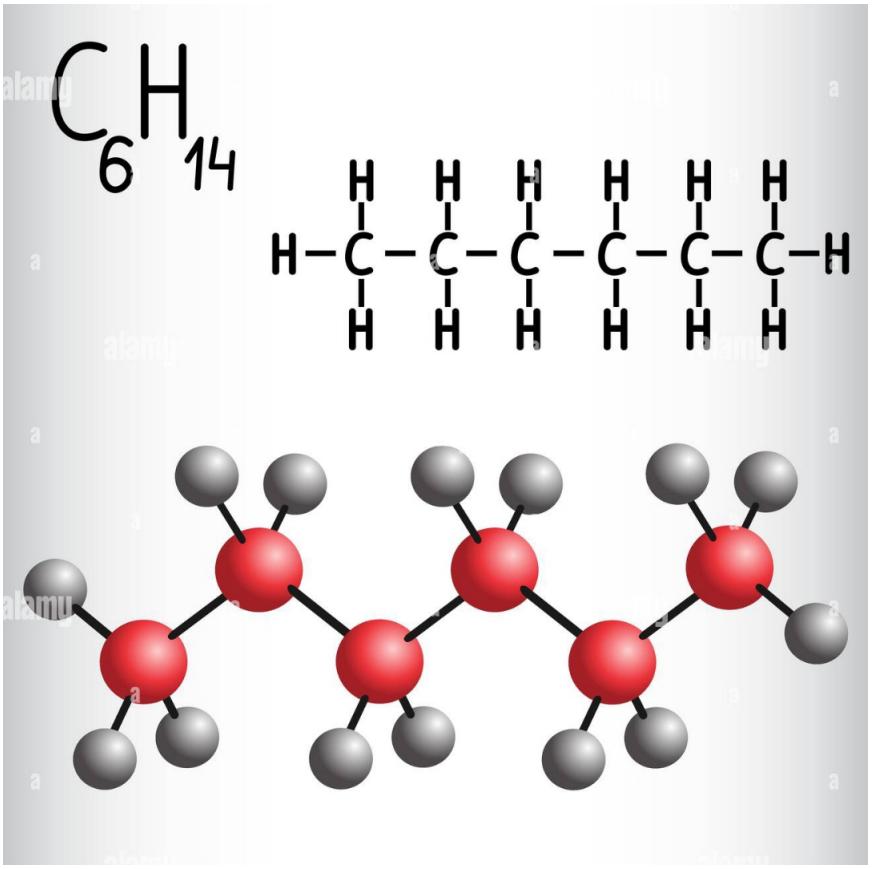
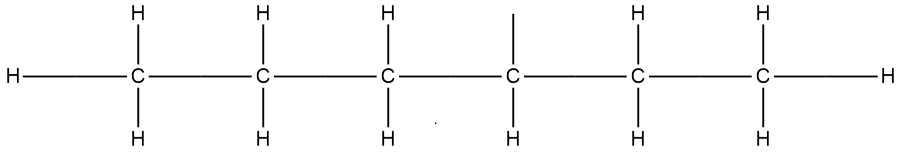


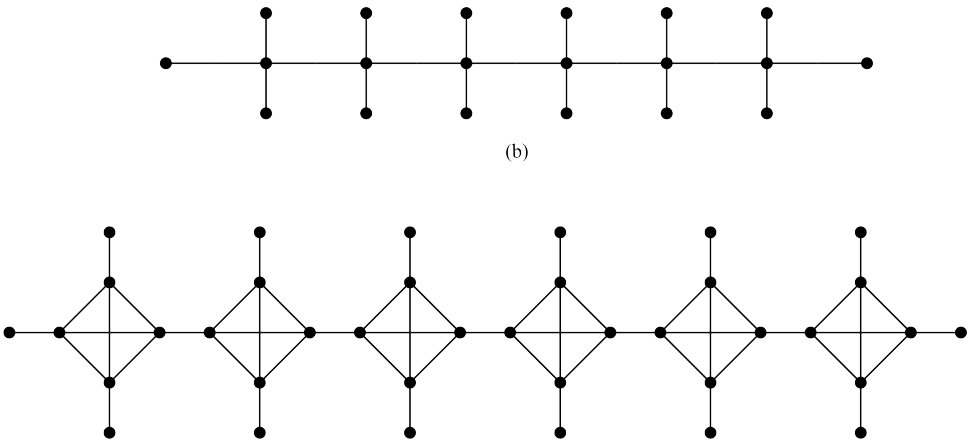
FIGURE 2. fig

The definition of the generic randic connection index G is [12].



(a)

FIGURE 3. (a)Molecular structure of hexane



(b)

(c)

FIGURE 4. (b) Molecular graph of hexane, (c) Tera-line graph of hexane

$$R_\alpha(G) = \sum_{x_1x_2 \in E(G)} (d_{x_1} d_{x_2})^\alpha \tag{1}$$

The first universal zagreb index was presented by Li and Zhao[22]:

$$M_\alpha(G) = \sum_{x_1 \in V(G)} (d_{x_1})^\alpha \tag{2}$$

The the general sum connectivity index of the G chart was introduced in 2010 [23]:

$$\chi_\alpha(G) = \sum_{x_1x_2 \in E(G)} (d_{x_1} + d_{x_2})^\alpha \tag{3}$$

The index (ABC) was proposed by Estrada [24]. It is expressed as follows for a graph G:

$$ABC(G) = \sum_{x_1x_2 \in E(G)} \sqrt{\frac{d_{x_1} + d_{x_2} - 2}{d_{x_1} d_{x_2}}} \tag{4}$$

The geometric-arithmetic index (GA) was introduced by Vukicevic and Furtula [25]. It is denoted as GA and is defined as follows for a graph G resently A. Asghar et.al[31]:

$$GA(G) = \sum_{x_1x_2 \in E(G)} \frac{2\sqrt{(d_{x_1} d_{x_2})}}{(d_{x_1} + d_{x_2})} \tag{5}$$

Ghorbani et al. [26] described another index belonging to the 4th class of indices, denoted as (ABC), which is defined as follows resently Zaib Hassan Niazi et.al[32]:

$$ABC_4(G) = \sum_{x_1x_2 \in E(G)} \sqrt{\frac{d_{S_1} + S_{x_2} - 2}{S_{x_1} S_{x_2}}} \tag{6}$$

Graovac et al. [27] introduced a fifth class of geometric-arithmetic indices denoted as GA_5, which is defined as follows:

$$GA_5(G) = \sum_{x_1x_2 \in E(G)} \frac{2\sqrt{(S_{x_1} S_{x_2})}}{(S_{x_1} + S_{x_2})} \tag{7}$$

Established the hyper-zagreb index in 2013 as follows resently Mukhtar Ahmad et.al[33]:

$$HM(G) = \sum_{x_1x_2 \in E(G)} (d_{x_1} + d_{x_2})^2 \tag{8}$$

In 2012, Ghorbani and Azimi introduced two new types of zagreb graph indices. The first is the first multiple zagreb index, denoted as $PM_1(G)$. The second multiple zagreb index is used, denoted as $PM_2(G)$. Additionally, the first and second zagreb polynomials, $M_1(G, p)$ and $M_2(G, p)$, respectively, are characterised as resently Mukhtar Ahmad et.al[34]:

$$PM_1(G) = \Pi_{x_1x_2 \in E(G)} (d_{x_1} + d_{x_2}) \tag{9}$$

$$PM_2(G) = \Pi_{x_1x_2 \in E(G)} (d_{x_1} \times d_{x_2}) \tag{10}$$

$$M_1(G, p) = \sum_{x_1x_2 \in E(G)} P^{(d_{x_1} + d_{x_2})} \tag{11}$$

$$M_2(G, p) = \sum_{x_1x_2 \in E(G)} P^{(d_{x_1} \times d_{x_2})} \tag{12}$$

2. Topological index of hexane para-line graphs

For an index that Schultz offered, Ranjini created the independent relations. Under the watchful eye of the Schultz index, these researchers looked at the subdivision of a number of graphs, including helm, ladder, tadpole and wheel [28]. They also looked at the ladder, tadpole and wheel hexane para-line graphs under the zagreb index [29]. In 2015, Xu and Su conducted an analysis of two indices specific to ladder, tadpole and wheel graphs constructed using hexane para-line graphs and named the total connectivity index of the sum and the co-index [30]. Nadim et al. calculated the atomic bond connectivity index and fifth class of geometric arithmetic indices for hexane para-line tadpole, wheel and ladder graphs. They also investigated several other indices, including randic general connectivity index, first zagreb general index, summation general connectivity index, atomic bond connectivity index, geometric arithmetic index, fifth class of geometric arithmetic indices, hyper zagreb index, the first and second multiple zagreb index for a hexane para-line graphs of linear [n]-pentacene and multiple pentacene., lattice plot in nanotorus $TUC_4C_8[p, q]$ and 2D nanotube .

In our study, we computed various indices, including randic general connectivity index, first zagreb general index, summation general connectivity index, atomic bond connectivity index, geometric arithmetic index, fifth class of geometric arithmetic indices, hyperzagreb index.

2.1. **Molecular characteristics of the linear [n]-pentacene hexane para-line graphs.** Figure 3 depicts the linear [n]-pentacene molecular graph, which is indicated by the symbol T_n. T_n consists of $84n-6$ edges and $66n$ vertices.

Theorem 2.1. Consider a hexane para-line graphs G derived from the graph T_n.

$M_\alpha(G^\star) = (9n+6)6^{\alpha+6} + 7^{\alpha+5}(36n-12)$.

Proof. In Figure 3, the graph G is displayed. There are $168n-12$ vertices in total in G, this has $108n-36$ vertices of degree and $60n+24$ vertices of degree 6, where

$M_\alpha(G) = (9n+6)6^{\alpha+6} + 7^{\alpha+5}(36n-12)$.

Theorem 2.2 Consider a hexane para-line graphs $G^\star$ derived from the graph T_n.

1. $R_\alpha(G^\star) = (30n+30)36^\alpha + (60n-12)42^\alpha + (132n-48)49^\alpha$.

2. $\chi_\alpha(G^\star) = (30n+30)12^\alpha + (60n-12)13^\alpha + (132n-48)14^\alpha$.

3. $ABC(G) = (45\sqrt{6} + \frac{264}{9})n + 7\sqrt{6} - \frac{96}{7}$.

4. $GA(G) = (162 + 24\sqrt{18})n - 18 - \frac{24}{17}\sqrt{18}$.

Proof. The total number of edges in G is determined by the formula $222n-30$. The edges in G can be divided into three sets, $E_1(G)$, $E_2(G^\star)$, and $E_3(G)$, which do not intersect with each other. The edge partition $E_1(G)$ contains $30n+30$ edges x_1, x_2, where $d_{x_1} = d_{x_2} = 6$, edge the partition $E_2(G)$ contains $60n-12$ edges x_1, x_2, where $d_{x_1} = 6$ and $d_{x_2} = 7$, and The edge partition $E_3(G)$ consists of $132n-48$ edges. This partition includes edges x_1 and x_2, where $d_{x_1} = d_{x_2} = 7$. By utilizing we get the required outcomes using formulae (1), (3), (4) and (5).

Theorem 2.3 Consider a hexane para-line graphs G derived from the graph T_n.

FIGURE 5. Linear Pentacene

1. $ABC_4(G) = (\sqrt{330} + 12\sqrt{6} + 6\sqrt{90} + \frac{48}{7})n + \frac{9}{6} + \frac{6}{9}\sqrt{105} - \frac{24}{9}\sqrt{6} - \frac{6}{7}\sqrt{90} - \frac{1}{9}\sqrt{330} - \frac{96}{27}$

2. $GA_5(G) = (90 + \frac{240}{39}\sqrt{30} + \frac{864}{51}\sqrt{6})n - 6 + \frac{48}{27}\sqrt{9} - \frac{48}{39}\sqrt{30} - \frac{288}{51}\sqrt{6}$

Proof. Assuming that the set of edges depends on the sum of the degrees of the neighbors of the end vertices, we can partition edges that divide $(G^\star)$ into seven distinct sets: $E_{12}(G)$, $E_{13}(G)$, ..., $E_{18}(G)$. Thus, we have $E(G) = \bigcup_{i=12}^{18} E_i(G)$. The edge assortment $E_{12}(G)$ comprises 18 edges x_1x_2, where $S_{x_1} = S_{x_2} = 12$, the edge collection $E_{13}(G)$ holds 12 edges x_1x_2, where $S_{x_1} = 12$ and $S_{x_2} = 13$, the edge collection $E_{14}(G)$ holds $18n-12$ edges x_1x_2, where $S_{x_1} = S_{x_2} = 13$, set of edges $E_{15}(G)$ contains $36n-12$ edges x_1x_2, where $S_{x_1} = 13$ and $S_{x_2} = 16$, edge the collection $E_{16}(G)$ contains $16n$ edges x_1x_2, where $S_{x_1} = S_{x_2} = 16$, the edge set $E_{17}(G)$ contains $48n-16$ edges x_1x_2,

where $S_{x_1} = 16$ and $S_{x_2} = 17$ and the set of edges $E_{18}(G)$ is satisfied $20n - 16$ edges x_1x_2, where $S_{x_1} = S_{x_2} = 17$. By utilizing we can get the required outcomes using formulae 6 and 7.

Theorem 2.4 Consider a hexane para-line graphs G derived from the graph T_n

1. $HM(G) = 40332n - 2412$.

2. $PM_1(G) = 12^{30n+30} \times 13^{60n-12} \times 14^{132n-24}$.

3. $PM_2(G) = 36^{30n+30} \times 42^{60n-12} \times 49^{132n-24}$.

Proof. Consider a hexane para-line graphs G of a linear pentacene. Based on the angles of the final vertex, the collection of edges $E(G)$ might be categorised as three distinct groups. The first category, $E_1(G)$, consists of $30n+30$ edges x_1x_2, where $d_{x_1} = d_{x_2}$ =6. The second category, $E_2(G)$, includes $60n - 12$ edges x_1x_2, where $d_{x_1} = 6$ and d_{x_2} =7. The third category, $E_3(G)$, comprises $132n - 24$ edges x_1x_2, where $d_{x_1} = d_{x_2} = 7$. Let $|E_1(G)| = e_{6,6}$, $|E_2(G)| = e_{6,7}$, and $|E_3(G)| = e_{7,7}$. Therefore,

1. $HM(G) = \sum_{x_1x_2 \in E(G)} (d_{x_1} + d_{x_2})^2$

$HM(G) = \sum_{x_1x_2 \in E_1(G)} [d_{x_1} + d_{x_2}]^2 + \sum_{x_1x_2 \in E_2(G)} [d_{x_1} + d_{x_2}]^2 + \sum_{x_1x_2 \in E_3(G)} [d_{x_1} + d_{x_2}]^2$

$HM(G) = 144|E_1(G)| + 169|E_2(G)| + 196|E_3(G)|$

$HM(G) = 144(30n + 30) + 169(60n - 12) + 196(132n - 24)$

$HM(G) = 4320n + 4320 + 10140n - 2028 + 25872n - 4704$

This implies that

$HM(G) = 40332n - 2412$.

2. $PM_1(G) = \Pi_{x_1x_2 \in E_1(G)} (d_{x_1} + d_{x_2}) \times \Pi_{x_1x_2 \in E_2(G)} (d_{x_1} + d_{x_2}) \times \Pi_{x_1x_2 \in E_3(G)} (d_{x_1} + d_{x_2})$

$PM_1(G) = 12^{|E_1(G)|} \times 13^{|E_2(G)|} \times 14^{|E_1(G)|}$

$PM_1(G) = 12^{30n+30} \times 13^{60n-12} \times 14^{132n-24}$.

3. $PM_2(G) = \Pi_{x_1x_2 \in E_1(G)} (d_{x_1} \times d_{x_2}) \times \Pi_{x_1x_2 \in E_2(G)} (d_{x_1} \times (d_{x_2}) \times \Pi_{x_1x_2 \in E_3(G)} (d_{x_1} \times d_{x_2})$

$PM_2(G) = 36^{|E_1(G)|} \times 42^{|E_2(G)|} \times 49^{|E_1(G)|}$

$PM_2(G) = 36^{|E_1(G)|} \times 42^{|E_2(G)|} \times 49^{|E_1(G)|}$

$PM_2(G) = 36^{30n+30} \times 42^{60n-12} \times 49^{132n-24}$.

Theorem 2.5 Consider a hexane para-line graphs $G^\star$ derived from the graph T_n

1. $M_1(G, p) = (30n + 30)P^{12} + (60n - 12)P^{13} + (132n - 24)P^{14}$.

2. $M_2(G, p) = (30n + 30)P^{36} + (60n - 12)P^{42} + (132n - 24)P^{49}$.

Proof. 1. $M_1(G, p) = \sum_{x_1x_2 \in E(G)} P^{(d_{x_1} + d_{x_2}}$

$M_1(G,p) = \sum_{x_1x_2\in E_1(G)} P^{(d_{x_1}+d_{x_2})} + \sum_{x_1x_2\in E_2(G)} P^{(d_{x_1}+d_{x_2})} \sum_{x_1x_2\in E_1(G)} P^{(d_{x_1}+d_{x_2})}$

$M_1(G,p) = \sum_{x_1x_2\in E_1(G)} P^{12} + \sum_{x_1x_2\in E_2(G)} P^{13} + \sum_{x_1x_2\in E_1(G)} P^{14}$

$M_1(G,p) = |E_1(G)|P^{12} + |E_2(G)|P^{13} + |E_3(G)|P^{14}$

$M_1(G,p) = (30n+30)P^{12} + (60n-12)P^{13} + (132n-24)P^{14}.$

2. $M_2(G,p) = \sum_{x_1x_2\in E(G)} P^{(d_{x_1}+d_{x_2}}$

$M_2(G,p) = \sum_{x_1x_2\in E_1(G)} P^{(d_{x_1}\times d_{x_2})} + \sum_{x_1x_2\in E_2(G)} P^{(d_{x_1}\times d_{x_2}} \sum_{x_1x_2\in E_1(G)} P^{(d_{x_1}\times d_{x_2})}$

$M_2(G,p) = \sum_{x_1x_2\in E_1(G)} P^{36} + \sum_{x_1x_2\in E_2(G)} P^{42} + \sum_{x_1x_2\in E_1(G)} P^{49}$

$M_2(G,p) = |E_1(G)|P^{36} + |E_2(G)|P^{42} + |E_3(G)|P^{49}$

$M_2(G,p) = (30n+30)P^{36} + (60n-12)P^{42} + (132n-24)P^{49}.$

This makes the proof whole.

FIGURE 6. Hexane para-line graphs linear Pentacene

2.2. **Molecular descriptors of hexane para-line graphs for multiple pentacenes.** The chemical diagram $T_{m,n}$ representing multiple pentacene is depicted in Figure 4. This graph consists of $66mn$ vertices and $99mn-6m-9n$ edges.

Theorem 2.6 Consider a hexane para-line graphs $G^\star$ derived from the graph $T_{m,n}$.

$M\alpha(G) = (9n+6)6^{\alpha+6} + 7^{\alpha+5}(36n-12).$

Proof. Figure 5 shows the graph $G^\star$ in a visual format. It has $168n-12$ worth of vertices in total, of which $60n+24$ and $108n-36$ have degrees of 6 and 7, respectively. Using formula 2, we can calculate $M\alpha(G)$.

Theorem 2.7 Consider a hexane para-line graphs G derived from the graph $T_{m,n}$.

1. $R_\alpha(G) = (10n+6m+4)36^\alpha + (4m+20n-8)42^\alpha + (99mn-20m-55n+4)49^\alpha.$

2. $\chi_\alpha(G) = (10n+6m+4)12^\alpha + (4m+20n-8)13^\alpha + (99mn-20m-55n+4)14^\alpha.$

3. $ABC(G) = (9\sqrt{6} - \frac{330}{7})n + (9\sqrt{6} - \frac{120}{7})m6\sqrt{6} + 198mn + \frac{24}{7}.$

Proof. The division graph $S(T_{m,n})$ comprises a total of $198mn-20m-50$ vertices and $99mn-10m-25n$ edges. There are $8m+20n$ vertices of degree 2 and $66mn-12m-30n$ vertices of degree 3, according to the vertex division. The edge set $E(G)$ of the hexane para-line graphs $E(G)$ consists of $99mn-20m-55n+4$ edges. Based on the angles of the end vertices, these edges

are divided into three groups, i.e, $E(G) = E_1(G) \cup E_2(G) \cup E_3(G)$. The edge separation $E_1(G)$ consists of $10n + 6m + 4$ edges x_1x_2. where $d_{x_1} = d_{x_2} = 4$. Edge Separation $4m + 20n - 8$ with $E_2(G)$ Edge x_1x_2, where $d_{x_1} = 4$ and $d_{x_2} = 5$. Lastly, Separating the edges $E_3(G)$ comprises $99mn - 20m - 55n + 4$ edges x_1x_2, where $d_{x_1} = d_{x_2} = 5$. By applying the required outcome may be produced using formulae (1), (3), (4) and (5).

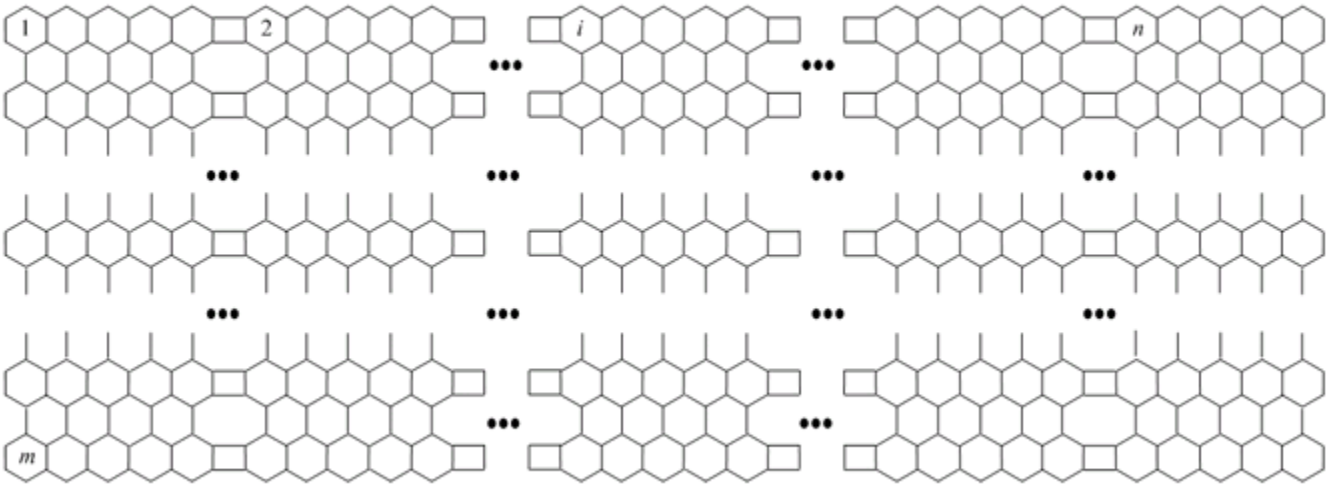


FIGURE 7. Multiple pentacene

Theorem 2.8 Consider a hexane para-line graphs G derived from the graph $T_{m,n}$.

1. $ABC_4(G) = (44m + \sqrt{14} + 4\sqrt{2} + \sqrt{110} + 2\sqrt{30} - \frac{116}{3})n + (\frac{1}{2}\sqrt{6}$
$+\frac{1}{5}\sqrt{110} + \frac{2}{5}\sqrt{35} - \frac{112}{9} + \frac{2}{3}\sqrt{30})m + 2\sqrt{6} - \frac{8}{5}\sqrt{2} - \frac{2}{5}\sqrt{110} - \frac{4}{3}\sqrt{30} + \frac{80}{9}$.

2. $GA_5(G) = (\frac{80}{13}\sqrt{10} + 99m + \frac{288}{17}\sqrt{2}69)n +$
$(-26 + \frac{16}{13}\sqrt{10} + \frac{16}{9}\sqrt{5} + \frac{96}{17}\sqrt{2})m - \frac{192}{17}\sqrt{10} - \frac{32}{13}\sqrt{10} + 24$

Proof. Seven distinct edge sets may be formed from the set of edges by taking into account the degree sum of end vertices' neighbours. $E_i(G)$, where $i = 6, 7, ..., 12$. Thus, we have $E(G^\star) = \bigcup_{i=6}^{12} E_i(G)$. The edge partition $E_6(G)$ contains $2m + 8$ edges x_1x_2, where $S_{x_1} = S_{x_2} = 6$. The edge partition $E_7(G)$ consists of $4m$ edges x_1x_2, where $S_{x_1} = 6$ and $S_{x_2} = 7$. Edge partition $E_8(G)$ contains $10n - 4$ edges x_1x_2. where $S_{x_1} = S_{x_2} = 7$. Edge partition $E_9(G)$ contains $20n + 4m - 8$ edges x_1x_2. where $S_{x_1} = 8$ and $S_{x_2} = 9$. Edge partition $E_{10}(G)$ consists of $10n$ edges x_1x_2. where $S_{x_1} = S_{x_2} = 9$. Edge partition $E_{11}(G)$ contains $8m + 24n - 16$ edge x_1x_2. where $S_{x_1} = 10$ and $S_{x_2} = 11$. Finally, edge partition $E_{12}(G)$ contains $99mn - 28m - 87n + 20$ edge x_1x_2, where $S_{x_1} = S_{x_2} = 11$. By utilizing formulas (6) and (7), we obtain the desired result.

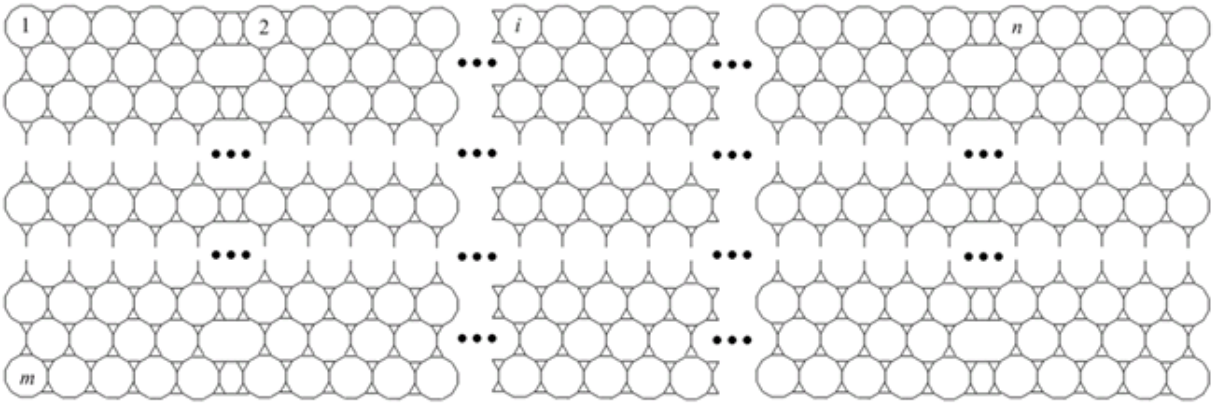


FIGURE 8. Hexane para-line graph multiple of pentacene

By performing computations on the chemical structures of multiple-pentacene, we obtain the following indices: $HM(G), PM_1(G), PM_2(G)$.

Theorem 2.9 Consider a hexane para-line graphs $G^\star$ derived from the graph $T_{m,n}$.

1. $HM(G) = 4851mn - 598m - 1495n4$.

2. $PM_1(G) = 12^{10n+6m+4} \times 13^{4m+20n-8} \times 14^{99mn-20m-55n+4}$.

3. $PM_2(G) = 36^{10n+6m+4} \times 42^{4m+20n-8} \times 47^{99mn-20m-55n+4}$.

4. $M_1(G,p) = (10n+6m+4)P^{12} + (4m+20n-8)P^{13} + (99mn-20m-55n+4)P^{14}$.

5. $M_2(G,p) = (10n+6m+4)P^{36} + (4m+20n-8)P^{42} + (99mn-20m-55n+4)P^{49}$.

Proof. Consider a graph G with its edges broken down into three parts categories due to the degrees of the final vertex. The initial category, denoted as $E_1(G)$, consists of $10n+6m+4$ edges x_1x_2, which both vertices x_1 and x_2 have a degree of 6. The second category, denoted as $E_2(G)$, contains $4m+20n-8$ edges x_1x_2, which x_1 has a degree of 6 and x_2 has a degree of 7. The third category, denoted as $E_3(G)$, includes $99mn-20m-55n+4$ edges x_1x_2, where both vertices x_1 and x_2 have a degree of 7. We can observe that the cardinality of $E_1(G)$ is equal to $e_{6,6}$, $E_2(G)$ is equal to $e_{6,7}$ and $E_3(G)$ is equal to $e_{7,7}$.

1. $HM(G) = \sum_{x_1x_2 \in E(G)} (d_{x_1} + d_{x_2})^2$

$HM(G) = \sum_{x_1x_2 \in E_1(G)} [d_{x_1} + d_{x_2}]^2 + \sum_{x_1x_2 \in E_2(G)} [d_{x_1} + d_{x_2}]^2 + \sum_{x_1x_2 \in E_3(G)} [d_{x_1} + d_{x_2}]^2$

$HM(G) = 36|E_1(G)| + 42|E_2(G)| + 49|E_3(G)|$

$HM(G) = 36(10n+6m+4) + 42(4m+20n-8) + 49(99mn-20m-55n+4)$

$HM(G) = 360n + 216m + 144 + 168m + 840n - 336 + 4851mn - 980m - 2695n + 196$

This implies that

$HM(G) = 4851mn - 598m - 1495n4$

Since,

2. $PM_1(G) = \Pi_{x_1x_2 \in E(G)}(d_{x_1} + d_{x_2})$

$PM_1(G) = \Pi_{x_1x_2 \in E_1(G)}(d_{x_1} + d_{x_2}) \times \Pi_{x_1x_2 \in E_2(G)}(d_{x_1} + d_{x_2}) \times \Pi_{x_1x_2 \in E_3(G)}(d_{x_1} + d_{x_2})$

$PM_1(G) = 12^{10n+6m+4} \times 13^{4m+20n-8} \times 14^{99mn-20m-55n+4}.$

Now that

3. $PM_2(G) = \Pi_{x_1x_2 \in E(G)}(d_{x_1} \times d_{x_2})$

$PM_2(G) = \Pi_{x_1x_2 \in E_1(G)}(d_{x_1}\ timesd_{x_2}) \times \Pi_{x_1x_2 \in E_2(G)}(d_{x_1} \times d_{x_2}) \times \Pi_{x_1x_2 \in E_3(G)}(d_{x_1} \times d_{x_2})$

$PM_2(G) = 36^{|E_1(G)|} \times 42^{|E_1(G)|} \times 49^{|E_1(G)|}$

$PM_2(G) = 36^{10n+6m+4} \times 42^{4m+20n-8} \times 49^{99mn-20m-55n+4}.$

4. $M_1(G,p) = \sum_{x_1x_2 \in E(G)} P^{(d_{x_1}+d_{x_2}}$

$M_1(G,p) = \sum_{x_1x_2 \in E_1(G)} P^{(d_{x_1}+d_{x_2})} + \sum_{x_1x_2 \in E_2(G)} P^{(d_{x_1}+d_{x_2})} \sum_{x_1x_2 \in E_1(G)} P^{(d_{x_1}+d_{x_2})}$

$M_1(G,p) = \sum_{x_1x_2 \in E_1(G)} P^{12} + \sum_{x_1x_2 \in E_2(G)} P^{13} + \sum_{x_1x_2 \in E_1(G)} P^{14}$

$M_1(G,p) = |E_1(G)|P^{12} + |E_2(G)|P^{13} + |E_3(G)|P^{14}$

$M_1(G,p) = (10n + 6m + 4)P^{12} + (4m + 20n - 8)P^{13} + (99mn - 20m - 55n + 4)P^{14}.$

5. $M_2(G,p) = \sum_{x_1x_2 \in E(G)} P^{(d_{x_1}+d_{x_2}}$

$M_2(G,p) = \sum_{x_1x_2 \in E_1(G)} P^{(d_{x_1} \times d_{x_2})} + \sum_{x_1x_2 \in E_2(G)} P^{(d_{x_1} \times d_{x_2}} \sum_{x_1x_2 \in E_1(G)} P^{(d_{x_1} \times d_{x_2})}$

$M_2(G,p) = \sum_{x_1x_2 \in E_1(G)} P^{36} + \sum_{x_1x_2 \in E_2(G)} P^{42} + \sum_{x_1x_2 \in E_1(G)} P^{49}$

$M_2(G,p) = |E_1(G)|P^{36} + |E_2(G)|P^{42} + |E_3(G)|P^{49}$

$M_2(G,p) = (10n + 6m + 4)P^{36} + (4m + 20n - 8)P^{42} + (99mn - 20m - 55n + 4)P^{49}.$

This makes the proof whole.

3. CONCLUSION

The research article examined mathematical indices essential to chemical informatics, specifically used in analyzing organic compounds. These indices include the randic general connectivity index, first zagreb general index, summation general connectivity index, atomic bond connectivity index, geometric arithmetic index, fifth class of geometric arithmetic indices, hyper zagreb index, as well as the initial and secondly multiple [n]-pentacene zagreb indices. The focus of our investigation involved heptane para-line graphs associated with two distinct types of pentacenes. The randic index (R_α) is a useful tool for understanding alkane physicochemical properties, while the ABC index predicts hydrocarbon stability for linear and branched alkanes. Cycloalkane stability can be assessed using this index, providing valuable insights. The GA index outperforms the ABC index in predicting physicochemical characteristics, chemical reactivity, and biological activities of pentacenes, enhancing our understanding through a philosophical approach. The study indicates that physical features can be linked to pentacenes' chemical structure, potentially benefiting the power industry and advancing advancements in the field.

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