

Connection-Based Multiplicative Zagreb Indices of Polycyclic Aromatic Hydrocarbon Structures

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Abstract

The topological index (TI) is a numerical quantity associated with a graph that describes its various physical and chemical properties. Wiener presented the first distance-based TI to determine the boiling point of paraffin. The degree-based indices were introduced in 1972 to discover the total π - electron energy of molecules in a molecular graph. In this paper, three different types (Hexa-peri-hexabenzocoronene, Dodeca-benzo-circumcoronene and Hexa-cata-hexabenzocoronene) of polycyclic aromatic hydrocarbon structures are studied with the help of the different multiplicative Zagreb indices based on connection number.

Keywords: Zagreb indices; zagreb connection indices; molecular graphs; topological index

1 Introduction

Chemical graph theory is a branch of mathematical chemistry in which we study the various structural and chemical properties of the chemical or molecular graph such as boiling point, volatility, melting point, chirality, stability, and connectivity with the help of different topological indices. Moreover, Topological indices (TIs) are used in the subject of cheminformatics to study the quantitative structures, activities and property relationships on the molecule structures (Kimberly Jordan Burch (Indiana Univ. of Pennsylvania).

Let $\delta = (V(\delta), E(\delta))$ be a graph, where $V(\delta)$ be a collection of vertices and $E(\delta)$ be collection of edges. For a vertex $u \in V(\delta)$ the degree $d\delta(u)$ is the number of those vertices that are distance at one from u and connection number $c\delta(u)$ is the number of such vertices that are at distance 2 from vertex u . View other graph theory ideas (Bell, 1992) and (Dechen, 2023).

In 1972, the first and second Zagreb indices were introduced by Gutman and Trinajstić (Gautam 2013; Gautam 1972). These are very well known and frequently used in the study of chemical graph theory. The symbols $(M_1(Z))$ and $(M_2(Z))$ represent the first and second Zagreb indices, respectively. Furtula and Gutman defined a third degree-based TI, which is represented by $(M_3(Z))$. A lot of research has been done on Zagreb indices due to their chemical importance.

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Javaid et al. (Javaid et al., 2021) initiated novel connection-based ZIs of different wheel related graphs. Haoer et al. ([Multiplicative Leap Zagreb Indices of T-Thorny Graphs, n.d.](#)) investigated the multiplicative leap ZIs. After that, in 2020, Cao et al. (Cao et al., 2020) computed ZCIs of molecular graphs. Recently, Ali et al. (Ali et al., 2020) calculated the modified ZCIs for T-sum graphs in 2020. Recently, Sattar et al. (Sattar et al., 2021a; Sattar, Javaid, & Alam, 2022; Sattar, Javaid, & Bonyah, 2022) computed the ZCIs of a dendrimer nanostar.

This paper consists of the following: Section 2 contains a couple of important definitions that are required to understand the concept of the current study and the construction of three different types (Hexa-peri-hexabenzocoronene, Dodeca-benzo-circumcoronene, and Hexacata-hexabenzocoronene) of polycyclic aromatic hydrocarbon structures; Section 3 contains the main results (Hexa-peri-hexabenzocoronene, Dodeca-benzo-circumcoronene and Hexacatahexabenzocoronene); Section 4 covers the conclusion.

2 Topological Indices Based on Connection Numbers

Definition 2.1. Let δ be a graph, then first multiplicative zagreb connection index ($M\hat{Z}C_1(\delta)$), second multiplicative zagreb connection index ($M\hat{Z}C_2(\delta)$), third multiplicative zagreb connection index ($M\hat{Z}C_3(\delta)$) and fourth multiplicative zagreb connection index ($M\hat{Z}C_4(\delta)$) are

$$(a) M\hat{Z}C_1(\delta) = \prod_{v \in V(\delta)} [c_\delta(v)]^2$$

$$(b) M\hat{Z}C_2(\delta) = \prod_{uv \in E(\delta)} [c_\delta(u) \times c_\delta(v)]$$

$$(c) M\hat{Z}C_3(\delta) = \prod_{uv \in V(\delta)} [d_\delta(u) \times c_\delta(v)]$$

$$(d) M\hat{Z}C_4(\delta) = \prod_{uv \in E(\delta)} [c_\delta(u) + c_\delta(v)]$$

3. Definition 2.2.

For a graph δ , modified first multiplicative Zagreb connection index ($M\hat{Z}C_1^*(\delta)$), modified second multiplicative Zagreb connection index ($M\hat{Z}C_2^*(\delta)$) and modified third multiplicative Zagreb connection index ($M\hat{Z}C_3^*(\delta)$) are

$$(a) M\hat{Z}C_1^*(\delta) = \prod_{uv \in E(\delta)} [d_\delta(u)c_\delta(v) + d_\delta(v)c_\delta(u)]$$

$$(b) M\hat{Z}C_2^*(\delta) = \prod_{uv \in E(\delta)} [d_\delta(u)c_\delta(u) + d_\delta(v)c_\delta(v)]$$

$$(c) M\hat{Z}C_3^*(\delta) = \prod_{uv \in E(\delta)} [d_\delta(u)c_\delta(v) \times d_\delta(v)c_\delta(u)] = \prod_{uv \in E(\delta)} [d_\delta(u)c_\delta(u) \times d_\delta(v)c_\delta(v)]$$

3.1. Hexa-peri-hexabenzocoronene ($HBC(t)$) Structure

Let $\delta \cong HBC(r)$ be a Hexa-peri-hexabenzocoronene structure for $r \geq 2$, where r represents its generation steps. $|V(\delta)| = 18r^2 + 18r + 6$ are the total number of vertices and $|E(\delta)| = 27r^2 + 21r + 6$ are the total number of edges of $HBC(r)$ as shown in Figure 1.

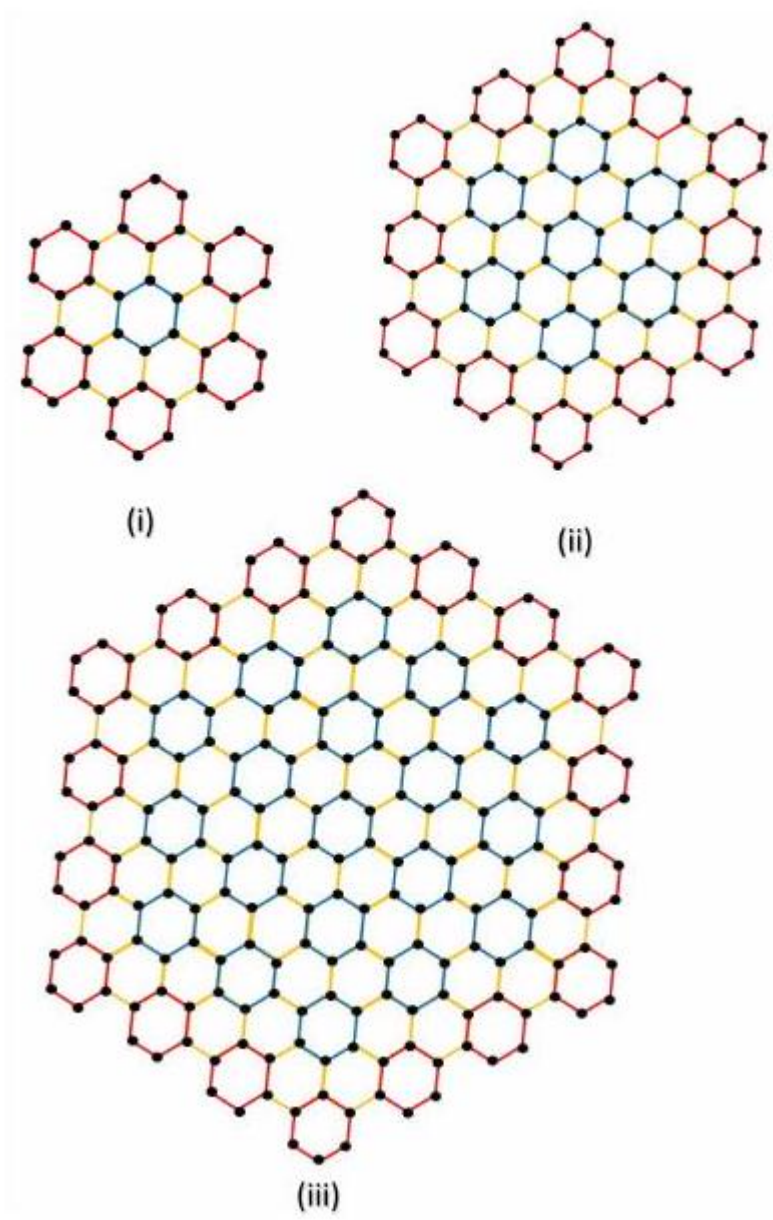


Figure 1: (i) $HBC(2)$; (ii) $HBC(3)$; (iii) $HBC(4)$

Using the connection number, we were able to determine the various subclasses of the set of edges as well as their cardinalities, as shown in Table 1. Using the degree-connection number, we also obtained the various subclasses of the set of edges and vertices along with their cardinalities in Tables 2 and Tables 3.

Table 1: $HBC(t)$ edges partition based on connection numbers.

$E_{c(t_1),c(t_2)}^c$	$ E_{c(t_1),c(t_2)}^c $
$E_{2,3}^c$	12
$E_{3,3}^c$	$6t - 6$
$E_{3,5}^c$	$12t$
$E_{5,5}^c$	$6t$
$E_{5,6}^c$	$12t$
$E_{6,6}^c$	$3t(9t - 5)$

Table 2: $HBC(t)$ edges partition based on degree-connection number.

$E_{d(u),d(v)}^{c(u),c(v)}$	$E_{d(u),d(v)}^{c(u),c(v)}$
$E_{2,2}^{2,3}$	12
$E_{2,2}^{3,3}$	$6t - 6$
$E_{2,3}^{3,5}$	$12t$
$E_{3,3}^{5,5}$	$6t$
$E_{3,3}^{5,6}$	$12t$
$E_{3,3}^{6,6}$	$3t(9t - 5)$

Table 3: $HBC(t)$ vertices partition based on degree-connection number.

$V_{d(u)}^{c(u)}$	$V_{d(u)}^{c(u)}$
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V_2^2	6
V_2^3	12t
V_3^5	12t
V_3^6	$6t(3t - 1)$

3.2. Dodeca-benzo-circumcoronene (*DBC(t)*) Structure

Let $\delta \cong DBC(r)$ be a Dodeca-benzo-circumcoronene structure for $r \geq 2$, where r represents its generation steps. $|V(\delta)| = 18r^2 + 6r$ are the total number of vertices and $|E(\delta)| = 27r^2 + 3r$ are total number of edges of *DBC(r)* as shown in Figure 2.

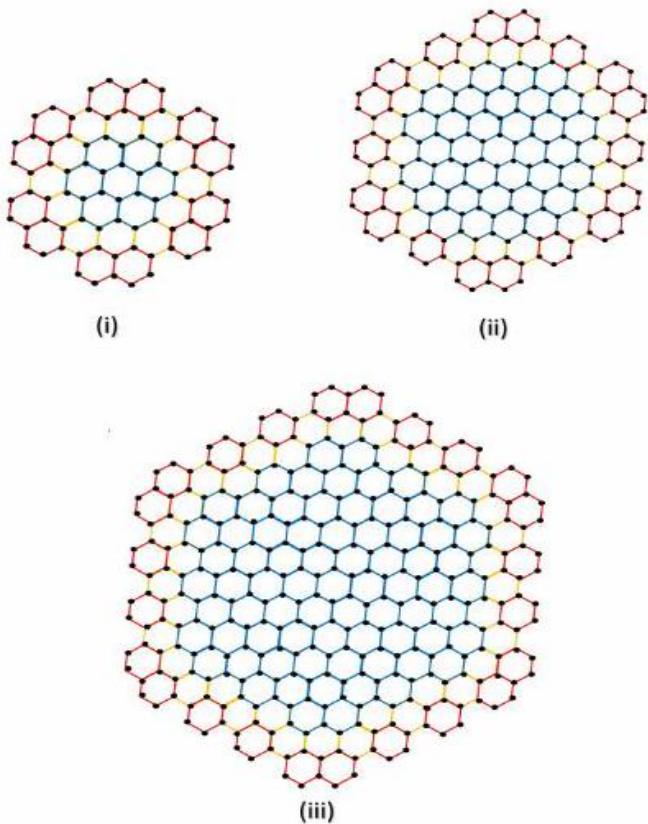


Figure 2: (i) *DBC(2)*; (ii) *DBC(3)*; (iii) *DBC(4)*

Using the connection number, we were able to determine the various subclasses of the set of

edges as well as their cardinalities, as shown in Table 4. Using the degree-connection number, we also obtained the various subclasses of the set of edges and vertices along with their cardinalities in Tables 5 and Tables 6. Table 4: $DBC(t)$ edges partition based on connection number

$E_{c(t_1),c(t_2)}^c$	$ E_{c(t_1),c(t_2)}^c $
$E_{3,3}^c$	$6t$
$E_{3,4}^c$	12
$E_{3,5}^c$	$12t - 12$
$E_{4,6}^c$	6
$E_{5,5}^c$	$6t - 6$
$E_{5,6}^c$	$12t - 12$
$E_{6,6}^c$	$27t^2 - 33t + 12$

Table 5: $DBC(t)$ edge partition based on degree-connection number.

$E_{d(u),d(v)}^{c(u),c(v)}$	$ E_{d(u),d(v)}^{c(u),c(v)} $
$E_{2,2}^{3,3}$	$6t$
$E_{2,3}^{3,4}$	12
$E_{2,3}^{3,5}$	$12t - 12$
$E_{3,3}^{4,6}$	6
$E_{3,3}^{5,5}$	$6t - 6$
$E_{3,3}^{5,6}$	$12t - 12$
$E_{3,3}^{6,6}$	$27t^2 - 33t + 12$

Table 6: $DBC(t)$ vertices partition based on degree-connection number.

$V_{d(u)}^{c(u)}$	$V_{d(u)}^{c(u)}$
V_2^3	$\overline{12t}$
V_3^4	6
V_3	$12t - 12$
	$18t^2 - 18t$

3.3. Hexa-cata-hexabenzocoronene ($chBC(t)$) Structure

Let $\delta \cong chBC(r)$ be a Hexa-cata-hexabenzocoronene structure for $r \geq 2$, where r represent its generation steps. $|V(\delta)| = 24r^2 - 30r + 12$ are the total number of vertices and $|E(\delta)| = 36r^2 - 54r + 24$ are the total number of edges of $chBC(r)$ as shown in Figure 3 .

Using the connection number, we were able to determine the various subclasses of the set of edges as well as their cardinalities, as shown in Table 7. Using the degree-connection number, we also obtained the various subclasses of the set of edges and vertices along with their cardinalities

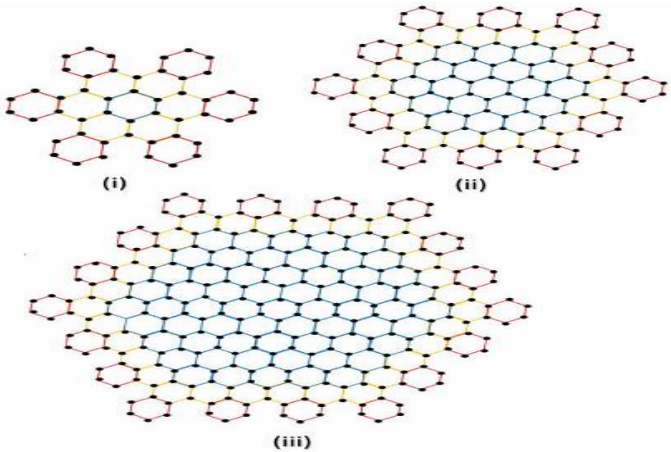


Figure 3: (i) $chBC(2)$;(ii) $chBC(3)$;(iii) $chBC(4)$

in Tables 8 and Tables 9.

Table 7: $chBC(t)$ edges Partition based on connection number.

$E_{c(n_1),c(n_2)}^c$	$ E_{c(n_1),c(n_2)}^c $
$E_{2,2}^c$	6
$E_{2,3}^c$	12t
$E_{3,5}^c$	12t
$E_{5,5}^c$	6
$E_{5,6}^c$	24t - 12
$E_{6,6}^c$	$36t^2 - 30t + 6$

Table 8: $cHBC(t)$ edges partition based on degree connection number.

$E_{d(u),d(v)}^{c(u),c(v)}$	$E_{d(u),d(v)}^{c(u),c(v)}$
$E_{2,2}^{2,2}$	6
$E_{2,2}^{2,3}$	12t
$E_{2,3}^{3,5}$	12t
$E_{3,3}^{5,5}$	6
$E_{3,3}^{5,6}$	24t - 12
$E_{3,3}^{6,6}$	$36t^2 - 30t + 6$

Table 9: $cHBC(t)$ vertices Partition based on degree-connection number.

$V_{d(u)}^{c(u)}$	$V_{d(u)}^{c(u)}$
V_2^2	6t + 6

V_3^3	$12t$
V_3^5	$12t$
V_3^6	$24t^2 - 12t$

4. Main results

This section deals with the results of the Connection number based multiplicative zagreb indices of the three different types (Hexa-peri-hexabenzocoronene, Dodeca-benzo-circumcoronene, and Hexa-cata-hexabenzocoronene) of molecular structure.

Theorem 3.1. Let $\delta \cong HBC(r)$ be a Hexa-peri-hexabenzocoronene structure. Then its first, second, third, and fourth multiplicative zagreb connection indices are

$$(a) M\hat{Z}C_1(\delta) = 2^{36t^2-12t+12} \times 3^{36t^2+12t} \times 5^{24t},$$

$$(b) M\hat{Z}C_2(\delta) = 2^{54t^2-18t+12} \times 3^{54t^2+6t} \times 5^{36t}$$

$$(c) M\hat{Z}C_3(\delta) = 2^{18t^2+6t+12} \times 3^{36t^2+12t} \times 5^{12t},$$

$$(d) M\hat{Z}C_4(\delta) = 2^{54t^2+18t-6} \times 3^{27t^2-9t-6} \times 5^{6t+12} \times 11^{12t}.$$

Proof. (a)

By the Definition 2.1,

$$M\hat{Z}C_1(\delta) = \prod_{v \in V(\delta)} [c_\delta(v)]^2$$

$$M\hat{Z}C_1(\delta) = \prod_{v \in V_1(\delta)} [c_\delta(v)]^2 \times \prod_{v \in V_2(\delta)} [c_\delta(v)]^2 \times \prod_{v \in V_3(\delta)} [c_\delta(v)]^2 \times \prod_{v \in V_4(\delta)} [c_\delta(v)]^2$$

We consider the partition of the vertices of the Hexa-peri-hexabenzocoronene structure with respect to their connection numbers

$$M\hat{Z}C_1(\delta) = (2)^{2|V_1|} \times (3)^{2|V_2|} \times (5)^{2|V_3|} \times (6)^{2|V_4|}$$

$$M\hat{Z}C_1(\delta) = 2^{2 \times 6} \times 3^{2 \times 12t} \times 5^{2 \times 12t} \times 6^{2 \times 6t(3t-1)}$$

By performing some calculations, We get

$$M\hat{Z}C_1(\delta) = 2^{36t^2-12t+12} \times 3^{36t^2+12t} \times 5^{24t}.$$

(b).

By Definition 2.1,

$$M\hat{Z}C_2(\delta) = \prod_{uv \in E(\delta)} [c_\delta(u) \times c_\delta(v)]$$

$$M\hat{Z}C_2(\delta) =$$

$$\begin{aligned} & \prod_{uv \in E_{2,3}^c} [c_\delta(u) \times c_\delta(v)] \times \prod_{uv \in E_{3,3}^c} [c_\delta(u) \times c_\delta(v)] \times \prod_{uv \in E_{3,5}^c} [c_\delta(u) \times c_\delta(v)] \\ & \times \prod_{uv \in E_{5,5}^c} [c_\delta(u) \times c_\delta(v)] \times \prod_{uv \in E_{5,6}^c} [c_\delta(u) \times c_\delta(v)] \times \prod_{uv \in E_{6,6}^c} [c_\delta(u) \times c_\delta(v)] \end{aligned}$$

Using Table 1,

$$M\hat{Z}C_2(\delta) = [2 \times 3]^{12} \times [3 \times 3]^{6t-6} \times [3 \times 5]^{12t} \times [5 \times 5]^{6t} \times [5 \times 6]^{12t} \times [6 \times 6]^{3t(9t-5)}$$

By performing some calculations, we get

$$M\hat{Z}C_2(\delta) = 2^{54t^2-18t+12} \times 3^{54t^2+6t} \times 5^{36t}.$$

(c)

By Definition 2.1,

$$M\hat{Z}C_3(\delta) = \prod_{v \in V(\delta)} [d_\delta(v) \times c_\delta(v)]$$

$$M\hat{Z}C_3(\delta) =$$

$$\begin{aligned} & \prod_{v \in V_1(\delta)} [d_\delta(v) \times c_\delta(v)] \times \prod_{v \in V_2(\delta)} [d_\delta(v) \times c_\delta(v)] \times \prod_{v \in V_3(\delta)} [d_\delta(v) \times c_\delta(v)] \\ & \times \prod_{v \in V_4(\delta)} [d_\delta(v) \times c_\delta(v)] \end{aligned}$$

Using table 3 ,

$$M\hat{Z}C_3(\delta) = (2 \times 2)^6 \times (2 \times 3)^{12t} \times (3 \times 5)^{12t} \times (3 \times 6)^{6t(3t-1)}$$

By performing some calculations, we get

$$M\hat{Z}C_3(\delta) = 2^{18t^2+6t+12} \times 3^{36t^2+12t} \times 5^{12t}.$$

(d).

By Definition 2.1,

$$M\hat{Z}C_4(\delta) =$$

$$\prod_{uv \in E_{2,3}^c} [c_\delta(u) + c_\delta(v)] \times \prod_{uv \in E_{3,3}^c} [c_\delta(u) + c_\delta(v)] \times \prod_{uv \in E_{3,5}^c} [c_\delta(u) + c_\delta(v)] \times \\ \prod_{uv \in E_{5,5}^c} [c_\delta(u) + c_\delta(v)] \times \prod_{uv \in E_{5,6}^c} [c_\delta(u) + c_\delta(v)] \times \prod_{uv \in E_{6,6}^c} [c_\delta(u) + c_\delta(v)]$$

Using Table 1,

$$M\hat{Z}C_4(\delta) = [2 + 3]^{12} \times [3 + 3]^{6t-6} \times [3 + 5]^{12t} \times [5 + 5]^{6t} \times [5 + 6]^{12t} \times [6 + 6]^{3t(9t-5)}.$$

By performing some calculations, we get

$$M\hat{Z}C_4(\delta) = 2^{54t^2+18t-6} \times 3^{27t^2-9t-6} \times 5^{6t+12} \times 11^{12t}.$$

Theorem 3.2. Let $\delta \cong HBC(r)$ be a Hexa-peri-hexabenzocoronene structure. Then the first, second, and third modified multiplicative zagreb connection indices are

$$(a) M\hat{Z}C_1^*(\delta) = 2^{54t^2-12t} \times 3^{54t^2-6t-6} \times 5^{6t+12} \times 11^{12t} \times 19^{12t},$$

$$(b) M\hat{Z}C_2^*(\delta) = 2^{54t^2-12t} \times 3^{54t^2+6t-6} \times 5^{6t+12} \times 7^{12t} \times 11^{12t},$$

$$(c) M\hat{Z}C_3^*(\delta) = 2^{54t^2+6t+24} \times 3^{108t^2+24t} \times 5^{36t}.$$

Proof. (a).

By the Definition 2.2,

$$M\hat{Z}C_1^*(\delta) = \prod_{uv \in E(\delta)} [d_\delta(u)c_\delta(v) + d_\delta(v)c_\delta(u)]$$

$$M\hat{Z}C_1^*(\delta) =$$

$$\prod_{uv \in E_{2,2}^{2,3}} [d_\delta(u)c_\delta(v) + d_\delta(v)c_\delta(u)] \times \prod_{uv \in E_{2,2}^{3,3}} [d_\delta(u)c_\delta(v) + d_\delta(v)c_\delta(u)] \\ \times \prod_{uv \in E_{2,3}^{3,5}} [d_\delta(u)c_\delta(v) + d_\delta(v)c_\delta(u)] \times \prod_{uv \in E_{3,3}^{5,5}} [d_\delta(u)c_\delta(v) + d_\delta(v)c_\delta(u)] \\ \times \prod_{uv \in E_{3,3}^{5,6}} [d_\delta(u)c_\delta(v) + d_\delta(v)c_\delta(u)] \times \prod_{uv \in E_{3,3}^{6,6}} [d_\delta(u)c_\delta(v) + d_\delta(v)c_\delta(u)]$$

Using table 2, we get

$$M\hat{Z}C_1^*(\delta) = [10]^{12} \times [12]^{6t-6} \times [19]^{12t} \times [30]^{6t} \times [33]^{12t} \times [36]^{3t(9t-5)}$$

By performing some calculations, we get

$$M\hat{Z}C_1^*(\delta) = 2^{54t^2-12t} \times 3^{54t^2-6t-6} \times 5^{6t+12} \times 11^{12t} \times 19^{12t}.$$

(b).

As we know from the Definition 2.2,

$$M\hat{Z}C_2^*(\delta) = \prod_{uv \in E(\delta)} [d_\delta(u)c_\delta(u) + d_\delta(v)c_\delta(v)]$$

$$M\hat{Z}C_2^*(\delta) =$$

$$\begin{aligned} & \prod_{uv \in E_{2,2}^{2,3}} [d_\delta(u)c_\delta(u) + d_\delta(v)c_\delta(v)] \times \prod_{uv \in E_{2,2}^{3,3}} [d_\delta(u)c_\delta(u) + d_\delta(v)c_\delta(v)] \\ & \times \prod_{uv \in E_{2,3}^{3,5}} [d_\delta(u)c_\delta(u) + d_\delta(v)c_\delta(v)] \times \prod_{uv \in E_{3,3}^{5,5}} [d_\delta(u)c_\delta(u) + d_\delta(v)c_\delta(v)] \\ & \times \prod_{uv \in E_{3,3}^{5,6}} [d_\delta(u)c_\delta(u) + d_\delta(v)c_\delta(v)] \times \prod_{uv \in E_{3,3}^{6,6}} [d_\delta(u)c_\delta(u) + d_\delta(v)c_\delta(v)] \end{aligned}$$

Using table 2,

$$M\hat{Z}C_2^*(\delta) = [10]^{12} \times [12]^{6t-6} \times [21]^{12t} \times [30]^{6t} \times [33]^{12t} \times [36]^{3t(9t-5)}$$

By performing some calculations, we get

$$M\hat{Z}C_2^*(\delta) = 2^{54t^2-12t} \times 3^{54t^2+6t-6} \times 5^{6t+12} \times 7^{12t} \times 11^{12t}.$$

5. (c).

By Definition 2.2,

$$M\hat{Z}C_3^*(\delta) = \prod_{uv \in E(\delta)} [d_\delta(u)c_\delta(u) \times d_\delta(v)c_\delta(v)]$$

$$M\hat{Z}C_3^*(\delta) =$$

$$\begin{aligned} & \prod_{uv \in E_{2,2}^{2,3}} [d_\delta(u)c_\delta(u) \times d_\delta(v)c_\delta(v)] \times \prod_{uv \in E_{2,2}^{3,3}} [d_\delta(u)c_\delta(u) \times d_\delta(v)c_\delta(v)] \\ & \times \prod_{uv \in E_{2,3}^{3,5}} [d_\delta(u)c_\delta(u) \times d_\delta(v)c_\delta(v)] \times \prod_{uv \in E_{3,3}^{5,5}} [d_\delta(u)c_\delta(u) \times d_\delta(v)c_\delta(v)] \\ & \times \prod_{uv \in E_{3,3}^{5,6}} [d_\delta(u)c_\delta(u) \times d_\delta(v)c_\delta(v)] \times \prod_{uv \in E_{3,3}^{6,6}} [d_\delta(u)c_\delta(u) \times d_\delta(v)c_\delta(v)] \end{aligned}$$

Using table 2,

$$M\hat{Z}C_3^*(\delta) = [24]^{12} \times [36]^{6t-6} \times [90]^{12t} \times [225]^{6t} \times [270]^{12t} \times [324]^{3t(9t-5)}$$

By performing some calculations, we get

$$M\hat{Z}C_3^*(\delta) = 2^{54t^2+6t+24} \times 3^{108t^2+24t} \times 5^{36t}.$$

Theorem 3.3. Let $\delta \cong DBC(r)$ be a Dodeca-benzo-circumcoronene structure. Then its first,

second, third, and fourth multiplicative zagreb connection indices are

$$(a) M\hat{Z}C_1(\delta) = 2^{36t^2-36t+36} \times 3^{36t^2-12t+12} \times 5^{24t-24},$$

$$(b) M\hat{Z}C_2(\delta) = 2^{54t^2-54t+54} \times 3^{54t^2-30t+18} \times 5^{36t-36}$$

$$(c) M\hat{Z}C_3(\delta) = 2^{18t^2-6t+18} \times 3^{36t^2-12t+6} \times 5^{12t-12}$$

$$(d) M\hat{Z}C_4(\delta) = 2^{54t^2-18t-12} \times 3^{27t^2-27t+12} \times 5^{6t} \times 11^{12t-12}.$$

Proof. (a)

By the Definition 2.1,

$$M\hat{Z}C_1(\delta) = \prod_{v \in V(\delta)} [c_\delta(v)]^2$$

$$M\hat{Z}C_1(\delta) = \prod_{v \in V_1(\delta)} [c_\delta(v)]^2 \times \prod_{v \in V_2(\delta)} [c_\delta(v)]^2 \times \prod_{v \in V_3(\delta)} [c_\delta(v)]^2 \times \prod_{v \in V_4(\delta)} [c_\delta(v)]^2$$

By using the partition of the vertices of the $DBC(t)$ with respect to their connection numbers, we get

$$M\hat{Z}C_1(\delta) = (3)^{2|V_1|} \times (4)^{2|V_2|} \times (5)^{2|V_3|} \times (6)^{2|V_4|}$$

$$M\hat{Z}C_1(\delta) = 3^{2 \times 12t} \times 4^{2 \times 6} \times 5^{2 \times (12t-12)} \times 6^{2 \times (18t^2-18t+6)}$$

By performing some calculations, We get

$$M\hat{Z}C_1(\delta) = 2^{36t^2-36t+36} \times 3^{36t^2-12t+12} \times 5^{24t-24}.$$

(b).

As we know from the Definition 2.1

$$M\hat{Z}C_2(\delta) = \prod_{uv \in E(\delta)} [c_\delta(u) \times c_\delta(v)]$$

$$M\hat{Z}C_2(\delta) =$$

$$\begin{aligned} & \prod_{uv \in E_{3,3}^c} [c_\delta(u) \times c_\delta(v)] \times \prod_{uv \in E_{3,4}^c} [c_\delta(u) \times c_\delta(v)] \times \prod_{uv \in E_{3,5}^c} [c_\delta(u) \times c_\delta(v)] \\ & \times \prod_{uv \in E_{4,6}^c} [c_\delta(u) \times c_\delta(v)] \times \prod_{uv \in E_{5,5}^c} [c_\delta(u) \times c_\delta(v)] \times \prod_{uv \in E_{5,6}^c} [c_\delta(u) \times c_\delta(v)] \\ & \times \prod_{uv \in E_{6,6}^c} [c_\delta(u) \times c_\delta(v)] \end{aligned}$$

Using Table 4

$$\begin{aligned} M\hat{Z}C_2(\delta) &= [3 \times 3]^{6t} \times [3 \times 4]^{12} \times [3 \times 5]^{12t-12} \times [4 \times 6]^6 \times [5 \times 5]^{6t-6} \times [5 \times 6]^{12t-12} \\ & \times [6 \times 6]^{27t^2-33t+12} \end{aligned}$$

By performing some calculations, we get

$$M\hat{Z}C_2(\delta) = 2^{54t^2-54t+54} \times 3^{54t^2-30t+18} \times 5^{36t-36}.$$

(c).

By Definition 2.1,

$$M\hat{Z}C_3(\delta) = \prod_{v \in V(\delta)} [d_\delta(v) \times c_\delta(v)]$$

$$M\hat{Z}C_3(\delta) =$$

$$\prod_{v \in V_1(\delta)} [d_\delta(v) \times c_\delta(v)] \times \prod_{v \in V_2(\delta)} [d_\delta(v) \times c_\delta(v)] \times \prod_{v \in V_3(\delta)} [d_\delta(v) \times c_\delta(v)] \\ \times \prod_{v \in V_4(\delta)} [d_\delta(v) \times c_\delta(v)]$$

$$\text{Using table 6, } M\hat{Z}C_3(\delta) = (2 \times 3)^{12t} \times (3 \times 4)^6 \times (3 \times 5)^{12t-12} \times (3 \times 6)^{18t^2-18t+6}$$

By performing some calculations, we get

$$M\hat{Z}C_3(\delta) = 2^{18t^2-6t+18} \times 3^{36t^2-12t+6} \times 5^{12t-12}.$$

(d)

By Definition 2.1,

$$M\hat{Z}C_4(\delta) =$$

$$\prod_{uv \in E_{3,3}^c} [c_\delta(u) + c_\delta(v)] \times \prod_{uv \in E_{3,4}^c} [c_\delta(u) + c_\delta(v)] \times \prod_{uv \in E_{3,5}^c} [c_\delta(u) + c_\delta(v)] \\ \times \prod_{uv \in E_{4,6}^c} [c_\delta(u) + c_\delta(v)] \times$$

$$\prod_{uv \in E_{5,5}^c} [c_\delta(u) + c_\delta(v)] \times \prod_{uv \in E_{5,6}^c} [c_\delta(u) + c_\delta(v)] \times \prod_{uv \in E_{6,6}^c} [c_\delta(u) + c_\delta(v)]$$

Using Table 4 ,

$$M\hat{Z}C_4(\delta) = [3 + 3]^{6t} \times [3 + 4]^{12} \times [3 + 5]^{12t-12} \times [4 + 6]^6 \times [5 + 5]^{6t-6} \times [5 + 6]^{12t-12} \times [6 + 6]^{27t^2-33t+12}.$$

By performing some calculations, we get

$$M\hat{Z}C_4(\delta) = 2^{54t^2-18t-12} \times 3^{27t^2-27t+12} \times 5^{6t} \times 11^{12t-12}.$$

Theorem 3.4. Let $\delta \cong DBC(r)$ be a Dodeca-benzo-circumcoronene structure. Then the first, second, and third modified multiplicative zagreb connection indices are

$$(a) M\hat{Z}C_1^*(\delta) = 2^{54t^2-48t+24} \times 3^{54t^2-42t+12} \times 5^{6t} \times 11^{12t-12} \times 17^{12} \times 19^{12t-12},$$

$$(b) M\hat{Z}C_2^*(\delta) = 2^{54t^2-48t+36} \times 3^{54t^2-30t+24} \times 5^{6t} \times 7^{12t-12} \times 11^{12t-12},$$

$$(c) M\hat{Z}C_3^*(\delta) = 2^{54t^2-30t+54} \times 3^{108t^2-48t+18} \times 5^{36t-36}.$$

Proof. (a).

By the Definition 2.2,

$$M\hat{Z}C_1^*(\delta) = \prod_{uv \in E(\delta)} [d_\delta(u)c_\delta(v) + d_\delta(v)c_\delta(u)]$$

$$M\hat{Z}C_1^*(\delta) =$$

$$\begin{aligned} & \prod_{uv \in E_{2,2}^{3,3}} [d_\delta(u)c_\delta(v) + d_\delta(v)c_\delta(u)] \times \prod_{uv \in E_{2,3}^{3,4}} [d_\delta(u)c_\delta(v) + d_\delta(v)c_\delta(u)] \\ & \times \prod_{uv \in E_{2,3}^{3,5}} [d_\delta(u)c_\delta(v) + d_\delta(v)c_\delta(u)] \times \prod_{uv \in E_{3,3}^{4,6}}^{2,3} [d_\delta(u)c_\delta(v) + d_\delta(v)c_\delta(u)] \\ & \quad \times \prod_{uv \in E_{3,3}^{5,5}} [d_\delta(u)c_\delta(v) + d_\delta(v)c_\delta(u)] \\ & \times \prod_{uv \in E_{3,3}^{5,6}}^{2,3} [d_\delta(u)c_\delta(v) + d_\delta(v)c_\delta(u)] \times \prod_{uv \in E_{3,3}^{6,6}} [d_\delta(u)c_\delta(v) + d_\delta(v)c_\delta(u)] \end{aligned}$$

Using table 7 ,we get

$$M\hat{Z}C_1^*(\delta) = [12]^{6t} \times [17]^{12} \times [19]^{12t-12} \times [30]^6 \times [30]^{6t-6} \times [33]^{12t-12} \times [36]^{27t^2-33t+12}$$

By performing some calculations, we get

$$M\hat{Z}C_1^*(\delta) = 2^{54t^2-48t+24} \times 3^{54t^2-42t+12} \times 5^{6t} \times 11^{12t-12} \times 17^{12} \times 19^{12t-12}.$$

(b).

As we know from the Definition 2.2,

$$M\hat{Z}C_2^*(\delta) = \prod_{uv \in E(\delta)} [d_\delta(u)c_\delta(u) + d_\delta(v)c_\delta(v)]$$

$$M\hat{Z}C_2^*(\delta) =$$

$$\begin{aligned} & \prod_{uv \in E_{2,2}^{3,3}} [d_\delta(u)c_\delta(u) + d_\delta(v)c_\delta(v)] \times \prod_{uv \in E_{2,3}^{3,4}} [d_\delta(u)c_\delta(u) + d_\delta(v)c_\delta(v)] \times \prod_{uv \in E_{2,3}^{3,5}} [d_\delta(u)c_\delta(u) + d_\delta(v)c_\delta(v)] \\ & \times \prod_{uv \in E_{3,3}^{4,6}} [d_\delta(u)c_\delta(u) + d_\delta(v)c_\delta(v)] \times \prod_{uv \in E_{3,3}^{5,5}} [d_\delta(u)c_\delta(u) + d_\delta(v)c_\delta(v)] \\ & \times \prod_{uv \in E_{3,3}^{5,6}} [d_\delta(u)c_\delta(u) + d_\delta(v)c_\delta(v)] \times \prod_{uv \in E_{3,3}^{6,6}} [d_\delta(u)c_\delta(u) + d_\delta(v)c_\delta(v)] \end{aligned}$$

Using table 7 ,

$$M\hat{Z}C_2^*(\delta) = [12]^{6t} \times [18]^{12} \times [21]^{12t-12} \times [30]^6 \times [30]^{6t-6} \times [33]^{12t-12} \times [36]^{27t^2-33t+12}$$

By performing some calculations, we get

$$M\hat{Z}C_2^*(\delta) = 2^{54t^2-48t+36} \times 3^{54t^2-30t+24} \times 5^{6t} \times 7^{12t-12} \times 11^{12t-12}.$$

(c)

By Definition 2.2,

$$M\hat{Z}C_3^*(\delta) = \prod_{uv \in E(\delta)} [d_\delta(u)c_\delta(u) \times d_\delta(v)c_\delta(v)]$$

$$M\hat{Z}C_3^*(\delta) =$$

$$\begin{aligned} & \prod_{uv \in E_{2,2}^{3,3}} [d_\delta(u)c_\delta(u) \times d_\delta(v)c_\delta(v)] \times \prod_{uv \in E_{2,3}^{3,4}} [d_\delta(u)c_\delta(u) \times d_\delta(v)c_\delta(v)] \\ & \times \prod_{uv \in E_{2,3}^{3,5}} [d_\delta(u)c_\delta(u) \times d_\delta(v)c_\delta(v)] \times \prod_{uv \in E_{3,3}^{4,6}} [d_\delta(u)c_\delta(u) \times d_\delta(v)c_\delta(v)] \\ & \times \prod_{uv \in E_{3,3}^{5,5}} [d_\delta(u)c_\delta(u) \times d_\delta(v)c_\delta(v)] \times \prod_{uv \in E_{3,3}^{5,6}} [d_\delta(u)c_\delta(u) \times d_\delta(v)c_\delta(v)] \\ & \times \prod_{uv \in E_{3,3}^{6,6}} [d_\delta(u)c_\delta(u) \times d_\delta(v)c_\delta(v)] \end{aligned}$$

Using table 7 ,

$$M\hat{Z}C_3^*(\delta) = [36]^{6t} \times [72]^{12} \times [90]^{12t-12} \times [216]^6 \times [225]^{6t-6} \times [270]^{12t-12} \times [324]^{27t^2-33t+12}$$

By performing some calculations, we get

$$M\hat{Z}C_3^*(\delta) = 2^{54t^2-30t+54} \times 3^{108t^2-48t+18} \times 5^{36t-36}.$$

Theorem 3.5. Let $\delta \cong CHBC(r)$ be a hexa-cata-hexabenzocoronene structure. Then its first, second, third, and fourth multiplicative zagreb connection indices are

$$(a) M\hat{Z}C_1(\delta) = 2^{48t^2+12t-12} \times 3^{48t^2} \times 5^{24t},$$

$$(b) M\hat{Z}C_2(\delta) = 2^{72t^2-24t+12} \times 3^{72t^2-12t} \times 5^{36t},$$

$$(c) M\hat{Z}C_3(\delta) = 2^{24t^2+12} \times 3^{48t^2+12t} \times 5^{12t},$$

$$(d) M\hat{Z}C_4(\delta) = 2^{72t^2-24t+30} \times 3^{36t^2-30t+6} \times 5^{12t+6} \times 11^{24t-12}.$$

Proof. (a)

By the Definition 2.1,

$$M\hat{Z}C_1(\delta) = \prod_{v \in V(\delta)} [c_\delta(v)]^2$$

$$M\hat{Z}C_1(\delta) = \prod_{v \in V_1(\delta)} [c_\delta(v)]^2 \times \prod_{v \in V_2(\delta)} [c_\delta(v)]^2 \times \prod_{v \in V_3(\delta)} [c_\delta(v)]^2 \times \prod_{v \in V_4(\delta)} [c_\delta(v)]^2$$

By using the partition of the vertices of the *cHBC* with respect to their connection numbers, we get

$$M\hat{Z}C_1(\delta) = (2)^{2|V_1|} \times (3)^{2|V_2|} \times (5)^{2|V_3|} \times (6)^{2|V_4|} \quad M\hat{Z}C_1(\delta) = 2^{2 \times (6t+6)} \times 3^{2 \times 12t} \times 5^{2 \times 12t} \times 6^{2 \times (24t^2-12t)}.$$

By performing some calculations, We get

$$M\hat{Z}C_1(\delta) = 2^{48t^2+12t-12} \times 3^{48t^2} \times 5^{24t}.$$

(b).

As we know from the Definition 2.1,

$$M\hat{Z}C_2(\delta) = \prod_{uv \in E(\delta)} [c_\delta(u) \times c_\delta(v)]$$

$$M\hat{Z}C_2(\delta) =$$

$$\prod_{uv \in E_{2,2}^c} [c_\delta(u) \times c_\delta(v)] \times \prod_{uv \in E_{2,3}^c} [c_\delta(u) \times c_\delta(v)] \times \prod_{uv \in E_{3,5}^c} [c_\delta(u) \times c_\delta(v)] \\ \times \prod_{uv \in E_{5,5}^c} [c_\delta(u) \times c_\delta(v)] \times \prod_{uv \in E_{5,6}^c}^{2,3} [c_\delta(u) \times c_\delta(v)] \times \prod_{uv \in E_{6,6}^c} [c_\delta(u) \times c_\delta(v)]$$

Using Table 7,

$$M\hat{Z}C_2(\delta) = [2 \times 2]^6 \times [2 \times 3]^{12t} \times [3 \times 5]^{12t} \times [5 \times 5]^6 \times [5 \times 6]^{24t-12} \times [6 \times 6]^{36t^2-30t+6}$$

By performing some calculations, we get

$$M\hat{Z}C_2(\delta) = 2^{72t^2-24t+12} \times 3^{72t^2-12t} \times 5^{36t}.$$

6. (c).

By Definition 2.1,

$$M\hat{Z}C_3(\delta) = \prod_{v \in V(\delta)} [d_\delta(v) \times c_\delta(v)]$$

$$M\hat{Z}C_3(\delta) =$$

$$\prod_{v \in V_1(\delta)} [d_\delta(v) \times c_\delta(v)] \times \prod_{v \in V_2(\delta)} [d_\delta(v) \times c_\delta(v)] \times \prod_{v \in V_3(\delta)} [d_\delta(v) \times c_\delta(v)] \\ \times \prod_{v \in V_4(\delta)} [d_\delta(u) \times c_\delta(v)]$$

Using table 9 ,

$$M\hat{Z}C_3(\delta) = (2 \times 2)^{6t+6} \times (3 \times 3)^{12t} \times (3 \times 5)^{12t} \times (3 \times 6)^{24t^2-12t}$$

By performing some calculations, we get

$$M\hat{Z}C_3(\delta) = 2^{24t^2+12} \times 3^{48t^2+12t} \times 5^{12t}$$

(d).

By Definition 2.1,

$$M\hat{Z}C_4(\delta) =$$

$$\prod_{uv \in E_{2,2}^c} [c_\delta(u) + c_\delta(v)] \times \prod_{uv \in E_{2,3}^c} [c_\delta(u) + c_\delta(v)] \times \prod_{uv \in E_{3,5}^c} [c_\delta(u) + c_\delta(v)] \times$$

$$\prod_{uv \in E_{5,5}^c} [c_\delta(u) + c_\delta(v)] \times \prod_{uv \in E_{5,6}^c} [c_\delta(u) + c_\delta(v)] \times \prod_{uv \in E_{6,6}^c} [c_\delta(u) + c_\delta(v)]$$

Using Table 7,

$$M\hat{Z}C_4(\delta) = [2 + 2]^6 \times [2 + 3]^{12t} \times [3 + 5]^{12t} \times [5 + 5]^6 \times [5 + 6]^{24t-12} \times [6 + 6]^{36t^2-30t+6}.$$

By performing some calculations, we get

$$M\hat{Z}C_4(\delta) = 2^{72t^2-24t+30} \times 3^{36t^2-30t+6} \times 5^{12t+6} \times 11^{24t-12}.$$

Theorem 3.6. Let $\delta \cong CHBC(r)$ be a hexa-cata-hexabenzocoronene structure. Then the first, second, and third modified multiplicative zagreb connection indices are

$$(a) M\hat{Z}C_1^*(\delta) = 2^{72t^2-48t+36} \times 3^{72t^2-36t+6} \times 5^{12t+6} \times 11^{24t-12} \times 19^{12t},$$

$$(b) M\hat{Z}C_2^*(\delta) = 2^{72t^2-48t+36} \times 3^{72t^2-24t+6} \times 5^{12t+6} \times 7^{12t} \times 11^{24t-12},$$

$$(c) M\hat{Z}C_3^*(\delta) = 2^{72t^2+12t+24} \times 3^{144t^2-12t} \times 5^{36t}.$$

Proof. (a).

By the Definition 2.2,

$$M\hat{Z}C_1^*(\delta) = \prod_{uv \in E(\delta)} [d_\delta(u)c_\delta(v) + d_\delta(v)c_\delta(u)]$$

$$M\hat{Z}C_1^*(\delta) =$$

$$\prod_{uv \in E_{2,2}^{2,2}} [d_\delta(u)c_\delta(v) + d_\delta(v)c_\delta(u)] \times \prod_{uv \in E_{2,2}^{2,3}} [d_\delta(u)c_\delta(v) + d_\delta(v)c_\delta(u)]$$

$$\times \prod_{uv \in E_{2,3}^{3,5}} [d_\delta(u)c_\delta(v) + d_\delta(v)c_\delta(u)] \times \prod_{uv \in E_{3,3}^{5,5}} [d_\delta(u)c_\delta(v) + d_\delta(v)c_\delta(u)]$$

$$\times \prod_{uv \in E_{3,3}^{5,6}} [d_\delta(u)c_\delta(v) + d_\delta(v)c_\delta(u)] \times \prod_{uv \in E_{3,3}^{6,6}} [d_\delta(u)c_\delta(v) + d_\delta(v)c_\delta(u)]$$

Using table 8 , we get

$$M\hat{Z}C_1^*(\delta) = [8]^6 \times [10]^{12t} \times [19]^{12t} \times [30]^6 \times [33]^{24t-12} \times [36]^{36t^2-30t+6}$$

By performing some calculations, we get

$$M\hat{Z}C_1^*(\delta) = 2^{72t^2-48t+36} \times 3^{72t^2-36t+6} \times 5^{12t+6} \times 11^{24t-12} \times 19^{12t}.$$

(b).

As we know from the Definition 2.2,

$$M\hat{Z}C_2^*(\delta) = \prod_{uv \in E(\delta)} [d_\delta(u)c_\delta(u) + d_\delta(v)c_\delta(v)]$$

$$M\hat{Z}C_2^*(\delta) =$$

$$\begin{aligned} & \prod_{uv \in E_{2,2}^{2,2}} [d_\delta(u)c_\delta(u) + d_\delta(v)c_\delta(v)] \times \prod_{uv \in E_{2,2}^{2,3}} [d_\delta(u)c_\delta(u) + d_\delta(v)c_\delta(v)] \\ & \times \prod_{uv \in E_{2,3}^{3,5}} [d_\delta(u)c_\delta(u) + d_\delta(v)c_\delta(v)] \times \prod_{uv \in E_{3,3}^{5,5}} [d_\delta(u)c_\delta(u) + d_\delta(v)c_\delta(v)] \\ & \times \prod_{uv \in E_{3,3}^{5,6}} [d_\delta(u)c_\delta(u) + d_\delta(v)c_\delta(v)] \times \prod_{uv \in E_{3,3}^{6,6}} [d_\delta(u)c_\delta(u) + d_\delta(v)c_\delta(v)] \end{aligned}$$

Using table 8

$$M\hat{Z}C_2^*(\delta) = [8]^6 \times [10]^{12t} \times [21]^{12t} \times [30]^6 \times [33]^{24t-12} \times [36]^{36t^2-30t+6}$$

By performing some calculations, we get

$$M\hat{Z}C_2^*(\delta) = 2^{72t^2-48t+36} \times 3^{72t^2-24t+6} \times 5^{12t+6} \times 7^{12t} \times 11^{24t-12}.$$

(c)

By Definition 2.2,

$$M\hat{Z}C_3^*(\delta) = \prod_{uv \in E(\delta)} [d_\delta(u)c_\delta(u) \times d_\delta(v)c_\delta(v)]$$

$$M\hat{Z}C_3^*(\delta) =$$

$$\prod_{uv \in E_{2,2}^{2,2}} [d_\delta(u)c_\delta(u) \times d_\delta(v)c_\delta(v)] \times \prod_{uv \in E_{2,2}^{2,3}} [d_\delta(u)c_\delta(u) \times d_\delta(v)c_\delta(v)]$$

$$\begin{aligned} & \times \prod_{uv \in E_{2,3}^{3,5}} [d_\delta(u)c_\delta(u) \times d_\delta(v)c_\delta(v)] \times \prod_{uv \in E_{3,3}^{5,5}} [d_\delta(u)c_\delta(u) \times d_\delta(v)c_\delta(v)] \\ & \times \prod_{uv \in E_{3,3}^{5,6}} [d_\delta(u)c_\delta(u) \times d_\delta(v)c_\delta(v)] \times \prod_{uv \in E_{3,3}^{6,6}} [d_\delta(u)c_\delta(u) \times d_\delta(v)c_\delta(v)] \end{aligned}$$

Using table 8

$$M\hat{Z}C_3^*(\delta) = [16]^6 \times [24]^{12t} \times [90]^{12t} \times [225]^6 \times [270]^{24t-12} \times [324]^{36t^2-30t+6}$$

By performing some calculations, we get

$$M\hat{Z}C_3^*(\delta) = 2^{72t^2+12t+24} \times 3^{144t^2-12t} \times 5^{36t}$$

3 Conclusion

In this paper, we constructed the partitions of the edges of three different types molecular graphs based on connection numbers (see Table 1, Table 4, and Table 7) and degree-connection numbers (see Table 2, Table 5, and Table 8) of their end vertices. furthermore, the partition of the vertex set of three different types molecular graphs is obtained based on degree-connection number considered at the same time (see Table 3, Table 6, and Table 9). Finally, we obtained the first, second, third, and fourth multiplicative zagreb connection indices as well as first, second, and third modified multiplicative zagreb connection indices, which are calculated for three different types molecular graphs.

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