Research Article **Open Access**

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Topological study of the para-line graphs of certain pentacene via topological indices

https://doi.org/10.1515/chem-2018-0126
Received June 5, 2018; accepted August 21, 2018

Abstract: A topological index is a map from molecular structure to a real number. It is a graph invariant and also used to describe the physio-chemical properties of the molecular structures of certain compounds. In this paper, we have investigated a chemical structure of pentacene. Our paper reflects the work on the following indices:R_α, M_α, χ_α, ABC, GA, ABC_4, GA_5, PM_1, PM_2, $M_1(G,p)$and $M_1(G,p)$ of the para-line graph of linear $[n]$-pentacene and multiple pentacene.

Keywords: Topological Indices, Para-line Graph, Nanostructures, Pentacene

1 Introduction and Preliminaries

Every Chemical compound has physical and chemical properties but some chemicals are biologically active, as well. In fact, many pharmaceutical companies are in search of new antibacterial agents. For this purpose they test thousands of compounds, but biological testing is expensive. To overcome this difficulty some other ways of investigating potential antibiotics involve the correlatiion of structures with biological activities or physical and chemical properties. Topological indices, also called molecular descriptors, can be used to explain physio-chemical properties of molecules. In recent years, many graph invariants have been developed for use in different fields of study, including structural chemistry, theoretical chemistry, environmental chemistry, toxicology, and pharmacology. Due to high industrial demand, researchers are motivated to work on topological indices. As a result of these efforts from researchers, more than 400 topological indices have been discovered. As the geometry of any chemical compound plays a vital role in defining the function of this compound, the topological structures of chemical compounds are being correlated with their chemical properties. Topological indices characterise the physio-chemical properties of molecular structures and are widely used in QSAR/QSPR modeling, chemical documentation, drug design, and database selection and for designing multilinear regression models. Molecular descriptors are generally classified into three types: degree-based indices [1–5], distance-based indices [6–11], and indices based on spectrum [12–15]. Indices based on both(Degrees and distances) are used in research reported in the literature (see [16–18]).

Pentacene is one of the most popular hydrocarbon semiconductors in chemistry [19]. The name pentacene is a combination of two words: penta, meaning five, and acene, which refers to polycyclic aromatic hydrocarbons with fused benzene rings. The importance of pentacene has dramatically increased in recent years due to its key roles in electronic devices and organic solar cells. As the price of energy rises day by day, researchers continue to look for cheaper sources of energy. Electricity, in particular, is produced in multiple ways, including with solar panels. Solar energy is costly because of the high price of developing traditional silicon-based solar cells, leading to a need to optimize organic solar cells, which can be cheaper than silicon-based cells. Researchers at the Georgia Institute of Technology have discovered a technique to create a lightweight organic solar cell. By using pentacene, researchers were able to transform sunlight into electricity with high efficiency. Pentacene, unlike other materials, is a good semiconductor due its crystalline properties. The importance of pentacene has motivated us to perform topological studies of pentacene and we have obtained some important results which will be useful in the study of

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chemical and physical properties of pentacene. For other topological studies on pentacene see [20, 21].

Let G be a simple graph (no loops and no multiple edges) including two sets: vertex set $V(G)$ and edge set $E(G)$, respectively. For $x \in V(G)$, N_x represents the set of its neighbours in G, and the valency (degree) of vertex $x$is $d_x = |N_x|$ and $S_x = \sum_{y \in N_x} ? d_y$. If we insert a vertex between every edge of any graph, then every edge of this graph will be divided into two edges, which yields a subdivision of the entire graph. This process is referred to as the subdivision of graphs, and it is denoted by $S(G)$. A line graph can be constructed from graph G by connecting adjacent edges of G with each other; these edges behave as vertices in a new graph. This new graph is denoted by $L(G)$. The line graph of the subdivision graph is termed the para-line graph of G, which is denoted by $L(S(G))$ (throughout this paper, we will use $G^\star$ instead of $L(S(G))$). On the other hand, we can build $G^\star$ from G in the following way:

1. Exchange every vertex $x \in V(G)$ by $K(x)$, the complete graph on d_x vertices;
2. There is an edge fitting together a vertex of $K(x_1)$ and a vertex of $K(x_2)$ in $G^\star$ if and only if there is an edge fitting together x_1 and x_2 in G;
3. For every vertex y of $K(x)$, the valency (degree) of y in $G^\star$ is the same as the valency(degree) of x in G.

These graphs are popular in structural chemistry. Para-line graphs have garnered less attention from researchers in recent years, however attention is increased these days. One reason for their popularity is the simplicty of construction. To construct any chemical compound, a researcher simply considers the carbon atom skeleton, and uses each atom to represent a vertex and each bond between every two atoms to represent an edge. For example, consider the hydrocarbon ethane (C_2H_6). The structure of Ethane is represented as molecular structure and molecular graph in Figure 1(a) and (b). A para-line graph of the molecular graph of ethane is shown in Figure 1(c).

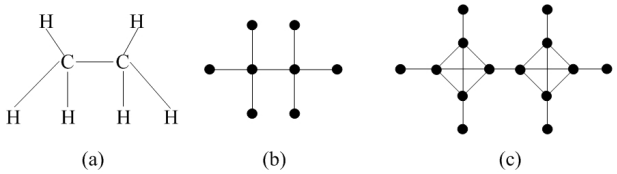

Figure 1: (a)molecular structure of Ethane, (b) molecular graph of Ethane, (c) Para-line graph of Ethane.

The general Randic connectivity index of G is defined as [12]

$$R_\alpha(G) = \sum_{xy \in E(G)} (d_x d_y)^\alpha \tag{1}$$

Where α represents a real number. If α is $-1/2$, then $R_{-1/2}(G)$ is said to be the Randic connectivity index of G. Li and Zhao presented the first general Zagreb index [22]:

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

In 2010, a general sum-connectivity index $\chi_\alpha(G)$ was invented [23]:

$$\chi_\alpha(G) = \sum_{xy \in E(G)} (d_x + d_y)^\alpha \tag{3}$$

The (ABC) index was presented by Estrada [24]. The ABC index of graph G is expressed as

$$ABC(G) = \sum_{xy \in E(G)} \sqrt{\frac{d_x + d_y - 2}{d_x d_y}} \tag{4}$$

Vukicevic and Furtula announced the geometric arithmetic (GA) index [25]. The geometric-arithmetic index, denoted by GA for graph G, is:

$$GA(G) = \sum_{xy \in E(G)} \frac{2\sqrt{d_x d_y}}{d_x + d_y} \tag{5}$$

Another index that belongs to the 4th class of (ABC) index was described by Ghorbani et al. [26] as:

$$ABC_4(G) = \sum_{xy \in E(G)} \sqrt{\frac{S_x + S_y - 2}{S_x S_y}} \tag{6}$$

The fifth class of geometric-arithmetic index, denoted by GA_5, was presented by Graovac et al. [27] as

$$GA_5(G) = \sum_{xy \in E(G)} \frac{2\sqrt{S_x S_y}}{S_x + S_y} \tag{7}$$

In 2013, the Hyper-Zagreb index was introduced as

$$HM(G) = \sum_{xy \in E(G)} (d_x + d_y)^2 \tag{8}$$

Ghorbani and Azimi proposed two new types of Zagreb indices of a graph G in 2012. $PM_1(G)$ is the first multiple Zagreb index, $PM_2(G)$ is the second multiple Zagreb index, and $M_1(G, p)$ and $M_2(G, p)$ are the first Zagreb polynomial and second Zagreb polynomial, respectively. These factors are defined as:

$$PM_1(G) = \prod_{xy \in E(G)} (d_x + d_y) \tag{9}$$

$$PM_2(G) = \prod_{xy \in E(G)} (d_x \times d_y) \tag{10}$$

$$M_1(G,p) = \sum_{xy \in E(G)} p^{(d_x+d_y)} \tag{11}$$

$$M_2(G,p) = \sum_{xy \in E(G)} p^{(d_x \times d_y)} \tag{12}$$

Ethical approval: The conducted research is not related to either human or animal use

2 Topological indices of para-line graphs

Ranjini designed the independent relations for an index that was presented by Schultz. These researchers investigated the subdivision of various graphs, including helm, ladder, tadpole and wheel, under the surveillance of the Schultz index [28]. They also investigated the para-line graph of ladder, tadpole and wheel under the Zagrib index [29]. Su and Xu evaluated two indices of para-line graphs of ladder, tadpole and wheel graphs, and named the general sum-connectivity index and co-index in 2015 [30]. Nadeem et.al. computed ABC_4 and GA_5 index of the para-line graphs of the tadpole, wheel and ladder graphs. They examined some indices, such as R_α, M_α, χ_α, ABC, GA, ABC_4 and GA_5 indices of the para-line graph of lattice in $2D$– nanotube and nanotorus $TUC_4C_8[p,q]$.

In our paper, we figured R_α, M_α, χ_α, ABC, GA, ABC_4, GA_5, PM_1, PM_2, $M_1(G,x)$, and $M_1(G,x)$ indices of the para-line graph of linear $[n]$-pentacene and multiple pentacene.

2.1 Molecular descriptors of the para-line graph of linear $[n]$-Pentacene

The molecular graph of linear $[n]$-pentacene is shown in Figure 2, and it is denoted by T_n. There are $22n$ vertices and $28n-2$ edges in T_n.

Theorem 2.1 *Let $G^\star$ be the para-line graph of T_n. Then*

$$M_\alpha(G^\star) = (5n+2)2^{\alpha+2} + 3^{\alpha+1}(12n-4).$$

Proof. The graph $G^\star$ is shown in Figure 3. In $G^\star$ there are a total of $56n-4$ vertices, among which $20n+8$ vertices are of degree 2 and $36n-12$ vertices are of degree because $M_\alpha(G^\star) = (5n+2)2^{\alpha+2} + 3^{\alpha+1}(12n-4)$. □

Theorem 2.2 *Let $G^\star$ be the para-line graph of T_n. Then*

1. $R_\alpha(G^\star) = (10n+10)4^\alpha + (20n-4)6^\alpha + (44n-16)9^\alpha$;
2. $\chi_\alpha(G^\star) = (10n+10)4^\alpha + (20n-4)5^\alpha + (44n-16)6^\alpha$;
3. $ABC(G^\star) = \left(15\sqrt{2} + \frac{88}{3}\right)n + 3\sqrt{2} - \frac{32}{3}$;
4. $GA(G^\star) = \left(54 + 8\sqrt{6}\right)n - 6 - \frac{8}{5}\sqrt{6}$.

Proof. The total cardinality of edges of $G^\star$ is $74n-10$. The edge set $E(G^\star)$characterized in the following three disjoint edge sets depends on the degrees of the end vertices, i.e. $E(G^\star) = E_1(G^\star) \cup E_2(G^\star) \cup E_3(G^\star)$. The edge partition $E_1(G^\star)$ holds $10n+10$ edges xy, where $d_x = d_y = 2$, the edge partition $E_2(G^\star)$ holds $20n-4$ edges xy, where $d_x = 2$ and $d_y = 3$, and the edge partition $E_3(G^\star)$ holds $44n-16$ edges xy, where $d_x = d_y = 3$. From formulas (1), (3), (4) and (5), we get the desired results. □

Theorem 2.3 *Let $G^\star$ be the para-line graph of T_n. Then*

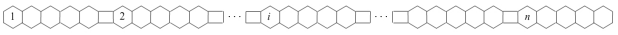

Figure 2: Linear Pentacene

1.

$$ABC_4(G^\star) = \left(\sqrt{110} + 4\sqrt{2} + 2\sqrt{30} + \frac{16}{3} + \sqrt{14}\right)n + 5/2\sqrt{6} + \frac{2}{5}\sqrt{35} - \frac{8}{5}\sqrt{2} - \frac{2}{3}\sqrt{30} - \frac{1}{5}\sqrt{110} - \frac{32}{9}$$

2.

$$GA_5(G^\star) = \left(30 + \frac{80}{13}\sqrt{10} + \frac{288}{17}\sqrt{2}\right)n - 2 + \frac{16}{9}\sqrt{5} - \frac{16}{13}\sqrt{10} - \frac{96}{17}\sqrt{2}.$$

Proof. If we suppose an edge collection depends on degree sum of neighbours of end vertices, then the set of edges $E(G^\star)$can be distributed into seven disjoint sets of edges $E_i(G^\star)$, $i = 4, 5, ?, 10$, i.e. $E(G^\star) = \cup_{i=4}^{10} E_i(G^\star)$. The edge collection $E_4(G^\star)$ holds 10 edges xy, where $S_x = S_y = 4$, the edge collection $E_5(G^\star)$ holds 4 edges xy, where $S_x = 4$ and $S_y = 5$, the edge collection $E_6(G^\star)$ holds $10n-4$ edges xy, where $S_x = S_y = 5$, the edge collection $E_7(G^\star)$ holds $20n-4$ edges xy, where $S_x = 5$ and $S_y = 8$, the edge collection $E_8(G^\star)$ holds $8n$ edges xy, where $S_x = S_y = 8$, the edge collection $E_9(G^\star)$ holds $24n-8$ edges xy, where $S_x = 8$ and $S_y = 9$, and the edge collection $E_{10}(G^\star)$ holds $12n-8$ edges xy, where $S_x = S_y = 9$. From formulas 6 and 7, we obtain the required results. □

Theorem 2.4 *Let $G^\star$ be the para-line graph of T_n. Then*
1. $HM(G^\star) = 2124\,n - 636$
2. $PM_1(G^\star) = 4^{10\,n+10} \times 5^{20\,n-4} \times 6^{44\,n-16}$
3. $PM_2(G^\star) = 4^{10\,n+10} \times 6^{20\,n-4} \times 9^{44\,n-16}$

Proof. Let $G^\star$ be the para-line graph of linear pentacene. The edge set $E(G^\star)$is distributed in three categories which depends on the degree of end vertices. The first disjoint edge set $E_1(G^\star)$ holds 10n+10 edges xy, where $d_x = d_y = 2$. The second disjoint set $E_2(G^\star)$ holds 20n-4 edges xy, where $d_x = 2, d_y = 3$.The third disjoint set $E_3(G^\star)$ holds 44n-16 edges xy, where $d_x = d_y = 3$. Now, $|E_1(G)| = e_{2,2}$, $|E_2(G)| = e_{2,3}$and $|E_3(G)| = e_{3,3}$. Since,

$$HM(G^\star) = \sum_{xy\in E(G)} (d_x + d_y)^2$$

$$HM(G^\star) = \sum_{xy\in E_1(G)} [d_x+d_y]^2 + \sum_{xy\in E_2(G)} [d_x+d_y]^2 + \sum_{xy\in E_3(G)} [d_x+d_y]^2$$

$$HM\left(G^\star\right) = 16\,|E_1\,(G)| + 25\,|E_2\,(G)| + 36\,|E_3\,(G)|$$

$$HM\left(G^\star\right) = 16(10n + 10) + 25(20n - 4) + 36(44n - 16)$$

This implies that

$$HM(G^\star) = 2124\,n - 636.$$

Since,

$$PM_1(G^\star) = \prod_{xy\in E(G)} (d_x + d_y)$$

$$PM_1(G^\star) = \prod_{xy\in E_1(G)} (d_x+d_y) \times \prod_{xy\in E_2(G)} (d_x+d_y) \times \prod_{xy\in E_3(G)} (d_x+d_y)$$

$$PM_1(G^\star) = 4^{|E_1(G)|} \times 5^{|E_2(G)|} \times 6^{|E_3(G)|}$$
$$= 4^{10n+10} \times 5^{20n-4} \times 6^{44n-16}$$

$$PM_1(G^\star) = 4^{10n+10} \times 5^{20n-4} \times 6^{44n-16}.$$

Now, since

$$PM_2(G^\star) = \prod_{xy\in E(G)} (d_x \times d_y)$$

$$PM_2(G^\star) = \prod_{xy\in E_1(G)} (d_x\times d_y) \times \prod_{xy\in E_2(G)} (d_x\times d_y) \times \prod_{xy\in E_3(G)} (d_x\times d_y)$$

$$PM_2(G^\star) = 4^{|E_1(G)|} \times 6^{|E_2(G)|} \times 9^{|E_3(G)|}$$
$$= 4^{10n+10} \times 6^{20n-4} \times 9^{44n-16}$$

□

Theorem 2.5 *Let $G^\star$ be the para-line graph of T_n. Then*
1. $M_1(G^\star, p) = (10\,n + 10)\,p^4 + (20\,n - 4)\,p^5 + (44\,n - 16)\,p^6$
2. $M_2(G^\star, p) = (10\,n + 10)\,p^4 + (20\,n - 4)\,p^6 + (44\,n - 16)\,p^9$

Proof.

$$M_1(G^\star, p) = \sum_{xy\in E(G)} p^{(d_x+d_y)}$$

$$M_1(G^\star, p) = \sum_{xy\in E_1(G)} p^{(d_x+d_y)} + \sum_{xy\in E_2(G)} p^{(d_x+d_y)} + \sum_{xy\in E_3(G)} p^{(d_x+d_y)}$$
$$= \sum_{xy\in E_1(G)} p^4 + \sum_{xy\in E_2(G)} p^5 + \sum_{xy\in E_3(G)} p^6$$
$$= |E_1(G)|p^4 + |E_2(G)|p^5 + |E_3(G)|p^6$$
$$= (10\,n + 10)\,p^4 + (20\,n - 4)\,p^5 + (44\,n - 16)\,p^6$$

$$M_2(G^\star, p) = \sum_{xy\in E(G)} p^{(d_x\times d_y)}$$

$$M_2(G^\star, x) = \sum_{xy\in E_1(G)} p^{(d_x\times d_y)} + \sum_{xy\in E_2(G)} p^{(d_x\times d_y)} + \sum_{xy\in E_3(G)} p^{(d_x\times d_y)}$$
$$= \sum_{xy\in E_1(G)} p^4 + \sum_{xy\in E_2(G)} p^6 + \sum_{xy\in E_3(G)} p^9$$
$$= |E_1(G)|p^4 + |E_2(G)|p^6 + |E_3(G)|p^9$$
$$= (10\,n + 10)\,p^4 + (20\,n - 4)\,p^6 + (44\,n - 16)\,p^9.$$

Hence proved. □

Figure 3: Paraline Graph of Linear Pentacene.

2.2 Molecular descriptors of the para-line graph of multiple Pentacene

The molecular graph of multiple pentacene is shown in Figure 4, and it is denoted by $T_{m,n}$. There are $22mn$ vertices and $33mn - 2m - 5n$ edges in $T_{m,n}$.

Theorem 2.6 *Let $G^\star$ be the para-line graph of $T_{m,n}$. Then*

$$M_\alpha(G^\star) = (5n + 2)2^{\alpha+2} + 3^{\alpha+1}(12n - 4).$$

Proof. The graph $G^\star$ is shown in Figure 5. In $G^\star$ there are total $56n-4$ vertices among which $20n+8$ degree 2 vertices and $36n - 12$ degree 3 vertices. Hence we get $M_\alpha(G^\star)$ by using formula 2. □

Theorem 2.7 *Let $G^\star$ be the para-line graph of $T_{m,n}$. Then*

1. $R(G^\star) = (10\,n + 6\,m + 4)\,4^\alpha + (4\,m + 20\,n - 8)\,6^\alpha + (99\,mn - 20\,m - 55\,n + 4)\,9^\alpha$;
2. $\chi_\alpha(G^\star) = (10\,n + 6\,m + 4)\,4^\alpha + (4\,m + 20\,n - 8)\,5^\alpha + (99\,mn - 20\,m - 55\,n + 4)\,6^\alpha$;
3. $ABC(G^\star) = \left(15\sqrt{2} - \frac{110}{3}\right)n + \left(5\sqrt{2} - \frac{40}{3}\right)m - 2\sqrt{2} + 66\,mn + 8/3$;
4. $GA(G^\star) = \left(-45 + 8\sqrt{6}\right)n + \left(8/5\sqrt{6} - 14\right)m + 99\,mn + 8 - \frac{16}{5}\sqrt{6}$.

Proof. The subdivision graph $S(T_{m,n})$ holds $99mn - 10m - 25n$ edges and $198mn - 20m - 50$ vertices in total. The division of the vertices is as follows: The number of vertices of degree two are $8m + 20n$ and the number of vertices of degree three are $66mn - 12m - 30n$. The cardinality edge set E of $G^\star$ are $99mn - 20m - 55n + 4$. The edge set $E(G^\star)$splits into three edge categories depends on the degrees of the end vertices, i.e. $E(G^\star) = E_1(G^\star) \cup E_2(G^\star) \cup E_3(G^\star)$. The edge partition $E_1(G^\star)$ holds $10n + 6m + 4$ edges xy, where $d_x = d_y = 2$, the edge partition $E_2(G^\star)$ holds $4m + 20n - 8$ edges xy, where $d_x = 2$ and $d_y = 3$, and the edge partition $E_3(G^\star)$ holds $99mn - 20m - 55n + 4$ edges xy, where $d_x = d_y = 3$. From formulas (1), (3), (4) and (5), Hence desired result is obtained. □

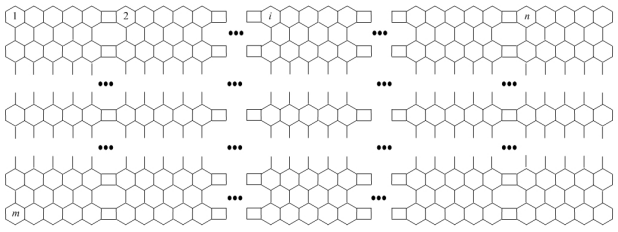

Figure 4: Multiple Pentacene.

Theorem 2.8 *Let $G^\star$ be the para-line graph of $T_{m,n}$. Then*

1. $ABC_4(G^\star) = \left(44\,m + \sqrt{14} + 4\sqrt{2} + \sqrt{110} + 2\sqrt{30} - \frac{116}{3}\right)n + \left(1/2\sqrt{6} + 1/5\sqrt{110} + 2/5\sqrt{35} - \frac{112}{9} + 2/3\sqrt{30}\right)m + 2\sqrt{6} - 8/5\sqrt{2} - 2/5\sqrt{110} - 4/3\sqrt{30} + \frac{80}{9}$
2. $GA_5(G^\star) = \left(\frac{80}{13}\sqrt{10} + 99\,m + \frac{288}{17}\sqrt{2} - 69\right)n + \left(-26 + \frac{16}{13}\sqrt{10} + \frac{16}{9}\sqrt{5} + \frac{96}{17}\sqrt{2}\right)m - \frac{192}{17}\sqrt{2} - \frac{32}{13}\sqrt{10} + 24$.

Proof. If the edge partition under consideration depends on degree sum of neighbours of end vertices then the set of edges $E(G^\star)$ can be classified into seven disjoint edge sets $E_i(G^\star)$, $i = 4, 5, \ldots, 10$, i.e. $E(G^\star) = \cup_{i=4}^{10} E_i(G^\star)$. The edge partition $E_4(G^\star)$ holds $2m + 8$ edges xy, where $S_x = S_y = 4$, the edge partition $E_5(G^\star)$ holds $4m$ edges xy, where $S_x = 4$ and $S_y = 5$, the edge partition $E_6(G^\star)$ holds $10n - 4$ edges xy, where $S_x = S_y = 5$, the edge partition $E_7(G^\star)$ holds $20n + 4m - 8$ edges xy, where $S_x = 5$ and $S_y = 8$, the edge partition $E_8(G^\star)$ holds $8n$ edges xy, where $S_x = S_y = 8$, the edge partition $E_9(G^\star)$ holds $8m + 24n - 16$ edges xy, where $S_x = 8$ and $S_y = 9$, and the edge partition $E_{10}(G^\star)$ holds $99mn - 28m - 87n + 20$ edges xy, where $S_x = S_y = 9$. From formulas (6) and (7), the required result is obtained. □

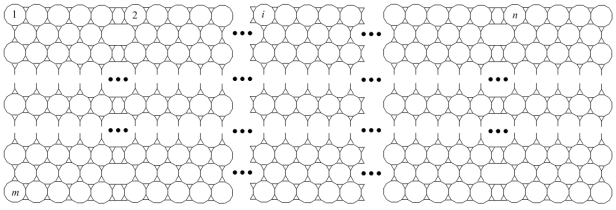

Figure 5: Paraline Graph of Multiple Pentacene.

We find the following indices $HM(G)$, $PM_1(G)$,$PM_2(G)$, Zagreb polynomials $M_1(G, x)$, $M_2(G, x)$by computation for chemical structures of multiple-pentacene.

Theorem 2.9 *Let $G^\star$ be the para-line graph of $T_{m,n}$.Then*

1. $HM(G^\star) = 3564\,mn - 596\,m - 1440\,n - 40$;
2. $PM_1(G^\star) = 4^{10\,n+6\,m+4} \times 5^{4\,m+20\,n-8} \times 6^{99\,mn-20\,m-55\,n+4}$;
3. $PM_2(G^\star) = 4^{10\,n+6\,m+4} \times 6^{4\,m+20\,n-8} \times 9^{99\,mn-20\,m-55\,n+4}$;
4. $M_1(G^\star, p) = (10\,n + 6\,m + 4)\,p^4 + (4\,m + 20\,n - 8)\,p^5 + (99\,mn - 20\,m - 55\,n + 4)\,p^6$;
5. $M_2(G^\star, p) = (10\,n + 6\,m + 4)\,p^4 + (4\,m + 20\,n - 8)\,p^6 + (99\,mn - 20\,m - 55\,n + 4)\,p^9$;

Proof. Let $G^\star$ be the graph. The edge set $E(G^\star)$classified into three edge categories based on degree of end vertices. The first edge partition $E_1(G)$ holds $10n + 6m + 4$ edges xy,where $d_x = d_y = 2$. The second edge partition $E_2(G)$ holds $4m + 20n - 8$ edges xy,where $d_x = 2$, $d_y = 3$.The third edge partition $E_3(G)$ holds $99mn - 20m - 55n + 4$ edges xy,where $d_x = 3$, $d_y = 3$.It is simple to observe that $|E_1(G)| = e_{2,2}$, $|E_2(G)| = e_{2,3}$and $|E_3(G)| = e_{3,3}$. Since,

$$HM(G^\star) = \sum_{xy \in E(G)} (d_x + d_y)^2$$

$$HM(G^\star) = \sum_{xy \in E_1(G)} [d_x + d_y]^2 + \sum_{xy \in E_2(G)} [d_x + d_y]^2 + \sum_{xy \in E_3(G)} [d_x + d_y]^2$$

$$HM\left(G^\star\right) = 16\,|E_1(G)| + 25\,|E_2(G)| + 36\,|E_3(G)|$$

$$=16(10n+6m+4)+25(20n+4m-8)$$
$$+36(99mn-20m-55n+4).$$

This implies that

$$HM(G^*)=3564\,mn-596\,m-1440\,n-40$$

Since,

$$PM_1(G^*)=\prod_{xy\in E(G)}(d_x+d_y)$$

$$PM_1(G^*)=\prod_{xy\in E_1(G)}(d_x+d_y)\times\prod_{xy\in E_2(G)}(d_x+d_y)\times\prod_{xy\in E_3(G)}(d_x+d_y)$$

$$PM_1(G^*)=4^{|E_1(G)|}\times5^{|E_2(G)|}\times6^{|E_3(G)|}$$
$$=4^{10n+6m+4}\times5^{20n+4m-8}\times6^{99mn-20m-55n+4}$$

Now, since

$$PM_2(G^*)=\prod_{xy\in E(G)}(d_x\times d_y)$$

$$PM_2\left(G^*\right)=\prod_{xy\in E_1(G)}(d_x\times d_y)\times\prod_{xy\in E_2(G)}(d_x\times d_y)$$
$$\times\prod_{xy\in E_3(G)}(d_x\times d_y)$$

$$PM_2(G^*)=4^{|E_1(G)|}\times6^{|E_2(G)|}\times9^{|E_3(G)|}$$
$$=4^{10n+6m+4}\times6^{20n+4m-8}\times9^{99mn-20m-55n+4}$$

As,

$$M_1(G^*,p)=\sum_{xy\in E(G)}p^{(d_x+d_y)}$$

$$M_1(G^*,p)=\sum_{xy\in E_1(G)}p^{(d_x+d_y)}+\sum_{xy\in E_2(G)}p^{(d_x+d_y)}+\sum_{xy\in E_3(G)}p^{(d_x+d_y)}$$
$$=\sum_{xy\in E_1(G)}p^4+\sum_{xy\in E_2(G)}p^5+\sum_{xy\in E_3(G)}p^6$$
$$=|E_1(G)|p^4+|E_2(G)|p^5+|E_3(G)|p^6$$
$$=(10\,n+6\,m+4)\,p^4+(4\,m+20\,n-8)\,p^5$$
$$+(99\,mn-20\,m-55\,n+4)\,p^6$$

$$M_2(G,p)=\sum_{xy\in E(G)}?p^{(d_x\times d_y)}$$

$$M_2(G,p)=\sum_{xy\in E_1(G)}p^{(d_x\times d_y)}+\sum_{xy\in E_2(G)}p^{(d_x\times d_y)}+\sum_{xy\in E_3(G)}p^{(d_x\times d_y)}$$
$$=\sum_{xy\in E_1(G)}p^4+\sum_{xy\in E_2(G)}p^6+\sum_{xy\in E_3(G)}p^9$$
$$=|E_1(G)|p^4+|E_2(G)|p^6+|E_3(G)|p^9$$
$$=(10\,n+6\,m+4)\,p^4+(4\,m+20\,n-8)\,p^6$$
$$+(99\,mn-20\,m-55\,n+4)\,p^9$$

Which completes the proof. □

3 Conclusion

In our paper, we have figured the indices R_α, M_α, χ_α, ABC, GA, ABC_4, GA_5, PM_1, PM_2, $M_1(G,x)$, and $M_1(G,x)$ of the para-line graph of linear $[n]$-pentacene and multiple pentacene. The Randic index is used in cheminformatics for studying organic compounds. This index has a better correlation with physio-chemical properties of alkanes, including boiling points, surface areas, and enthalpies of formation. For the stability of any hydrocarbons such as linear and branched alkanes, the ABC index offers a good model. This index also has a correlation with the stability of strain energy of cycloalkane. For some physiochemical properties, GA index can predict physical properties, chemical reactivity and biological activities better than ABC index. We have studied pentacene theoretically, not experimentally. Our theoretical study on pentacene can be very useful and helpful in understanding the physical properties, chemical reactivity and biological activities of pentacenes. The main results obtained in this paper make it possible to correlate the chemical structure of pentacenes with the large amount of information about their physical features, and these results may be useful in the power industry.

Conflict of interest: Authors declare no conflict of interest.

References

[1] Li X., Shi Y., A survey on the Randic' index, MATCH Commun. Math. Comput. Chem. 2008, 59(1), 127-156.

[2] Li X., Shi Y., Wang L., An updated survey on the Randic' index, in: B.F. I. Gutman (Ed.), Recent Results in the Theory of Randic Index, University of Kragujevac and Faculty of Science Kragujevac, 2008, 9-47.

[3] Mufti Z.S., Zafar S., Zahid Z., Nadeem M. F., Study of the para-line graphs of certain Benzenoid structures using topological indices. MAGNT Research Report, 2017, 4(3), 110-116.

[4] Rada J., Cruz R., Vertex-degree-based topological indices over graphs, MATCH Commun. Math. Comput. Chem. 2014, 72, 603-616.

[5] Hinz A.M,. Parisse D., The average eccentricity of Sierpiński graphs, Graphs and Combinatorics, 2012, 28(5), 671-686.

[6] Devillers J,. Balaban A.T., Topological indices and related descriptors in QSAR and QSPAR. CRC Press, 2000.

[7] Azari M., Iranmanesh A., Harary index of some nano-structures, MATCH Commum. Math. Comput. Chem., 2014, 71, 373-382.

[8] Feng L., Liu W., Yu G., Li S., The hyper-Wiener index of graphs with given bipartition, Utilitas Math. 2014, 95, 23-32.

[9] Ali A., Nazeer W., Munir M., Kang S.M., M-Polynomials and Topological Indices Of Zigzag and Rhombic Benzenoid Systems. Open Chemistry, 2018, 16(1), 73-78.

[10] Knor M., Lužar B., Škrekovski R., Gutman I., On Wiener index of common neighborhood graphs, MATCH Commum. Math. Comput. Chem., 2014, 72, 321-332.
[11] Xu K., Liu M., Das K., Gutman I., Furtula B., A survey on graphs extremal with respect to distance-based topological indices, MATCH Commun. Math. Comput. Chem. 2014, 71, 461-508.
[12] Schultz H.P., Topological organic chemistry, Graph theory and topological indices of alkanes. Journal of Chemical Information and Computer Sciences, 1989, 29(3), 227-228.
[13] Xu K., Das K.C., Liu H., Some extremal results on the connective eccentricity index of graphs. Journal of Mathematical Analysis and Applications, 2016, 433(2), 803-817.
[14] Kanna M.R., Jagadeesh R., Topological Indices of Vitamin A., Int. J. Math. And Appl., 2018, 6(1B), 271-279.
[15] Virk A., Nazeer W., Kang S.M., On Computational Aspects of Bismuth Tri-Iodide., Preprints, 2018, 2018060209, doi: 10.20944/preprints201806.0209.v1.
[16] Dehmer M., Emmert-Streib F., Grabner M., A computational approach to construct a multivariate complete graph invariant, Inform. Sci. 2014, 260, 200-208.
[17] Feng L., Liu W., Ilic' A., Yu G., The degree distance of unicyclic graphs with given matching number, Graphs Comb., 2013, 29, 449-462.
[18] Gutman I., Selected properties of the Schultz molecular topological index, J. Chem. Inf. Comput. Sci., 1994, 34, 1087-1089.
[19] Farahani M. R., Nadeem M. F., Zafar S., , Zahid Z., , Husin M. N., Study of the topological indices of the line graphs of hpantacenic nanotubes. New Front. Chem., 2017, 26(1), 31-38.
[20] Soleimani N., Mohseni E., Maleki N., Imani N., Some topological indices of the family of nanostructures of polycyclic aromatic hydrocarbons (PAHs). J. Natl. Sci Found. Sri., 2018, 46(1).
[21] Soleimani N., Nikmehr MJ., Tavallaee HA., Theoretical study of nanostructures using topological indices. Stud. U. Babes-Bol, Che., 2014, 59(4), 139-148.
[22] Li X., Zhao H., Trees with the first three smallest and largest generalized topological indices, MATCH Commun. Math. Comput. Chem., 2004, 50, 57-62.
[23] Zhou B., Trinajstic N., On general sum-connectivity index, J. Math. Chem., 2010, 47, 210-218.
[24] Estrada E., Torres L., Rodriguez L., Gutman I., An atom-bond connectivity index: Modelling the enthalpy of formation of alkanes. Indian J. Chem., 1998, 37A, 849-855.
[25] Vukicevic D., Furtula B., Topological index based on the ratios of geometrical and arithmetical means of end-vertex degrees of edges, J. Math. Chem., 2009, 46, 1369-1376.
[26] Ghorbani M., Hosseinzadeh M.A., Computing ABC_4index of nanostar dendrimers, Optoelectron. Adv. Mater.-Rapid Commun., 2010, 4(9), 1419-1422.
[27] Graovac A., Ghorbani M., Hosseinzadeh M.A., Computing fifth geometric-arithmetic index for nanostar dendrimers, J. Math. Nanosci, 2011, 1, 33-42.
[28] Ranjini P.S., Lokesha V., Rajan M.A., On the Schultz index of the subdivision graphs, Adv. Stud. Contemp. Math., 2011, 21(3), 279-290.
[29] Ranjini P.S., Lokesha V., Cangül I.N., On the Zagreb indices of the line graphs of the subdivision graphs, Appl. Math. Comput., 2011, 218, 699-702.
[30] Su G., Xu L., Topological indices of the line graph of subdivision graphs and their Schur-bounds, Appl. Math. Comput., 2015, 253, 395-401.