

Article

# Computation of topological indices of linear chains of perylene and coronene using M-polynomial

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**Abstract:** The M-polynomial yields degree based topological indices that anticipate different physical and chemical properties of material being scrutinized. In this work, M-polynomial of linear chains of perylene and coronene are acquired. From M-polynomial, some degree based topological dicriptors are determined. Some topological indices of these compounds are compared by plotting graphs.

**Keywords:** topological indices; graph polynomials; subdivision graph; semi-total point graph

## 1. Introduction

In this article, connected graphs with parallel edges and no loops are taken into consideration. Let the vertex set and edge set of a graph be  $V(G)$  and  $E(G)$  respectively. The number of edges that are incident to determines a vertex's degree, given by the symbol  $d_v$ . Chemical graph theory is primarily concerned with the relationship between a compound's molecular graph and its various properties and functions. The physico-chemical properties and biological activities of substances are related to their chemical structures using mathematical models known as quantitative structure-property/quantitative structure-activity relationships (QSPR/QSAR). The topological index for the chemical graph is the end result of a mathematical and logical process that converts chemical information about a molecular structure into a usable integer. A degree dependent topological index is a subclass of topological index in which the index is calculated using the degrees of vertexs of the chemical compound's molecular graph. These indices are commonly used to study structural activity relationships, computer-aided design, medication creation, and forecast the topological properties of chemical graphs and networks. Topological indices can be estimated using their standard definitions, which is time-consuming if multiple indices of a given class of graphs have to be obtained. To overcome this difficulty, many researchers had introduced graph polynomials [1–3], whose differentiation or integration or a blending of both, at particular values yields required indices. Recently, Deutsch and Klavzar [4] made an analogous advancement in the form of the M-polynomial, which is widely utilized today to get several degree-based indices of molecular graphs of various chemical compounds. Using M-polynomials, many researchers [5–7] have determined the molecular descriptors of diverse chemical compounds. We concentrate on the combinatorial and topological characteristics of linear chains of perylene and coronene in the current work. We specifically establish closed forms for the M-polynomials of molecular graph of n-perylene and n-coronene and their subdivision [8] and semitotal vertex graphs [9] and then, using successive calculus operations, we obtain formulas for the topological indices of these graphs. In section II one can find the brief information of the different topological indices (Table 1) and their respective M-polynomials that will be used to generate these topological indices of n-perylene and n-coronene. In Section

III the simple methodology used for computation is explained. The main results of this work are shown in section IV, where the computation of different M-polynomials for various graph invariants are expressed in the form of theorems.

### 2. Preliminaries

Topological indices based on degree of end vertices of each edge of graph  $G$  is defined as follows:

$$I(G) = \sum_{uv \in E(G)} f(d_u, d_v)$$

where  $d_u$  and  $d_v$  are degrees of vertices  $u$  and  $v$  in graph  $G$  respectively.

**Table 1.** Some degree-based topological indices.

Topological index	$f(d_u, d_v)$
First Zagreb index, $M_1(G)$ [10]	$d_u + d_v$
Second Zagreb index $M_2(G)$ [10]	$d_u d_v$
Second Modified Zagreb index, $M_2^*(G)$ [11]	$\frac{1}{d_u d_v}$
General Randic connectivity index, $R_\alpha(G)$ [12, 13]	$(d_u d_v)^\alpha$
Symmetric Division degree index, $SDD(G)$ [14]	$\frac{d_u^\alpha + d_v^\alpha}{d_u d_v}$
Harmonic index, $H(G)$ [15]	$\frac{2}{d_u + d_v}$
Inverse sum index, $ISI(G)$ [16]	$\frac{d_u d_v}{d_u + d_v}$

For further information on degree based topological indices, one can refer following articles [17, 18]. M-polynomial of graph  $G$  is given by the following formula

$$M(G; x, y) = \sum_{i \leq j} m_{ij}(G) x^i y^j$$

where,  $m_{ij}(G)$ ,  $(i, j \geq 1)$  is the number of edges  $e = uv$  such that  $(i, j) = (d_u, d_v)$ .

where,  $D_x f(x, y) = x \frac{\partial(f(x, y))}{\partial x}$ ,  $D_y f(x, y) = y \frac{\partial(f(x, y))}{\partial y}$ ,  $S_x f(x, y) = \int_0^x \frac{f(t, y)}{t} dt$ ,  $S_y f(x, y) = \int_0^y \frac{f(x, t)}{t} dt$ ,  $Jf(x, y) = f(x, y)$ .

**Table 2.** Derivation of some degree-based topological indices from M-polynomial.

Topological index	$f(x, y)$	Derivation from $M(G; x, y)$
First Zagreb index	$x + y$	$(D_x + D_y) M(G; x, y) _{x=y=1}$
Second Zagreb index	$xy$	$(D_x D_y) M(G; x, y) _{x=y=1}$
Second Modified Zagreb index	$\frac{1}{xy}$	$(S_x S_y) M(G; x, y) _{x=y=1}$
Randic index	$(xy)^\alpha$	$(D_x^\alpha D_y^\alpha) M(G; x, y) _{x=y=1}$
Symmetric Division degree index	$\frac{x^\alpha + y^\alpha}{xy}$	$(D_x S_y + S_x D_y) M(G; x, y) _{x=y=1}$
Harmonic index	$\frac{2}{x+y}$	$(2S_x J) M(G; x, y) _{x=y=1}$
Inverse sum index	$\frac{xy}{x+y}$	$(S_x J D_x D_y) M(G; x, y) _{x=y=1}$

### 3. Methodology

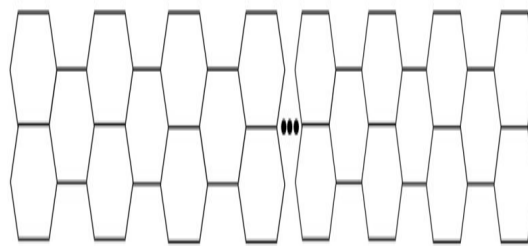
The computation of degree-based indices of n-perylene and n-coronene, as well as their subdivision and semitotal vertex graphs, are the subjects of the current work. To begin with, The M-polynomials are computed, and then various degree-based indices are determined using several calculus operators. For the purpose of obtaining the results, we use edge partition technique. Maple 2018 is used to display the results in graphical form.

### 4. Main results

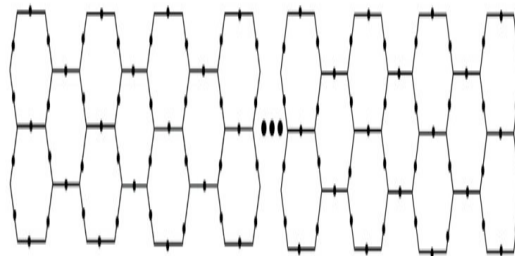
This section is subdivided into two section, where we present our main results coresponding to linear chains of perylene and coronene respectively.

#### 4.1. computational aspects of n-perylene

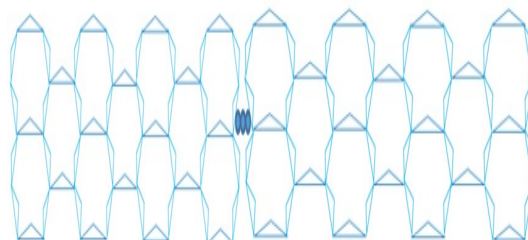
The graphical structures of n-perylene and it's subdivision graph and semitotal point graphs are represented in the **Figure 1**. The graph of n-perylene has  $nq+2(n-1)$  edges and  $np$  vertices, where  $p=20$ ,  $q=24$  and  $n = 1, 2, 3, \dots$



(a) molecular graph of n-perylene



(b) subdivision graph of n-perylene



(c) semitotal point graph of n-perylene

**Figure 1.** Graphs of n-perylene and it's subdivision and semi-total point graphs.

**Table 3.** The edge partition of n-perylene based on degree of end vertices of each edge.

$(d_u, d_v)$	(2,2)	(2,3)	(3,3)
Number of edges	$4n+4$	$8n$	$14n-6$

**Table 4.** The edge partition of subdivision graph of n-perylene based on degree of end vertices of each edge.

$(d_u, d_v)$	(2,2)	(2,3)
Number of edges	$16n+8$	$36n-12$

**Table 5.** The edge partition of semi total point graph of n-perylene based on degree of end vertices of each edge.

$(d_u, d_v)$	(2,4)	(2,6)	(4,4)	(4,6)	(6,6)
Number of edges	$16n+8$	$36n-12$	$4n+4$	$8n$	$14n-6$

**Theorem 1.** Let  $G$  be a graph of n-perylene and  $n=1,2,3\dots$  then the  $M$ -polynomial is

$$M(G; x, y) = (4n + 4)x^2y^2 + 8nx^2y^3 + (14n - 6)x^3y^3.$$

**Proof.** From **Figure 2**, The number of vertices and edges of n-perylene are  $np$  and  $nq+(2n-1)$  respectively.

The edge set can be partitioned into following three sets based on degree of end vertices of each edge.

$$E_{2,2} = \{uv \in E(G) | d_u = 2, d_v = 2\}$$

$$E_{2,3} = \{uv \in E(G) | d_u = 2, d_v = 3\}$$

$$E_{3,3} = \{uv \in E(G) | d_u = 3, d_v = 3\}$$

From **Table 3**, we have

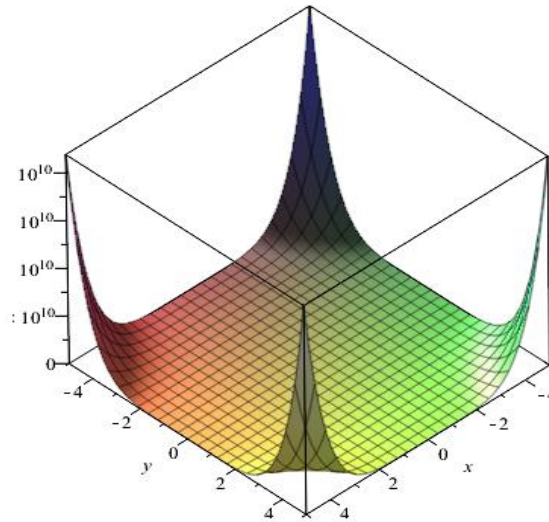
$$|E_{2,2}| = 2n + 4$$

$$|E_{2,3}| = 12n$$

$$|E_{3,3}| = 18n - 6.$$

Thus  $M$  polynomial of n-perylene is

$$\begin{aligned} M(G; x, y) &= \sum_{i \leq j} m_{ij}(G)x^i y^j \\ &= |E_{2,2}|x^2y^2 + |E_{2,3}|x^2y^3 + |E_{3,3}|x^3y^3 \\ &= (4n + 4)x^2y^2 + (8n)x^2y^3 + (14n - 6)x^3y^3. \quad \square \end{aligned}$$



**Figure 2.** M-polynomial of n-perylene for n=10.

**Theorem 2.** Let  $G$  be the graph of n-perylene and  $n=1, 2, 3, \dots$ , then

1.  $M_1(G) = 140n - 20$
2.  $M_2(G) = 190n - 38$
3.  $M_2^*(G) = \frac{35n + 3}{9}$
4.  $SDD(G) = \frac{160n - 12}{3}$
5.  $H(G) = \frac{148n}{15}$
6.  $ISI(G) = \frac{111n - 11}{2}$
7.  $R_\alpha(G) = 2^{2\alpha+2}(n + 1) + 2^{\alpha+3}3^\alpha n + 3^{2\alpha}(14n - 6)$ .

**Proof.** The required results are obtained by substituting **Table 2** results into the M-polynomial of n-perylene.  $\square$

**Theorem 3.** Let  $H$  be a subdivision graph of n-perylene then the M-polynomial of  $H$  is

$$M(H; x, y) = (16n + 8)x^2y^2 + (36n - 12)x^2y^3.$$

**Proof.** The number of vertices and edges of subdivision graph of n-perylene are  $n(p+q+2)-2$  and  $2nq+4(n-1)$  respectively. The edge set can be partitioned into following two sets based on degree of end vertices of each edge.

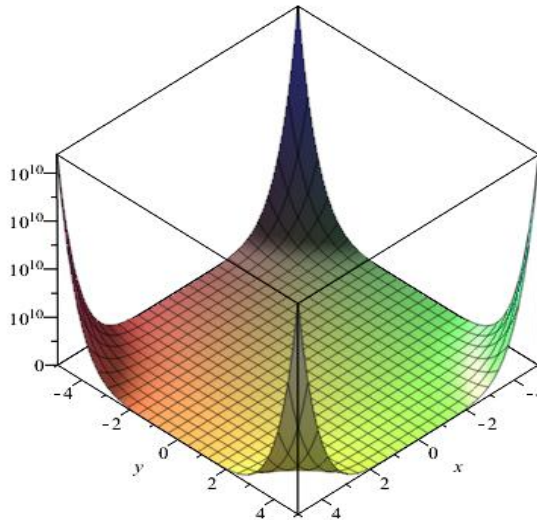
$$E_{2,2} = \{uv \in E(H) | d_u = 2, d_v = 2\}$$

$$E_{2,3} = \{uv \in E(H) | d_u = 2, d_v = 3\}$$

From **Table 4**, we have

$$|E_{2,2}| = 16n + 8$$

$$|E_{2,3}| = 36n - 12$$



**Figure 3.** M-polynomial of subdivision graph of n-perylene for n=10.

Thus  $M$  polynomial of subdivision graph of n-perylene is

$$\begin{aligned}
 M(H; x, y) &= \sum_{i \leq j} m_{ij}(G) x^i y^j \\
 &= |E_{2,2}| x^2 y^2 + |E_{2,3}| x^2 y^3 \\
 &= (16n + 8) x^2 y^2 + (36n - 12) x^2 y^3. \quad \square
 \end{aligned}$$

**Theorem 4.** Let  $H$  be the subdivision graph of n-perylene then

1.  $M_1(H) = 244n - 28$
2.  $M_2(H) = 280n - 40$
3.  $M_2^*(H) = 10n$
4.  $SDD(H) = 110n - 10$
5.  $H(H) = \frac{112n - 4}{5}$
6.  $ISI(H) = 104n - 8$
7.  $R_\alpha(H) = 2^{2\alpha+3}(2n + 1) + 2^{\alpha+2}3^{\alpha+1}(3n - 1)$ .

**Proof.** The required results are obtained by substituting **Table 2** results into the M-polynomial of subdivision graph of n-perylene.  $\square$

**Theorem 5.** Let  $P$  be a semi total point graph of n-perylene then the M-polynomial of  $P$  is

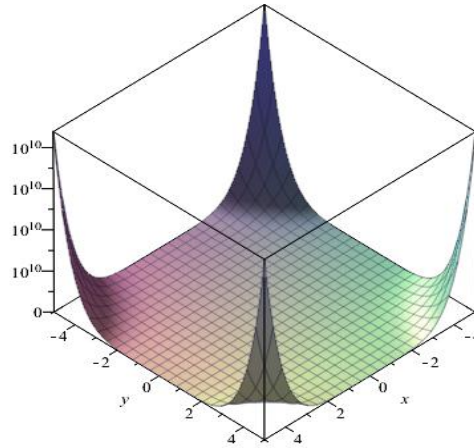
$$\begin{aligned}
 M(P; x, y) &= (16n + 8)x^2y^4 + (36n - 12)x^2y^6 \\
 &+ (4n + 4)x^4y^4 + (8n)x^4y^6 + (14n - 6)x^6y^6
 \end{aligned}$$

**Proof.** The number of vertices and edges of semi total point graph of n-perylene are  $n(p+q+2)-2$  and  $3nq+6(n-1)$  respectively. The edge set can be partitioned into following sets based on degree of end vertices of each edge.

$$E_{2,4} = \{uv \in E(H) | d_u = 2, d_v = 2\}$$

$$E_{2,6} = \{uv \in E(H) | d_u = 2, d_v = 3\}$$

$$E_{4,4} = \{uv \in E(H) | d_u = 2, d_v = 2\}$$



**Figure 4.** M-polynomial of semi total point graph of n-perylene for n=10.

$$E_{4,6} = \{uv \in E(H) | d_u = 2, d_v = 3\}$$

$$E_{6,6} = \{uv \in E(H) | d_u = 2, d_v = 2\}$$

From **Table 5**, we have

$$|E_{2,4}| = 16n + 8$$

$$|E_{2,6}| = 36n - 12$$

$$|E_{4,4}| = 4n + 4$$

$$|E_{4,6}| = 8n$$

$$|E_{6,6}| = 14n - 6$$

Thus M polynomial of semi total point graph of n-perylene is

$$\begin{aligned} M(H; x, y) &= \sum_{i \leq j} m_{ij}(G) x^i y^j \\ &= |E_{2,4}| x^2 y^4 + |E_{2,6}| x^2 y^6 + |E_{4,4}| x^4 y^4 + |E_{4,6}| x^4 y^6 + |E_{6,6}| x^6 y^6 \\ &= (16n + 8) x^2 y^4 + (36n - 12) x^2 y^6 + (4n + 4) x^4 y^4 + (8n) x^4 y^6 \\ &\quad + (14n - 6) x^6 y^6. \quad \square \end{aligned}$$

**Theorem 6.** Let  $P$  be the semi total point graph of n-perylene then

1.  $M_1(P) = 664n - 88$

2.  $M_2(P) = 1320n - 232$

3.  $M_2^*(P) = \frac{215n+3}{36}$

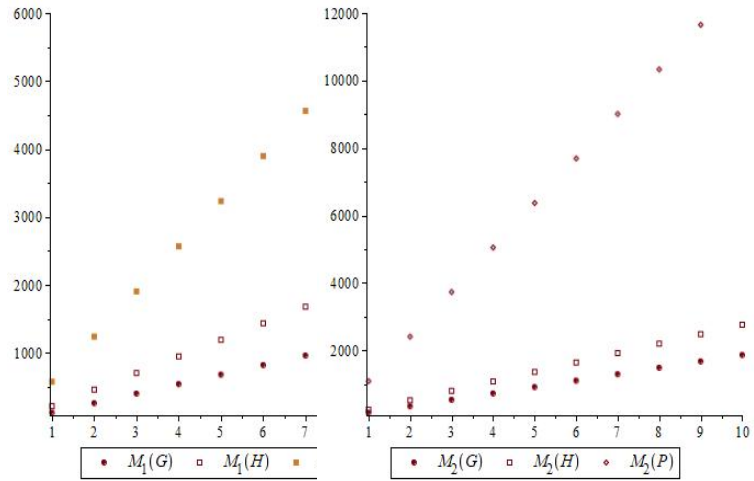
4.  $SDD(P) = \frac{676n+144}{3}$

5.  $H(P) = \frac{289n-5}{15}$

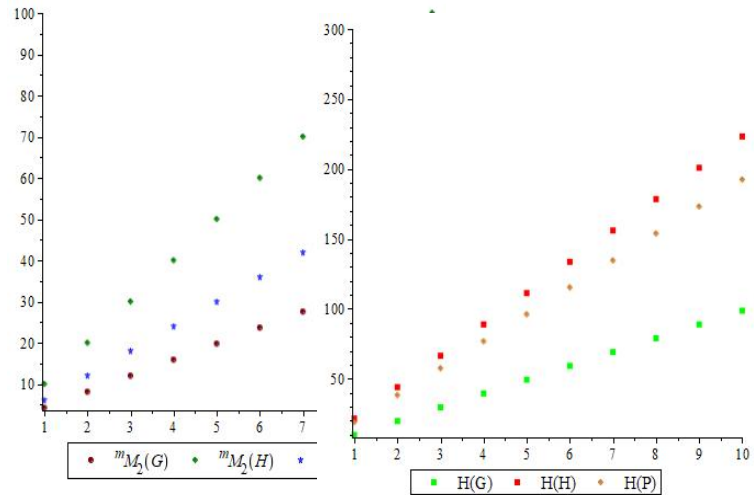
6.  $ISI(P) = \frac{2836n-284}{15}$

7.  $R_\alpha(P) = 2^{3\alpha+3}(2n+1) + 2^{3\alpha} 3^{\alpha+1}(3n-1) + 2^{4\alpha+2}(n+1) + 2^{3\alpha+3} 3^\alpha n + 2^{2\alpha+1} 3^{2\alpha}(7n-3).$

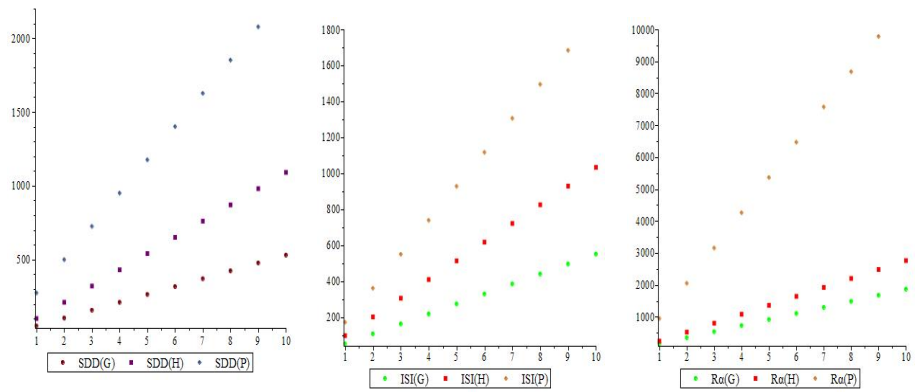
**Proof.** The required results are obtained by substituting **Table 2** results into the M-polynomial of semi total point graph of n-perylene.  $\square$



(a) First Zagreb index (b) Second Zagreb index



(c) Second modified Zagreb index (d) Harmonic index



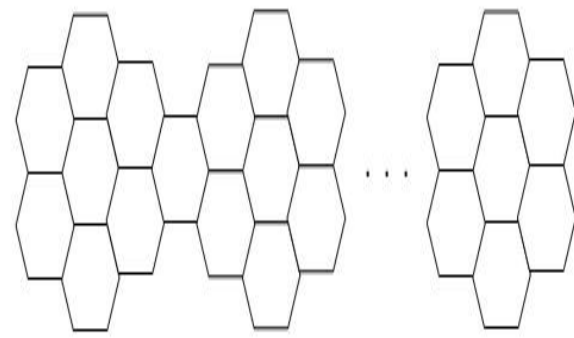
(e) Symmetric division degree index (f) Inverse sum index (g) Randic index

**Figure 5.** Plot of individual topological indices for n-perylene graph, it's subdivision and semi total point graph upto n=10.

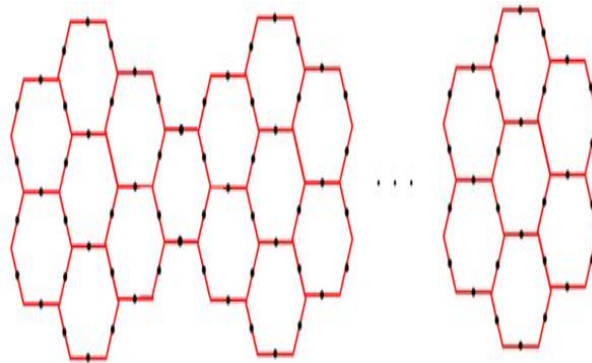
### 4.2. Computational aspects of n-coronene

The graphical structure of n-coronene is represented in the **Figure 2**. The graph of n-coronene has  $nq+2(n-1)$  edges and  $np$  vertices, where  $p=24$ ,  $q=30$  and  $n=1,2,3,\dots$

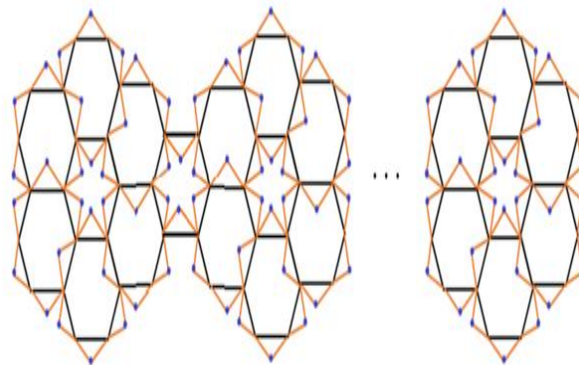




(a) n-coronene



(b) subdivision graph of n-coronene



(c) semi total point graph of n-coronene

**Figure 6.** Graphs of n-coronene and it's subdivision and semittotal point graphs.

**Table 6.** The edge partition of n-coronene based on degree of end vertices of each edge.

$(d_u, d_v)$	(2,2)	(2,3)	(3,3)
Number of edges	$2n+4$	$12n$	$18n-6$

**Table 7.** The edge partition of subdivision graph of n-coronene based on degree of end vertices of each edge.

$(d_u, d_v)$	(2,2)	(2,3)
Number of edges	$16n+8$	$48n-12$

**Table 8.** The edge partition of semi total point graph of n-coronene based on degree of end vertices of each edge.

$(d_u, d_v)$	(2,4)	(2,6)	(4,4)	(4,6)	(6,6)
Number of edges	16n+8	48n-12	2n+4	12n	18n-6

**Theorem 7.** Let  $G$  be a graph of n-coronene and  $n=1,2,3\dots$  then the M-polynomial is

$$M(G; x, y) = (2n + 4)x^2y^2 + 12nx^2y^3 + (18n - 6)x^3y^3.$$

**Proof.** From **Figure 6**, The number of vertices and edges of n-coronene are  $np$  and  $nq+(2n-1)$  respectively. The edge set can be partitioned into following three sets based on degree of end vertices of each edge.

$$E_{2,2} = \{uv \in E(G) | d_u = 2, d_v = 2\}$$

$$E_{2,3} = \{uv \in E(G) | d_u = 2, d_v = 3\}$$

$$E_{3,3} = \{uv \in E(G) | d_u = 3, d_v = 3\}.$$

From **Table 6**, we have

$$|E_{2,2}| = 2n + 4$$

$$|E_{2,3}| = 12n$$

$$|E_{3,3}| = 18n - 6.$$

Thus  $M$  polynomial of n-coronene is

$$\begin{aligned} M(G; x, y) &= \sum_{i \leq j} m_{ij}(G)x^i y^j \\ &= |E_{2,2}|x^2y^2 + |E_{2,3}|x^2y^3 + |E_{3,3}|x^3y^3 \\ &= (2n + 4)x^2y^2 + (12n)x^2y^3 + (18n - 6)x^3y^3. \quad \square \end{aligned}$$

**Theorem 8.** Let  $G$  be the graph of n-coronene and  $n=1, 2, 3, \dots$ , then

1.  $M_1(G) = 176n - 20$

2.  $M_2(G) = 242n - 38$

3.  ${}^m M_2(G) = \frac{27n + 2}{6}$

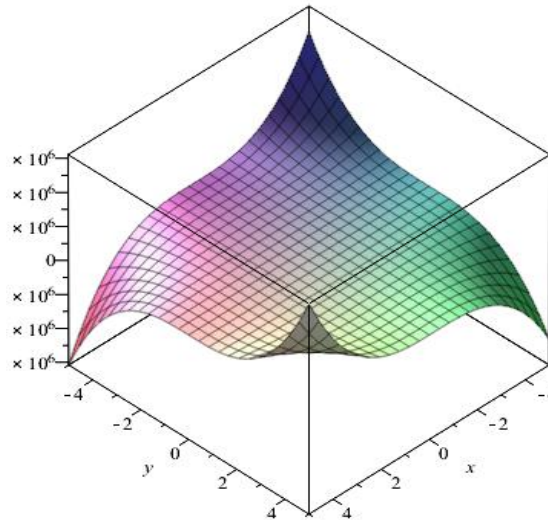
4.  $SDD(G) = 66n - 4$

5.  $H(G) = \frac{59n}{5}$

6.  $ISI(G) = \frac{137n - 11}{2}$

7.  $R_\alpha(G) = 2^{2\alpha+1}(n + 2) + 2^{\alpha+2}3^{\alpha+1}n + 3^{2\alpha+1}(6n - 2).$

**Proof.** The required results are obtained by substituting **Table 2** results into the M-polynomial of n-coronene.  $\square$



**Figure 7.** M-polynomial of n-coronene for n=10.

**Theorem 9.** Let  $H$  be a subdivision graph of n-coronene then the M-polynomial of  $H$  is

$$M(H; x, y) = (16n + 8)x^2y^2 + (48n - 12)x^2y^3.$$

**Proof.** From **Figure 6**, The number of vertices and edges of subdivision graph of n-coronene are  $n(p+q+2)-2$  and  $2nq+4(n-1)$  respectively. The edge set can be partitioned into following two sets based on degree of end vertices of each edge.

$$E_{2,2} = \{uv \in E(G) | d_u = 2, d_v = 2\}$$

$$E_{2,3} = \{uv \in E(G) | d_u = 2, d_v = 3\}$$

From **Table 7**, we have

$$|E_{2,2}| = 16n + 8$$

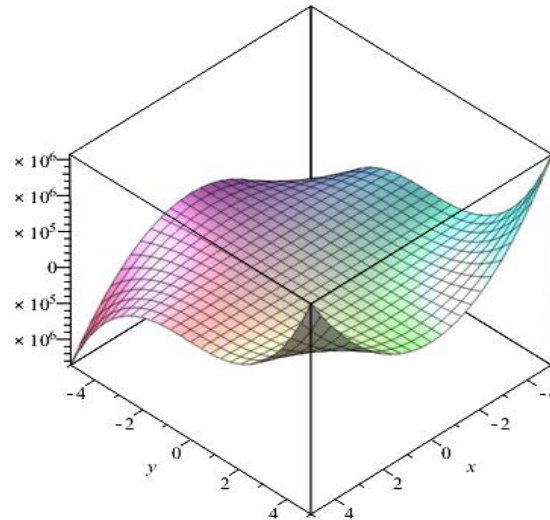
$$|E_{2,3}| = 48n - 12$$

Thus M polynomial of subdivision graph of n-coronene is

$$\begin{aligned} M(H; x, y) &= \sum_{i \leq j} m_{ij}(G)x^i y^j \\ &= |E_{2,2}|x^2y^2 + |E_{2,3}|x^2y^3 \\ &= (16n + 8)x^2y^2 + (48n - 12)x^2y^3. \quad \square \end{aligned}$$

**Theorem 10.** Let  $H$  be the subdivision graph of n-coronene then

1.  $M_1(H) = 304n - 28$
2.  $M_2(H) = 352n - 40$
3.  ${}^m M_2(H) = 12n$
4.  $SDD(H) = 136n - 10$
5.  $H(H) = \frac{136n - 4}{5}$
6.  $ISI(H) = 128n - 8$
7.  $R_\alpha(H) = 2^{2\alpha+3}(2n + 1) + 2^{\alpha+2}3^{\alpha+1}(2n - 1).$



**Figure 8.** M-polynomial of subdivision graph of n-coronene for n=10.

**Proof.** The required results are obtained by substituting **Table 2** results into the M-polynomial of subdivision graph of n-coronene. □

**Theorem 11.** Let  $P$  be a semi total point graph of n-coronene then the M-polynomial of  $P$  is

$$M(P; x, y) = (16n + 8)x^2y^4 + (48n - 12)x^2y^6 + (2n + 4)x^4y^4 + 12nx^4y^6 + (18n - 6)x^6y^6.$$

**Proof.** From **Figure 6**, The number of vertices and edges of semi total point graph of n-coronene are  $n(p+q+2)-2$  and  $3nq+6(n-1)$  respectively. The edge set can be partitioned into following five sets based on degree of end vertices of each edge.

$$E_{2,4} = \{uv \in E(G) | d_u = 2, d_v = 4\}$$

$$E_{2,6} = \{uv \in E(G) | d_u = 2, d_v = 6\}$$

$$E_{4,4} = \{uv \in E(G) | d_u = 4, d_v = 4\}$$

$$E_{4,6} = \{uv \in E(G) | d_u = 4, d_v = 6\}$$

$$E_{6,6} = \{uv \in E(G) | d_u = 6, d_v = 6\}$$

From **Table 8**, we have

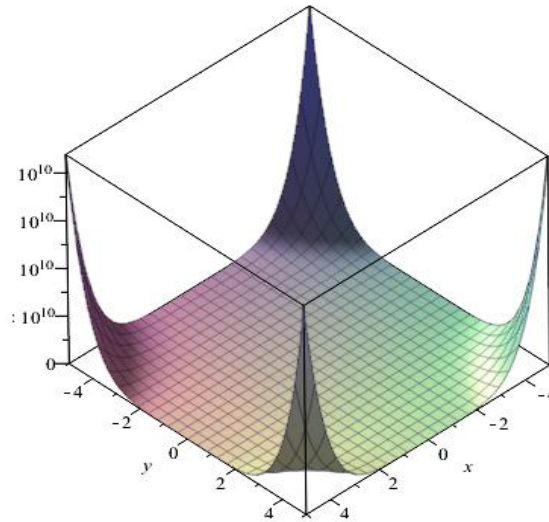
$$|E_{2,4}| = 16n + 8$$

$$|E_{2,6}| = 48n - 12$$

$$|E_{4,4}| = 2n + 4$$

$$|E_{4,6}| = 12n$$

$$|E_{6,6}| = 18n - 6$$



**Figure 9.** M-polynomial of semi total point graph of n-coronene for n=10.

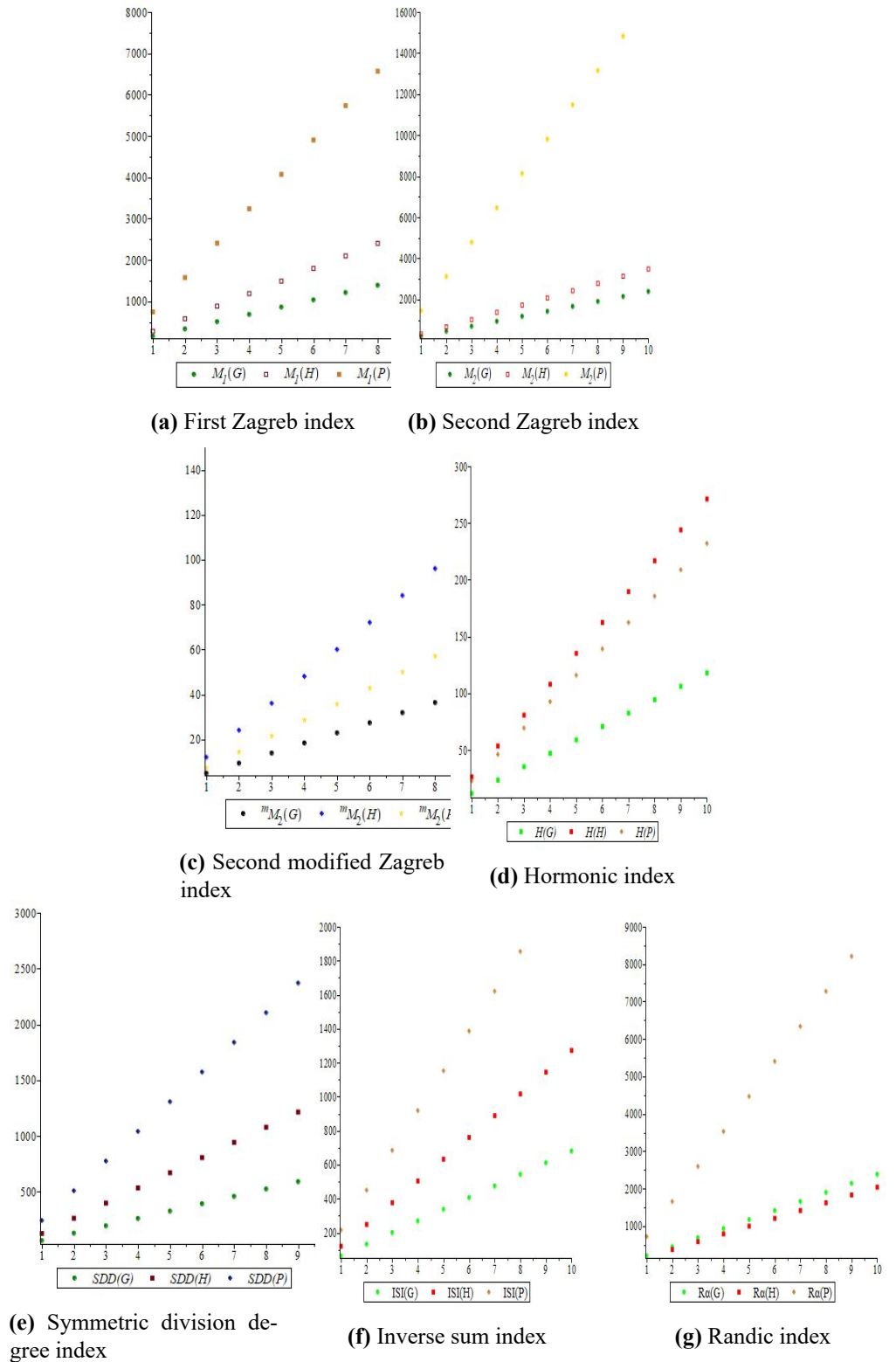
Thus M polynomial of semi total point graph of n-coronene is

$$\begin{aligned}
 M(P; x, y) &= \sum_{i \leq j} m_{ij}(G) x^i y^j \\
 &= |E_{2,4}| x^2 y^4 + |E_{2,6}| x^2 y^6 + |E_{4,4}| x^4 y^4 + |E_{4,6}| x^4 y^6 + |E_{6,6}| x^6 y^6 \\
 &= (16n + 8) x^2 y^4 + (48n - 12) x^2 y^6 + (2n + 4) x^4 y^4 + (12n) x^4 y^6 \\
 &+ (18n - 6) x^6 y^6. \quad \square
 \end{aligned}$$

**Theorem 12.** Let  $P$  be the semi total point graph of n-coronene then

1.  $M_1(P) = 832n - 88$
2.  $M_2(P) = 1672n - 232$
3.  ${}^m M_2(P) = \frac{171n + 2}{24}$
4.  $SDD(P) = 266n - 24$
5.  $H(P) = \frac{697n - 10}{30}$
6.  $ISI(P) = \frac{3512n - 284}{15}$
7.  $R_\alpha(P) = 2^{3\alpha+2} 3^{\alpha+1} n + 2^{2\alpha+1} 3^{2\alpha+1} (3n - 1)$ .

**Proof.** The required results are obtained by substituting **Table 2** results into the M-polynomial of semi total point graph of n-coronene.  $\square$



**Figure 10.** Plot of individual topological indices for n-coronene graph, it’s subdivision and semi total point graph upto n=10.

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