

Degree-Based Molecular Descriptors of Chain Biphenylene

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Abstract: With the fast advancement of the industry, including the drug and medical fields, Irregularity Descriptors may help to measure the physicochemical and Nano-properties, which are necessary for a growing industry. Biphenylene is a two-dimensional polymeric material that is among the most active areas of investigation in chemistry, biology, and physics. In our article, in view of structure analysis and mathematical derivation, we studied some topological descriptors such as the General Harmonic index, Redefined version of Zagreb indices, the Sombor index SO , the General sum-connectivity index, First and Second multiplicative Zagreb index, Geometric arithmetic index, Ordinary Geometric-arithmetic index Atom-bond connectivity (ABC) index and Irregularity Descriptors of molecular chain graphs of Biphenylene D_n . Furthermore, by the concepts of well-known degree-based descriptors, we introduced new degree-based descriptors such as (the Yemen-Sombor index) ($YS - index$), Second General sum-connectivity index (χ_2^α), Third General sum-connectivity index (χ_3^α), Generalized General sum-connectivity index (χ_α^α) of chain Biphenylene. These numerical values correlate with structural facts and chemical reactivity, biological activities, and physical properties. The results obtained could help us learn more about the characteristics of the chain Biphenylene.

Keywords: irregularity indices; molecular structures; degree-based molecular descriptors; chain biphenylene.

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1. Introduction

Topological descriptors describe the design of the molecular structure and significantly impact different properties and activities like entropy, acentric factor, stability, boiling point, molar refraction, etc., of chemical compounds [1–3]. There is a wide range of topological descriptors: degree-based, distance-based, eigenvalue-based, matching-based, and mixed-based [4–6]. Hundred-degree-based descriptors are introduced to study compounds' properties, which have been used in chemical, medical and pharmacy engineering. Gutman and Trinajstić [7,8] presented the first degree-based structure descriptors (first and second Zagreb indices) in (1972). The first and second Zagreb indices were introduced by Ashrafi *et al.* in (2010) [9]. Furtula *et al.* (2015) introduced the forgotten index and coindex (F-index, F-coindex) [10,11].

Alameri *et al.* [12,13] (2020) defined new degree-based structure descriptors the (*Y – index*) and (*Y – coindex*). The Harmonic index was introduced by Zhong [14]. Recently, in order to extend the harmonic index for more chemical applications, Yan *et al.* [15] introduced the General Harmonic index, which is defined in Equation 1.

$$H_k(\Gamma) = \sum_{uv \in E(\Gamma)} \left(\frac{2}{\delta(u) + \delta(v)} \right)^k, \tag{1}$$

Ranjini *et al.* [16] defined the Redefined first, second and third Zagreb indices for a graph *G*, and these are manifested as:

$$\begin{aligned} ReZG_1(\Gamma) &= \sum_{uv \in E(\Gamma)} \frac{\delta(u) + \delta(v)}{\delta(u)\delta(v)}, & ReZG_2(\Gamma) &= \sum_{uv \in E(\Gamma)} \frac{\delta(u)\delta(v)}{\delta(u) + \delta(v)}, \\ ReZG_3(\Gamma) &= \sum_{uv \in E(\Gamma)} (\delta(u) \delta(v))(\delta(u) + \delta(v)), \end{aligned} \tag{2}$$

The Sombor index *SO* was introduced by Gutman [17], which is defined as

$$SO(\Gamma) = \sum_{uv \in E(\Gamma)} \sqrt{\delta_\Gamma^2(u) + \delta_\Gamma^2(v)}, \tag{3}$$

The General sum-connectivity index [18] is defined as

$$\chi^\alpha(\Gamma) = \sum_{uv \in E(\Gamma)} [\delta_\Gamma(u) + \delta_\Gamma(v)]^\alpha, \tag{4}$$

The first multiplicative Zagreb index introduced by Gutman [19]

$$PM_1(\Gamma) = \prod_{uv \in E(\Gamma)} [\delta_\Gamma(u) + \delta_\Gamma(v)], \tag{5}$$

The second multiplicative Zagreb index defined by Ghorbani and Azimi [20]

$$PM_2(\Gamma) = \prod_{uv \in E(\Gamma)} [\delta_\Gamma(u) \delta_\Gamma(v)], \tag{6}$$

The geometric arithmetic index introduced by Ghorbani and Azimi [21]

$$GA(\Gamma) = \sum_{uv \in E(\Gamma)} \frac{2\sqrt{\delta(u)\delta(v)}}{\delta(u) + \delta(v)}, \tag{7}$$

As the extension of the geometric-arithmetic index, Eliasi *et al.* [22] proposed the Ordinary Geometric-arithmetic index

$$OGA_k(\Gamma) = \sum_{uv \in E(\Gamma)} \left(\frac{2\sqrt{\delta(u)\delta(v)}}{\delta(u) + \delta(v)} \right)^k, \tag{8}$$

Atom-bond connectivity (ABC) index defined by Estrada *et al.* [23]

$$ABC(\Gamma) = \sum_{uv \in E(\Gamma)} \sqrt{\frac{\delta(u) + \delta(v) - 2}{\delta(u)\delta(v)}}, \tag{9}$$

And by the concepts of the Yemen index (*Y – index*) and the Sombor index *SO*, we introduce a new degree-based index named (the Yemen-Sombor index) denoted by (*YS – index*) and define by:

$$YS(\Gamma) = \sum_{uv \in E(\Gamma)} \sqrt{\delta_\Gamma^3(u) + \delta_\Gamma^3(v)}, \tag{10}$$

Moreover, by the definition of the General sum-connectivity index, we introduce new degree-based indices denoted by (Second General sum-connectivity index $\chi_2^\alpha(\Gamma)$), (Third

General sum-connectivity index $\chi_3^\alpha(\Gamma)$, (Generalized General sum-connectivity index $\chi_\alpha^\alpha(\Gamma)$) and define respectively by:

$$\chi_2^\alpha(\Gamma) = \sum_{uv \in E(\Gamma)} [\delta_\Gamma^2(u) + \delta_\Gamma^2(v)]^\alpha, \tag{11}$$

$$\chi_3^\alpha(\Gamma) = \sum_{uv \in E(\Gamma)} [\delta_\Gamma^3(u) + \delta_\Gamma^3(v)]^\alpha, \tag{12}$$

$$\chi_\alpha^\alpha(\Gamma) = \sum_{uv \in E(\Gamma)} [\delta_\Gamma^\alpha(u) + \delta_\Gamma^\alpha(v)]^\alpha, \tag{13}$$

Irregularity indices are used to express the irregularity of graphs. For regular graphs, the irregularity descriptor vanishes, and it will be non-zero for non-regular graphs. Many researchers computed the irregularity descriptors for various chemical structures. Table 1 shows twelve degree-based irregularity indices.

Table 1. Irregularity indices.

Irregularity indices	Form of index
AL index [24]	$AL(\Gamma) = \sum_{uv \in E(\Gamma)} \delta_\Gamma(u) - \delta_\Gamma(v) $
IRR_t index [25]	$IRR_t(\Gamma) = \frac{1}{2} \sum_{uv \in E(\Gamma)} \delta_\Gamma(u) - \delta_\Gamma(v) $
IRF index [26]	$IRF(\Gamma) = \sum_{uv \in E(\Gamma)} (\delta_\Gamma(u) - \delta_\Gamma(v))^2$
IRB index [27]	$IRB(\Gamma) = \sum_{uv \in E(\Gamma)} (\sqrt{\delta_\Gamma(u)} - \sqrt{\delta_\Gamma(v)})^2$
IRA index [27]	$IRA(\Gamma) = \sum_{uv \in E(\Gamma)} \left(\frac{1}{\sqrt{\delta_\Gamma(u)}} - \frac{1}{\sqrt{\delta_\Gamma(v)}} \right)^2$
IRL index [28]	$IRL(\Gamma) = \sum_{uv \in E(\Gamma)} \ln(\delta_\Gamma(u)) - \ln(\delta_\Gamma(v)) $
IRDIF index [27]	$IRDIF(\Gamma) = \sum_{uv \in E(\Gamma)} \left \frac{\delta_\Gamma(u)}{\delta_\Gamma(v)} - \frac{\delta_\Gamma(v)}{\delta_\Gamma(u)} \right $
IRLU index [28]	$IRLU(\Gamma) = \sum_{uv \in E(\Gamma)} \frac{ \delta_\Gamma(u) - \delta_\Gamma(v) }{\min\{\delta_\Gamma(u), \delta_\Gamma(v)\}}$
IRLF index [27]	$IRLF(\Gamma) = \sum_{uv \in E(\Gamma)} \frac{ \delta_\Gamma(u) - \delta_\Gamma(v) }{\sqrt{\delta_\Gamma(u)\delta_\Gamma(v)}}$
IRLA index [27]	$IRLA(\Gamma) = \sum_{uv \in E(\Gamma)} \frac{ \delta_\Gamma(u) - \delta_\Gamma(v) }{(\delta_\Gamma(u) + \delta_\Gamma(v))}$
IRDI index [27]	$IRDI(\Gamma) = \sum_{uv \in E(\Gamma)} \ln[1 + \delta_\Gamma(u) - \delta_\Gamma(v)]$
IRGA index [27]	$IRGA(\Gamma) = \sum_{uv \in E(\Gamma)} \ln\left(\frac{\delta_\Gamma(u) + \delta_\Gamma(v)}{2\sqrt{\delta_\Gamma(u)\delta_\Gamma(v)}}\right)$

Consequently, graphene is an allotrope of carbon molecules constructed on a honeycomb grid (hexagonal pattern). Graphene has good heat and electric conductive strength. Many researchers have computed topological indices of graphene and its applications [29].

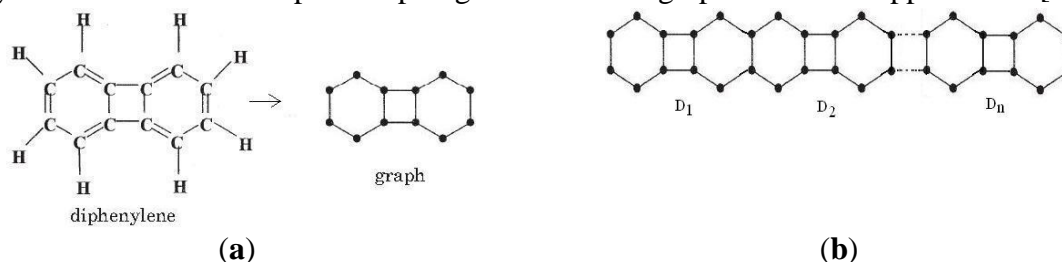


Figure 1. (a) Biphenylene and its graph; (b) The chain biphenylene graphs D_n .

Recently, a novel carbon allotrope named Biphenylene (see Figure. 1) was successfully fabricated. Biphenylene has attracted considerable attention owing to its promising applications in various fields [30].

A chain biphenylene where any two of Biphenylene intersect by one edge (see Figure. 1a and b). In this study, in view of structure analysis and mathematical derivation, we evaluated the General Harmonic index, Redefined version of the Zagreb indices, the Sombor index SO , the General sum-connectivity index, the First and Second multiplicative Zagreb index, Geometric arithmetic index, Ordinary Geometric-arithmetic index Atom-bond connectivity (ABC) index and Irregularity Descriptors of molecular chain graphs of Biphenylene D_n . Furthermore, we derive their corresponding polynomials formulae of chain Biphenylene. We refer the interested reader to [31–40].

2. Main Results

In this section, we study the General Harmonic index, Redefined version of the Zagreb indices, the Sombor index SO , the General sum-connectivity index, the First and Second multiplicative Zagreb index, the Geometric arithmetic index, the Ordinary Geometric-arithmetic index, Atom-bond connectivity (ABC) index and Irregularity Descriptors of molecular chain graphs of Biphenylene D_n . Moreover, the polynomial formulae for all the above-mentioned topological descriptors have been introduced.

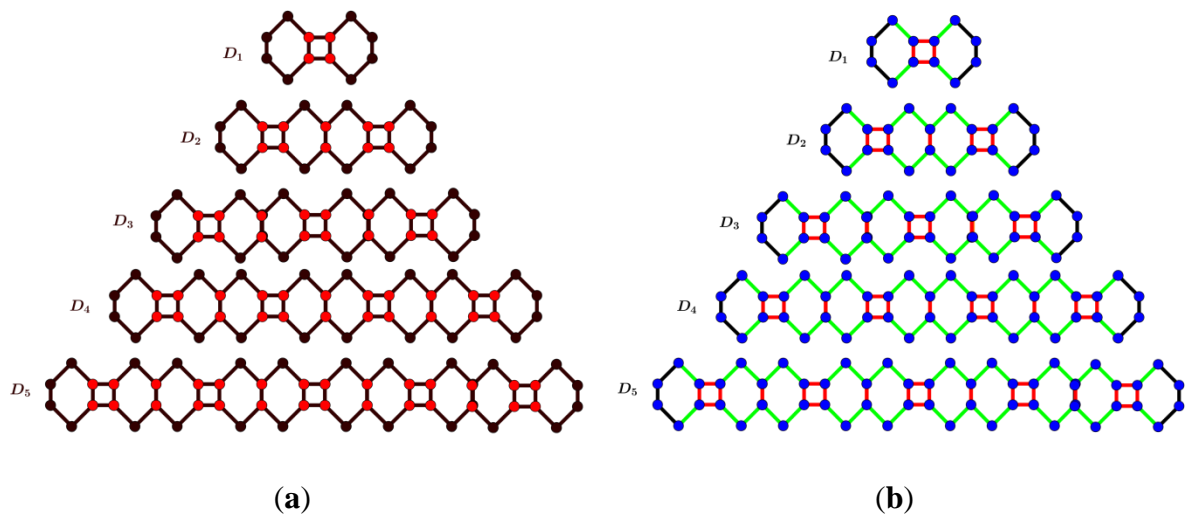


Figure 2. (a) The vertex color in D_n ; (b) The edge color in D_n .

Theorem 2.1. Let D_n be the n th level in chain of Biphenylene. Then,

1. $H_k(D_n) = \frac{6}{2^k} + 4\left(\frac{2}{5}\right)^k [2n - 1] + \frac{1}{3^k} [5n - 1]$
2. $SO(D_n) = 12\sqrt{2} + 4\sqrt{13}[2n - 1] + 3\sqrt{2}[5n - 1]$
3. $\chi^\alpha(D_n) = 6 \cdot 4^\alpha + 4[2n - 1] \cdot 5^\alpha + [5n - 1] \cdot 6^\alpha$
4. $PM_1(D_n) = 4^6 \times 5^{8n-4} \times 6^{5n-1}$.
5. $PM_2(D_n) = 4^6 \times 6^{8n-4} \times 9^{5n-1}$
6. $GA(D_n) = 6 + 8\frac{\sqrt{6}}{5} [2n - 1] + [5n - 1]$
7. $OGA_k(D_n) = 4\left(\frac{2\sqrt{6}}{5}\right)^k [2n - 1] + 5[n + 1]$

8. $ABC(D_n) = \sqrt{\frac{1}{2}}[8n + 2] + \frac{2}{3}[5n - 1]$
9. $YS(D_n) = 24 + 4\sqrt{35}[2n - 1] + 3\sqrt{6}[5n - 1]$
10. $ReZG_1(D_n) = 6 + \frac{5}{6}[8n - 4] + \frac{2}{3}[5n - 1]$
11. $ReZG_2(D_n) = 6 + \frac{6}{5}[8n - 4] + \frac{3}{2}[5n - 1]$
12. $ReZG_3(D_n) = 96 + 30[8n - 4] + 54[5n - 1]$
13. $\chi_2^\alpha(D_n) = 6 \cdot 8^\alpha + 4[2n - 1] \cdot 13^\alpha + [5n - 1] \cdot 18^\alpha$
14. $\chi_3^\alpha(D_n) = 6 \cdot 16^\alpha + 4[2n - 1] \cdot 35^\alpha + [5n - 1] \cdot 54^\alpha$
15. $\chi_\alpha^\alpha(D_n) = 6 \cdot 2^{\alpha^2+\alpha} + 4[2n - 1][2^\alpha + 3^\alpha]^\alpha + [5n - 1] \cdot 2^\alpha \cdot 3^{\alpha^2}$

Proof. By (Fig.2 (b)), we see that

$$\delta_{D_n}(a)\delta_{D_n}(b) = \begin{cases} 3 \times 3 & ab \text{ of color red} \\ 2 \times 3 & ab \text{ of color green} \\ 2 \times 2 & ab \text{ of color black} \end{cases}$$

Therefore, we can write the number of edges and degree of vertices incident on edges in the chain of Biphenylene at D_n as follows:

$$E_{2,2}(D_n) = \{ab \in E(D_n) : \delta(a) = 2, \delta(b) = 2, \delta(a)\delta(b) = 4\}, \quad E_{2,3}(D_n) = \{ab \in E(D_n) : \delta(a) = 2, \delta(b) = 3, \delta(a)\delta(b) = 6\},$$

$$E_{3,3}(D_n) = \{ab \in E(D_n) : \delta(a) = 3, \delta(b) = 3, \delta(a)\delta(b) = 9\},$$

And easily by (Fig.2 (b)), the number of the edges $|E(D_n)|$ are given in (Table. 2),

Table 2. The edge partitions in the chain of Biphenylene D_n .

Edge partition	Cardinality
$E_{2,2}$	6
$E_{2,3}$	$8n - 4$
$E_{3,3}$	$5n - 1$

And by the definition of the General Harmonic index, Sombor index, General sum-connectivity index, First and Second multiplicative Zagreb indices, Geometric arithmetic index, Ordinary Geometric-arithmetic index, Atom-bond connectivity index, Yemen-Sombor index (YS), Redefined first, second and third Zagreb indices, Second, Third and Generalized General sum-connectivity indices, respectively, we have

1.
$$H_k(D_n) = \sum_{ab \in E(D_n)} \left(\frac{2}{\delta_{D_n}(a) + \delta_{D_n}(b)}\right)^k = \sum_{ab \in E_{2,2}(D_n)} \left(\frac{2}{\delta_{D_n}(a) + \delta_{D_n}(b)}\right)^k$$

$$+ \sum_{ab \in E_{2,3}(D_n)} \left(\frac{2}{\delta_{D_n}(a) + \delta_{D_n}(b)}\right)^k + \sum_{ab \in E_{3,3}(D_n)} \left(\frac{2}{\delta_{D_n}(a) + \delta_{D_n}(b)}\right)^k$$

$$= \left(\frac{2}{2+2}\right)^k |E_{2,2}(D_n)| + \left(\frac{2}{2+3}\right)^k |E_{2,3}(D_n)| + \left(\frac{2}{3+3}\right)^k |E_{3,3}(D_n)|$$

$$= \frac{6}{2^k} + 4\left(\frac{2}{5}\right)^k [2n - 1] + \frac{1}{3^k} [5n - 1].$$
2.
$$SO(D_n) = \sum_{ab \in E(D_n)} \sqrt{\delta_{D_n}^2(a) + \delta_{D_n}^2(b)}$$

$$\begin{aligned}
 &= \sum_{ab \in E_{2,2}(D_n)} \sqrt{\delta_{D_n}^2(a) + \delta_{D_n}^2(b)} + \sum_{ab \in E_{2,3}(D_n)} \sqrt{\delta_{D_n}^2(a) + \delta_{D_n}^2(b)} \\
 &\quad + \sum_{ab \in E_{3,3}(D_n)} \sqrt{\delta_{D_n}^2(a) + \delta_{D_n}^2(b)} \\
 &= \sqrt{2^2 + 2^2} |E_{2,2}(D_n)| + \sqrt{2^2 + 3^2} |E_{2,3}(D_n)| + \sqrt{3^2 + 3^2} |E_{3,3}(D_n)| \\
 &\quad = 12\sqrt{2} + 4\sqrt{13}[2n - 1] + 3\sqrt{2}[5n - 1]. \\
 3. \quad \chi^\alpha(D_n) &= \sum_{ab \in E(D_n)} [\delta_{D_n}(a) + \delta_{D_n}(b)]^\alpha = \\
 &\quad \sum_{ab \in E_{2,2}(D_n)} [\delta_{D_n}(a) + \delta_{D_n}(b)]^\alpha + \sum_{ab \in E_{2,3}(D_n)} [\delta_{D_n}(a) + \delta_{D_n}(b)]^\alpha \\
 &\quad + \sum_{ab \in E_{3,3}(D_n)} [\delta_{D_n}(a) + \delta_{D_n}(b)]^\alpha \\
 &= [2 + 2]^\alpha |E_{2,2}(D_n)| + [2 + 3]^\alpha |E_{2,3}(D_n)| + [3 + 3]^\alpha |E_{3,3}(D_n)| \\
 &\quad = 6 \cdot 4^\alpha + 4[2n - 1] \cdot 5^\alpha + [5n - 1] \cdot 6^\alpha. \\
 4. \quad PM_1(D_n) &= \prod_{ab \in E(D_n)} [\delta_{D_n}(a) + \delta_{D_n}(b)] = \\
 &\quad \prod_{ab \in E_{2,2}(D_n)} [\delta_{D_n}(a) + \delta_{D_n}(b)] \times \prod_{ab \in E_{2,3}(D_n)} [\delta_{D_n}(a) + \delta_{D_n}(b)] \\
 &\quad \times \prod_{ab \in E_{3,3}(D_n)} [\delta_{D_n}(a) + \delta_{D_n}(b)] \\
 &= [2 + 2]^{|E_{2,2}(D_n)|} \times [2 + 3]^{|E_{2,3}(D_n)|} \times [3 + 3]^{|E_{3,3}(D_n)|} \\
 &\quad = 4^6 \times 5^{8n-4} \times 6^{5n-1}. \\
 5. \quad PM_2(D_n) &= \prod_{ab \in E(D_n)} [\delta_{D_n}(a)\delta_{D_n}(b)] = \prod_{ab \in E_{2,2}(D_n)} [\delta_{D_n}(a)\delta_{D_n}(b)] \\
 &\quad \times \prod_{ab \in E_{2,3}(D_n)} [\delta_{D_n}(a)\delta_{D_n}(b)] \times \prod_{ab \in E_{3,3}(D_n)} [\delta_{D_n}(a) + \delta_{D_n}(b)] \\
 &\quad = [2 \cdot 2]^{|E_{2,2}(D_n)|} \times [2 \cdot 3]^{|E_{2,3}(D_n)|} \times [3 \cdot 3]^{|E_{3,3}(D_n)|} \\
 &\quad = 4^6 \times 6^{8n-4} \times 9^{5n-1}. \\
 6. \quad GA(D_n) &= \sum_{ab \in E(D_n)} \frac{2\sqrt{\delta(a)\delta(b)}}{\delta(a) + \delta(b)} = \sum_{ab \in E_{2,2}(D_n)} \frac{2\sqrt{\delta(a)\delta(b)}}{\delta(a) + \delta(b)} \\
 &\quad + \sum_{ab \in E_{2,3}(D_n)} \frac{2\sqrt{\delta(a)\delta(b)}}{\delta(a) + \delta(b)} + \sum_{ab \in E_{3,3}(D_n)} \frac{2\sqrt{\delta(a)\delta(b)}}{\delta(a) + \delta(b)} \\
 &= \frac{2\sqrt{2 \times 2}}{2 + 2} |E_{2,2}(D_n)| + \frac{2\sqrt{2 \times 3}}{2 + 3} |E_{2,3}(D_n)| + \frac{2\sqrt{3 \times 3}}{3 + 3} |E_{3,3}(D_n)| \\
 &\quad = 6 + 8 \frac{\sqrt{6}}{5} [2n - 1] + [5n - 1]. \\
 7. \quad OGA_k(D_n) &= \sum_{ab \in E(D_n)} \left(\frac{2\sqrt{\delta(a)\delta(b)}}{\delta(a) + \delta(b)} \right)^k = \sum_{ab \in E_{2,2}(D_n)} \left(\frac{2\sqrt{\delta(a)\delta(b)}}{\delta(a) + \delta(b)} \right)^k
 \end{aligned}$$

$$\begin{aligned}
 & + \sum_{ab \in E_{2,3}(D_n)} \left(\frac{2\sqrt{\delta(a)\delta(b)}}{\delta(a) + \delta(b)} \right)^k + \sum_{ab \in E_{3,3}(D_n)} \left(\frac{2\sqrt{\delta(a)\delta(b)}}{\delta(a) + \delta(b)} \right)^k \\
 = & \left(\frac{2\sqrt{2 \times 2}}{2 + 2} \right)^k |E_{2,2}(D_n)| + \left(\frac{2\sqrt{2 \times 3}}{2 + 3} \right)^k |E_{2,3}(D_n)| + \left(\frac{2\sqrt{3 \times 3}}{3 + 3} \right)^k |E_{3,3}(D_n)| \\
 = & 4 \left(\frac{2\sqrt{6}}{5} \right)^k [2n - 1] + 5[n + 1].
 \end{aligned}$$

$$\begin{aligned}
 8. \quad ABC(D_n) = & \sum_{ab \in E(D_n)} \sqrt{\frac{\delta(a) + \delta(b) - 2}{\delta(a)\delta(b)}} = \sum_{ab \in E_{2,2}(D_n)} \sqrt{\frac{\delta(a) + \delta(b) - 2}{\delta(a)\delta(b)}} \\
 & + \sum_{ab \in E_{2,3}(D_n)} \sqrt{\frac{\delta(a) + \delta(b) - 2}{\delta(a)\delta(b)}} + \sum_{ab \in E_{3,3}(D_n)} \sqrt{\frac{\delta(a) + \delta(b) - 2}{\delta(a)\delta(b)}} \\
 = & \sqrt{\frac{2 + 2 - 2}{2 \cdot 2}} |E_{2,2}(D_n)| + \sqrt{\frac{2 + 3 - 2}{2 \cdot 3}} |E_{2,3}(D_n)| + \sqrt{\frac{3 + 3 - 2}{3 \cdot 3}} |E_{3,3}(D_n)| \\
 = & 6 \cdot \sqrt{\frac{1}{2}} + \sqrt{\frac{1}{2}} [8n - 4] + \frac{2}{3} [5n - 1].
 \end{aligned}$$

$$\begin{aligned}
 9. \quad YS(D_n) = & \sum_{ab \in E(D_n)} \sqrt{\delta_{D_n}^3(a) + \delta_{D_n}^3(b)} = \\
 & \sum_{ab \in E_{2,2}(D_n)} \sqrt{\delta_{D_n}^3(a) + \delta_{D_n}^3(b)} + \sum_{ab \in E_{2,3}(D_n)} \sqrt{\delta_{D_n}^3(a) + \delta_{D_n}^3(b)} \\
 & + \sum_{ab \in E_{3,3}(D_n)} \sqrt{\delta_{D_n}^3(a) + \delta_{D_n}^3(b)} \\
 = & \sqrt{2^3 + 2^3} |E_{2,2}(D_n)| + \sqrt{2^3 + 3^3} |E_{2,3}(D_n)| + \sqrt{3^3 + 3^3} |E_{3,3}(D_n)| \\
 = & 24 + 4\sqrt{35} [2n - 1] + 3\sqrt{6} [5n - 1].
 \end{aligned}$$

$$\begin{aligned}
 10. \quad ReZG_1(D_n) = & \sum_{ab \in E(D_n)} \frac{\delta(a) + \delta(b)}{\delta(a)\delta(b)} = \sum_{ab \in E_{2,2}(D_n)} \frac{\delta(a) + \delta(b)}{\delta(a)\delta(b)} \\
 & + \sum_{ab \in E_{2,3}(D_n)} \frac{\delta(a) + \delta(b)}{\delta(a)\delta(b)} + \sum_{ab \in E_{3,3}(D_n)} \frac{\delta(a) + \delta(b)}{\delta(a)\delta(b)} \\
 = & \frac{2 + 2}{2 \cdot 2} |E_{2,2}(D_n)| + \frac{2 + 3}{2 \cdot 3} |E_{2,3}(D_n)| + \frac{3 + 3}{3 \cdot 3} |E_{3,3}(D_n)| \\
 = & 6 + \frac{5}{6} [8n - 4] + \frac{2}{3} [5n - 1].
 \end{aligned}$$

$$\begin{aligned}
 11. \quad ReZG_2(D_n) = & \sum_{ab \in E(D_n)} \frac{\delta(a)\delta(b)}{\delta(a) + \delta(b)} = \sum_{ab \in E_{2,2}(D_n)} \frac{\delta(a)\delta(b)}{\delta(a) + \delta(b)} \\
 & + \sum_{ab \in E_{2,3}(D_n)} \frac{\delta(a)\delta(b)}{\delta(a) + \delta(b)} + \sum_{ab \in E_{3,3}(D_n)} \frac{\delta(a)\delta(b)}{\delta(a) + \delta(b)} \\
 = & \frac{2 \cdot 2}{2 + 2} |E_{2,2}(D_n)| + \frac{2 \cdot 3}{2 + 3} |E_{2,3}(D_n)| + \frac{3 \cdot 3}{3 + 3} |E_{3,3}(D_n)| \\
 = & 6 + \frac{6}{5} [8n - 4] + \frac{3}{2} [5n - 1].
 \end{aligned}$$

$$\begin{aligned}
 12. \text{ReZG}_3(D_n) &= \sum_{ab \in E(D_n)} (\delta(a)\delta(b))[\delta(a) + \delta(b)] = \\
 &\sum_{ab \in E_{2,2}(D_n)} (\delta(a)\delta(b))[\delta(a) + \delta(b)] + \sum_{ab \in E_{2,3}(D_n)} (\delta(a)\delta(b))[\delta(a) + \delta(b)] \\
 &\quad + \sum_{ab \in E_{3,3}(D_n)} (\delta(a)\delta(b))[\delta(a) + \delta(b)] \\
 &= (2 \cdot 2)[4]|E_{2,2}(D_n)| + (2 \cdot 3)[5]|E_{2,3}(D_n)| + (3 \cdot 3)[6]|E_{3,3}(D_n)| \\
 &= 96 + 30[8n - 4] + 54[5n - 1].
 \end{aligned}$$

$$\begin{aligned}
 13. \chi_2^\alpha(D_n) &= \sum_{ab \in E(D_n)} [\delta_{D_n}^2(a) + \delta_{D_n}^2(b)]^\alpha = \\
 &\sum_{ab \in E_{2,2}(D_n)} [\delta_{D_n}^2(a) + \delta_{D_n}^2(b)]^\alpha + \sum_{ab \in E_{2,3}(D_n)} [\delta_{D_n}^2(a) + \delta_{D_n}^2(b)]^\alpha \\
 &\quad + \sum_{ab \in E_{3,3}(D_n)} [\delta_{D_n}^2(a) + \delta_{D_n}^2(b)]^\alpha \\
 &= [2^2 + 2^2]^\alpha |E_{2,2}(D_n)| + [2^2 + 3^2]^\alpha |E_{2,3}(D_n)| + [3^2 + 3^2]^\alpha |E_{3,3}(D_n)| \\
 &= 6 \cdot 8^\alpha + 4[2n - 1] \cdot 13^\alpha + [5n - 1] \cdot 18^\alpha.
 \end{aligned}$$

$$\begin{aligned}
 14. \chi_3^\alpha(D_n) &= \sum_{ab \in E(D_n)} [\delta_{D_n}^3(a) + \delta_{D_n}^3(b)]^\alpha = \\
 &\sum_{ab \in E_{2,2}(D_n)} [\delta_{D_n}^3(a) + \delta_{D_n}^3(b)]^\alpha + \sum_{ab \in E_{2,3}(D_n)} [\delta_{D_n}^3(a) + \delta_{D_n}^3(b)]^\alpha \\
 &\quad + \sum_{ab \in E_{3,3}(D_n)} [\delta_{D_n}^3(a) + \delta_{D_n}^3(b)]^\alpha \\
 &= [2^3 + 2^3]^\alpha |E_{2,2}(D_n)| + [2^3 + 3^3]^\alpha |E_{2,3}(D_n)| + [3^3 + 3^3]^\alpha |E_{3,3}(D_n)| \\
 &= 6 \cdot 16^\alpha + 4[2n - 1] \cdot 35^\alpha + [5n - 1] \cdot 54^\alpha.
 \end{aligned}$$

$$\begin{aligned}
 15. \chi_\alpha^\alpha(D_n) &= \sum_{ab \in E(D_n)} [\delta_{D_n}^\alpha(a) + \delta_{D_n}^\alpha(b)]^\alpha = \\
 &\sum_{ab \in E_{2,2}(D_n)} [\delta_{D_n}^\alpha(a) + \delta_{D_n}^\alpha(b)]^\alpha + \sum_{ab \in E_{2,3}(D_n)} [\delta_{D_n}^\alpha(a) + \delta_{D_n}^\alpha(b)]^\alpha \\
 &\quad + \sum_{ab \in E_{3,3}(D_n)} [\delta_{D_n}^\alpha(a) + \delta_{D_n}^\alpha(b)]^\alpha \\
 &= [2^\alpha + 2^\alpha]^\alpha |E_{2,2}(D_n)| + [2^\alpha + 3^\alpha]^\alpha |E_{2,3}(D_n)| + [3^\alpha + 3^\alpha]^\alpha |E_{3,3}(D_n)| \\
 &= 6 \cdot 2^{\alpha^2 + \alpha} + 4[2n - 1][2^\alpha + 3^\alpha]^\alpha + [5n - 1] \cdot 2^\alpha \cdot 3^{\alpha^2}.
 \end{aligned}$$

Corollary 2.2 Let D_n be the n th level in the chain of Biphenylene. Then,

1. $H_k(D_n, x) = 6x^{6/2^k} + 4[2n - 1]x^{(2/5)^k} + [5n - 1]x^{(1/3^k)}$.
2. $SO(D_n, x) = 6 \cdot x^{2\sqrt{2}} + [8n - 4] \cdot x^{\sqrt{13}} + [5n - 1] \cdot x^{3\sqrt{2}}$.
3. $\chi^\alpha(D_n, x) = 6x^{4^\alpha} + 4[2n - 1]x^{5^\alpha} + [5n - 1]x^{6^\alpha}$.
4. $PM_1(D_n, x) = x^{4^6} \times x^{5^{8n-4}} \times x^{6^{5n-1}}$.
5. $PM_2(D_n) = x^{4^6} \times x^{6^{8n-4}} \times x^{9^{5n-1}}$.
6. $GA(D_n) = 6x + [8n - 4]x^{(2\sqrt{6}/5)} + [5n - 1]x$.
7. $OGA_k(D_n) = 6x + 4[2n - 1]x^{(2\sqrt{6}/5)^k} + [5n - 1]x$.

8. $ABC(D_n) = [8n + 2]x^{(1/\sqrt{2})} + [5n - 1]x^{(2/3)}$.
9. $YS(D_n) = 6x^4 + 4[2n - 1]x^{\sqrt{35}} + [5n - 1]x^{3\sqrt{6}}$.
10. $ReZG_1(D_n) = 6x + [8n - 4]x^{(5/6)} + [5n - 1]x^{(2/3)}$.
11. $ReZG_2(D_n) = 6x + [8n - 4]x^{(6/5)} + [5n - 1]x^{(3/2)}$.
12. $ReZG_3(D_n) = 6x^{16} + [8n - 4]x^{30} + [5n - 1]x^{54}$.
13. $\chi_2^\alpha(D_n) = 6x^{8\alpha} + 4[2n - 1]x^{13\alpha} + [5n - 1]x^{18\alpha}$.
14. $\chi_3^\alpha(D_n) = 6x^{16\alpha} + 4[2n - 1]x^{35\alpha} + [5n - 1]x^{54\alpha}$.
15. $\chi_\alpha^\alpha(D_n) = 6x^{2^{\alpha^2+\alpha}} + 4[2n - 1]x^{[2^\alpha+3^\alpha]^\alpha} + [5n - 1]x^{2^\alpha \cdot 3^{\alpha^2}}$.

Theorem 2.3. Let D_n be the n th level in the chain of Biphenylene. Then the irregularity indices of D_n are given as follows:

- | | |
|---|--|
| 1. $AL(D_n) = 8n - 4,$ | 2. $IRR_t(D_n) = \frac{1}{2}[8n - 4],$ |
| 3. $IRF(D_n) = [8n - 4],$ | 4. $IRB(D_n) = [\sqrt{2} - \sqrt{3}]^2[8n - 4],$ |
| 5. $IRA(D_n) = \left[\frac{1}{\sqrt{2}} - \frac{1}{\sqrt{3}}\right]^2[8n - 4],$ | 6. $IRL(D_n) = \ln 2 - \ln 3 [8n - 4],$ |
| 7. $IRDIF(D_n) = \left[\frac{2}{3} - \frac{3}{2}\right][8n - 4],$ | 8. $IRLU(D_n) = \frac{1}{2}[8n - 4],$ |
| 9. $IRLF(D_n) = \frac{1}{\sqrt{6}}[8n - 4],$ | 10. $IRLA(D_n) = \frac{1}{5}[8n - 4],$ |
| 11. $IRDI(D_n) = \ln 2 \cdot [8n - 4],$ | 12. $IRLF(D_n) = \frac{5}{2\sqrt{6}}[8n - 4].$ |

Proof. By the concepts of Irregularity indices as (Table 1) and the number of the edges $|E(D_n)|$ are given in (Table 2), we have

$$\begin{aligned}
 1. \quad AL(D_n) &= \sum_{ab \in E(D_n)} |\delta(a) - \delta(b)| = \sum_{ab \in E_{2,2}(D_n)} |\delta(a) - \delta(b)| \\
 &+ \sum_{ab \in E_{2,3}(D_n)} |\delta(a) - \delta(b)| + \sum_{ab \in E_{3,3}(D_n)} |\delta(a) - \delta(b)| \\
 &= |2 - 2||E_{2,2}(D_n)| + |2 - 3||E_{2,3}(D_n)| + |3 - 3||E_{3,3}(D_n)| \\
 &= 8n - 4.
 \end{aligned}$$

$$\begin{aligned}
 2. \quad IRR_t(D_n) &= \frac{1}{2} \sum_{ab \in E(D_n)} |\delta(a) - \delta(b)| = \frac{1}{2} \sum_{ab \in E_{2,2}(D_n)} |\delta(a) - \delta(b)| \\
 &+ \frac{1}{2} \sum_{ab \in E_{2,3}(D_n)} |\delta(a) - \delta(b)| + \frac{1}{2} \sum_{ab \in E_{3,3}(D_n)} |\delta(a) - \delta(b)| \\
 &= \frac{1}{2}|2 - 2||E_{2,2}(D_n)| + \frac{1}{2}|2 - 3||E_{2,3}(D_n)| + \frac{1}{2}|3 - 3||E_{3,3}(D_n)| \\
 &= \frac{1}{2}[8n - 4].
 \end{aligned}$$

$$\begin{aligned}
 3. \quad IRF(D_n) &= \sum_{ab \in E(D_n)} [\delta(a) - \delta(b)]^2 = \sum_{ab \in E_{2,2}(D_n)} [\delta(a) - \delta(b)]^2 \\
 &+ \sum_{ab \in E_{2,3}(D_n)} [\delta(a) - \delta(b)]^2 + \sum_{ab \in E_{3,3}(D_n)} [\delta(a) - \delta(b)]^2 \\
 &= [2 - 2]^2|E_{2,2}(D_n)| + [2 - 3]^2|E_{2,3}(D_n)| + [3 - 3]^2|E_{3,3}(D_n)| \\
 &= 8n - 4.
 \end{aligned}$$

$$\begin{aligned}
 4. \quad IRB(D_n) &= \sum_{ab \in E(D_n)} [\sqrt{\delta(a)} - \sqrt{\delta(b)}]^2 = \\
 &\sum_{ab \in E_{2,2}(D_n)} [\sqrt{\delta(a)} - \sqrt{\delta(b)}]^2 + \sum_{ab \in E_{2,3}(D_n)} [\sqrt{\delta(a)} - \sqrt{\delta(b)}]^2 \\
 &\quad + \sum_{ab \in E_{3,3}(D_n)} [\sqrt{\delta(a)} - \sqrt{\delta(b)}]^2 \\
 &= [\sqrt{2} - \sqrt{2}]^2 |E_{2,2}(D_n)| + [\sqrt{2} - \sqrt{3}]^2 |E_{2,3}(D_n)| + [\sqrt{3} - \sqrt{3}]^2 |E_{3,3}(D_n)| \\
 &= [\sqrt{2} - \sqrt{3}]^2 [8n - 4]. \\
 5. \quad IRA(D_n) &= \sum_{ab \in E(D_n)} \left[\frac{1}{\sqrt{\delta(a)}} - \frac{1}{\sqrt{\delta(b)}} \right]^2 = \sum_{ab \in E_{2,2}(D_n)} \left[\frac{1}{\sqrt{\delta(a)}} - \frac{1}{\sqrt{\delta(b)}} \right]^2 \\
 &\quad + \sum_{ab \in E_{2,3}(D_n)} \left[\frac{1}{\sqrt{\delta(a)}} - \frac{1}{\sqrt{\delta(b)}} \right]^2 + \sum_{ab \in E_{3,3}(D_n)} \left[\frac{1}{\sqrt{\delta(a)}} - \frac{1}{\sqrt{\delta(b)}} \right]^2 \\
 &= \left[\frac{1}{\sqrt{2}} - \frac{1}{\sqrt{2}} \right]^2 |E_{2,2}(D_n)| + \left[\frac{1}{\sqrt{2}} - \frac{1}{\sqrt{3}} \right]^2 |E_{2,3}(D_n)| + \left[\frac{1}{\sqrt{3}} - \frac{1}{\sqrt{3}} \right]^2 |E_{3,3}(D_n)| \\
 &= \left[\frac{1}{\sqrt{2}} - \frac{1}{\sqrt{3}} \right]^2 [8n - 4]. \\
 6. \quad IRL(D_n) &= \sum_{ab \in E(D_n)} |\ln(\delta(a)) - \ln(\delta(b))| = \\
 &\sum_{ab \in E_{2,2}(D_n)} |\ln(\delta(a)) - \ln(\delta(b))| + \sum_{ab \in E_{2,3}(D_n)} |\ln(\delta(a)) - \ln(\delta(b))| \\
 &\quad + \sum_{ab \in E_{3,3}(D_n)} |\ln(\delta(a)) - \ln(\delta(b))| \\
 &= |\ln 2 - \ln 2| |E_{2,2}(D_n)| + |\ln 2 - \ln 3| |E_{2,3}(D_n)| + |\ln 3 - \ln 3| |E_{3,3}(D_n)| \\
 &= |\ln 2 - \ln 3| [8n - 4]. \\
 7. \quad IRDIF(D_n) &= \sum_{ab \in E(D_n)} \left[\frac{\delta(a)}{\delta(b)} - \frac{\delta(b)}{\delta(a)} \right] = \sum_{ab \in E_{2,2}(D_n)} \left[\frac{\delta(a)}{\delta(b)} - \frac{\delta(b)}{\delta(a)} \right] \\
 &\quad + \sum_{ab \in E_{2,3}(D_n)} \left[\frac{\delta(a)}{\delta(b)} - \frac{\delta(b)}{\delta(a)} \right] + \sum_{ab \in E_{3,3}(D_n)} \left[\frac{\delta(a)}{\delta(b)} - \frac{\delta(b)}{\delta(a)} \right] \\
 &= \left[\frac{2}{2} - \frac{2}{2} \right] |E_{2,2}(D_n)| + \left[\frac{2}{3} - \frac{3}{2} \right] |E_{2,3}(D_n)| + \left[\frac{3}{3} - \frac{3}{3} \right] |E_{3,3}(D_n)| \\
 &= \left[\frac{2}{3} - \frac{3}{2} \right] [8n - 4]. \\
 8. \quad IRLU(D_n) &= \sum_{ab \in E(D_n)} \frac{|\delta(a) - \delta(b)|}{\min\{\delta(a), \delta(b)\}} = \sum_{ab \in E_{2,2}(D_n)} \frac{|\delta(a) - \delta(b)|}{\min\{\delta(a), \delta(b)\}} \\
 &\quad + \sum_{ab \in E_{2,3}(D_n)} \frac{|\delta(a) - \delta(b)|}{\min\{\delta(a), \delta(b)\}} + \sum_{ab \in E_{3,3}(D_n)} \frac{|\delta(a) - \delta(b)|}{\min\{\delta(a), \delta(b)\}} \\
 &= \frac{|2 - 2|}{\min\{2,2\}} |E_{2,2}(D_n)| + \frac{|2 - 3|}{\min\{2,3\}} |E_{2,3}(D_n)| + \frac{|3 - 3|}{\min\{3,3\}} |E_{3,3}(D_n)| \\
 &= \frac{1}{2} [8n - 4].
 \end{aligned}$$

$$\begin{aligned}
 9. \quad IRLF(D_n) &= \sum_{ab \in E(D_n)} \frac{|\delta(a) - \delta(b)|}{\sqrt{\delta(a) \cdot \delta(b)}} = \sum_{ab \in E_{2,2}(D_n)} \frac{|\delta(a) - \delta(b)|}{\sqrt{\delta(a) \cdot \delta(b)}} \\
 &+ \sum_{ab \in E_{2,3}(D_n)} \frac{|\delta(a) - \delta(b)|}{\sqrt{\delta(a) \cdot \delta(b)}} + \sum_{ab \in E_{3,3}(D_n)} \frac{|\delta(a) - \delta(b)|}{\sqrt{\delta(a) \cdot \delta(b)}} \\
 &= \frac{|2-2|}{\sqrt{2 \cdot 2}} |E_{2,2}(D_n)| + \frac{|2-3|}{\sqrt{2 \cdot 3}} |E_{2,3}(D_n)| + \frac{|3-3|}{\sqrt{3 \cdot 3}} |E_{3,3}(D_n)| \\
 &= \frac{1}{\sqrt{6}} [8n - 4].
 \end{aligned}$$

$$\begin{aligned}
 10. \quad IRLA(D_n) &= \sum_{ab \in E(D_n)} \frac{|\delta(a) - \delta(b)|}{\delta(a) + \delta(b)} = \sum_{ab \in E_{2,2}(D_n)} \frac{|\delta(a) - \delta(b)|}{\delta(a) + \delta(b)} \\
 &+ \sum_{ab \in E_{2,3}(D_n)} \frac{|\delta(a) - \delta(b)|}{\delta(a) + \delta(b)} + \sum_{ab \in E_{3,3}(D_n)} \frac{|\delta(a) - \delta(b)|}{\delta(a) + \delta(b)} \\
 &= \frac{|2-2|}{2+2} |E_{2,2}(D_n)| + \frac{|2-3|}{2+3} |E_{2,3}(D_n)| + \frac{|3-3|}{3+3} |E_{3,3}(D_n)| \\
 &= \frac{1}{5} [8n - 4].
 \end{aligned}$$

$$\begin{aligned}
 11. \quad IRDI(D_n) &= \sum_{ab \in E(D_n)} \ln[1 + |\delta(a) - \delta(b)|] = \\
 &\sum_{ab \in E_{2,2}(D_n)} \ln[1 + |\delta(a) - \delta(b)|] + \sum_{ab \in E_{2,3}(D_n)} \ln[1 + |\delta(a) - \delta(b)|] \\
 &+ \sum_{ab \in E_{3,3}(D_n)} \ln[1 + |\delta(a) - \delta(b)|] \\
 &= \ln[1 + |2-2|] |E_{2,2}(D_n)| + \ln[1 + |2-3|] |E_{2,3}(D_n)| \\
 &+ \ln[1 + |3-3|] |E_{3,3}(D_n)| = \ln 2 \cdot [8n - 4].
 \end{aligned}$$

$$\begin{aligned}
 12. \quad IRLF(D_n) &= \sum_{ab \in E(D_n)} \ln\left(\frac{\delta(a) + \delta(b)}{2\sqrt{\delta(a) \cdot \delta(b)}}\right) = \sum_{ab \in E_{2,2}(D_n)} \ln\left(\frac{\delta(a) + \delta(b)}{2\sqrt{\delta(a) \cdot \delta(b)}}\right) \\
 &+ \sum_{ab \in E_{2,3}(D_n)} \ln\left(\frac{\delta(a) + \delta(b)}{2\sqrt{\delta(a) \cdot \delta(b)}}\right) + \sum_{ab \in E_{3,3}(D_n)} \ln\left(\frac{\delta(a) + \delta(b)}{2\sqrt{\delta(a) \cdot \delta(b)}}\right) \\
 &= \ln\left(\frac{2+2}{2\sqrt{2 \cdot 2}}\right) |E_{2,2}(D_n)| + \ln\left(\frac{2+3}{2\sqrt{2 \cdot 3}}\right) |E_{2,3}(D_n)| \\
 &+ \ln\left(\frac{3+3}{2\sqrt{3 \cdot 3}}\right) |E_{3,3}(D_n)| = \frac{5}{2\sqrt{6}} [8n - 4].
 \end{aligned}$$

Corollary 2.4 Let D_n be the n th level in the chain of Biphenylene. Then the irregularity polynomials of D_n are given as follows:

1. $AL(D_n, x) = 5(n + 1) + [8n - 4]x,$
2. $IRR_t(D_n, x) = 5n + 2 + \frac{1}{2} [8n - 4]x,$
3. $IRF(D_n, x) = 5(n + 1) + 4[2n - 1]x,$
4. $IRB(D_n, x) = 5(n + 1) + 4[2n - 1]x^{[\sqrt{2}-\sqrt{3}]^2},$
5. $IRA(D_n, x) = 5(n + 1) + [8n - 4]x^{[1/\sqrt{2}-1/\sqrt{3}]^2},$
6. $IRL(D_n, x) = 5(n + 1) + [8n - 4]x^{|\ln 2 - \ln 3|},$
7. $IRDIF(D_n, x) = 5(n + 1) + [8n - 4]x^{-5/6},$

8. $IRLU(D_n, x) = 5(n + 1) + [8n - 4]x^{1/2}$,
9. $IRLF(D_n, x) = 5(n + 1) + [8n - 4]x^{1/\sqrt{6}}$,
10. $IRLA(D_n, x) = 5(n + 1) + [8n - 4]x^{1/5}$,
11. $IRDI(D_n, x) = 5(n + 1) + [8n - 4]x^{\ln 2}$,
12. $IRLF(D_n, x) = 5(n + 1) + [8n - 4]x^{5/2\sqrt{6}}$.

4. Conclusions

The present study has studied some topological descriptors such as the General Harmonic index, Redefined version of Zagreb indices, the Sombor index SO , the General sum-connectivity index, the First and Second multiplicative Zagreb index, the Geometric arithmetic index, Ordinary Geometric-arithmetic index Atom-bond connectivity (ABC) index and Irregularity Descriptors of molecular chain graphs of Biphenylene D_n . Moreover, by the concepts of well-known degree-based descriptors, we introduced new degree-based descriptors such as the Yemen-Sombor index ($YS - index$), Second General sum-connectivity index (χ_2^α), Third General sum-connectivity index (χ_3^α), Generalized General sum-connectivity index (χ_α^α) of chain Biphenylene. Furthermore, we derived their corresponding polynomials formulae of chain Biphenylene. Therefore, the results obtained in this study could help us learn more about the characteristics of the chain Biphenylene and can also perform a valuable role in the findings on the significance of the considered structures.

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Conflicts of Interest

The authors declare no conflict of interest.

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