Research Article

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M-polygonal and topological indices of zigzag edge coronoid fused by starphene

Abstract: Chemical graph theory is a subfield of graph theory that studies the topological indices for chemical graphs that have a good correlation with chemical properties of a chemical molecule. In this study, we have computed M-polygonal of zigzag edge coronoid fused by starphene. We also investigate various topological indices related to this graph by using their M-polygonal.

Keywords: M-polygonal, zigzag-edge coronoid fused by starphene, topological indices.

MSC 2010: Primary: 97Kxx, Secondary: 97K30

1 Introduction

Graph theory is applied in numerous fields of engineering and science such as computer science, chemistry, and biology [27]. Chemical graph theory has become a major subfield in the area of mathematical chemistry, which is innovated by Trinajstic [17,22,28], Gutman and Trinajstic [17], Graovac [16], Randić [24] and Balaban [5]. Chemical graph theory compacts with the graph of the molecular structure, for example, we can find the mathematical study of a chemical graph and try to improve the method to calculate the topological indices that have many applications in the quantitative structure activity and property relationship. Similarly, the chemical behavior of graph theory have applications in quantum chemistry and stereochemistry [6,29].

Topics that are studied in chemical graph theory are topological and differential geometric characterization of molecules, novel approaches to structure property relationships, mathematical theory of chemical transformations, fractal characterization of supramolecular microstructures, computational algorithms for the analysis of chemical data, renormalization group technology for chemistry, chemical applications of group theory, chemical enumerations, and combinatorial methods in chemistry and computational modeling of molecular structures [28].

The topological index or the descriptor of a chemical structure, which is represented by graph, is the last outcome of logical and mathematical operations, which convert facts store in a chemical molecule into a beneficial number. These topological descriptors have many application during the studies of QSAR and QSPR. Topological descriptor is a real numerical parameter calculated from the graph, representing the structure of a molecule that characterizes the molecular properties, and is a graph invariant.

A major perception of chemistry is structural characteristics of some molecules that are accountable for its properties. A chemical reaction represents the formation of a product from the reactants by forming or breaking a bridge between the vertices of the reactants. Hence, chemical graph theory plays a role in the study of the mechanism of the chemical reaction. Topological indices study the physical characteristics such as melting point, molar refraction, boiling point, surface tension, heats of vaporization, and molar volume [18]. Topological indices also describe the biological behavior of chemical species such as lipophilicity, toxicity, stimulation of cell growth, pH regulation, and nutritive. Hence, the topological indices may be helpful to know the physical and chemical characteristics and chemical and biological behaviors [12,18,23].

A degree-dependent topological descriptor is the specific type of topological indices in which the index of the chemical structure is computed by using the degrees of vertices of a chemical graph. Here, we call $E(G_i)$ as the set of edges and $V(G_i)$ as set of vertices. The degree of
First index is the Wiener index familiarized by H. Wiener index describes the boiling point of paraffin and defined as the sum of the distances between all pairs of vertices in G1 [31]. The first and second Zagreb indices for a graph G1, denoted by $M_1(G_1)$ and $M_2(G_1)$, respectively, are the popular, oldest, and utmost extensively studied vertex degree-dependent topological indices. In 1972, these indices were acquainted in the study by Gutman and Trinajstić during the analysis of the structure-dependency of the total $\varphi$-electron energy [17]. Both provide greater and smaller weights to inner and outer vertices and edges, respectively.

$$M_1(G_1) = \sum_{uv \in E(G_1)} (d_u + d_v).$$

$$M_2(G_1) = \sum_{uv \in E(G_1)} (d_u \cdot d_v).$$

Results attained in the theory of Zagreb indices are outlined in the review “The Zagreb Indices 30 Years After” written by Nikolić et al. in 2003 [22] and defined the modified first and second Zagreb index as follows:

$$^mM_1(G_1) = \sum_{uv \in E(G_1)} \left( \frac{1}{d_u + d_v} \right).$$

$$^mM_2(G_1) = \sum_{uv \in E(G_1)} \left( \frac{1}{d_u \cdot d_v} \right).$$

Randić introduced in 1975 a bond-additive topological index to describe the characterizing of the molecular branching [24]. The Randić index is a remarkably widespread, mostly applied, and frequently examined index among all former topological descriptors. In 1998, Bollobas and Erdos suggested the general Randić index [7]. This topic has been comprehensively discussed by both theoretical mathematicians and chemists. The appropriateness of the Randić index for drug making was accepted immediately; finally, this descriptor was utilized for this objective. Although numerous more or less reasonable explanations were offered, yet the physical explanation for realization of such a chemical graph invariant is a paradox, but currently, it has been utilized on many occasions [14,20]. Randić also present two reviews on the Randić index [25,26].

$$R_{1/2}(G_1) = \sum_{uv \in E(G_1)} \left( \frac{1}{\sqrt{d_u \cdot d_v}} \right).$$

$$R_d(G_1) = \sum_{uv \in E(G_1)} (d_u \cdot d_v)^d.$$

$$RR_d(G_1) = \sum_{uv \in E(G_1)} \left( \frac{1}{d_u \cdot d_v} \right)^a.$$

The symmetric division index (SDD) is taken from 148 discrete Adriatic indices. Also, it is a best forecaster to find the total surface area for polychlorobiphenyls [30].

$$SDD(G_1) = \sum_{uv \in E(G_1)} \left( \frac{d_u + d_v}{d_u \cdot d_v} \right).$$

In 1987, Fajtlowicz familiarized another index called harmonic index $H(G_1)$ [15], Favaron et al. in 1993 formulated the relationship between eigenvalues of graphs and harmonic index [1].

$$H(G_1) = \sum_{uv \in E(G_1)} \left( \frac{2}{d_u + d_v} \right).$$

The inverse sum index $I(G_1)$ is an invariant that was designated in 1982 by Balaban [5], as an important predictor to calculate the total surface area of extremal graphs and also for octane isomers, which have a principally simple and well-designed structure. This can be easily calculated with the help of MathChem.

$$I(G_1) = \sum_{uv \in E(G_1)} \left( \frac{d_u \cdot d_v}{d_u + d_v} \right).$$

The augmented Zagreb index $A(G_1)$ of $G_1$ offered by Furtula et al. [16]. This graph theoretical descriptor has confirmed to be a good forecasting descriptor during the analysis of the heat of development in octanes and heptanes (alkanes).

$$A(G_1) = \sum_{uv \in E(G_1)} \left( \frac{d_u \cdot d_v}{d_u + d_v - 2} \right)^3.$$

The graph polynomial is a mathematical tool affiliated to a graph, which ordinarily explains the graph at least under graph isomorphism [13]. In the past, many algebraic graph polynomials were formulated. Typically topological descriptors are calculated by the means of definitions. A solid general technique that can generate topological indices of a specific class is that firstly compute the graph polynomial and then by taking the integral or a derivative or both of the graph polynomial at some specific point provided the topological descriptor. The procedure of this method is called the Hosoya polynomial [11]. This is the best knowing general graph polynomial in the perspective of resolving the topological descriptor that is dependent on the distance of vertices. So the computation of distance-dependent topological indices shorten by computing individual graph polynomial.

The M-polynomial behaves like a Hosoya polynomial and provides functions that are related to the topological indices dependent on the degree of the vertex. M-polynomial is a best graph polynomial established until now.
It indicates that by understanding the knowledge of M-polynomial for some provided chemical structure, we can find a closed formula for some specific index normally. In the present article, all graphs under observations are connected and simple. The M-polynomial for a graph $G_1$ formulated in 2015 [10] is explained as follows:

$$M(G_1, x, y) = \sum_{\delta \leq i \leq \Delta} m_{ij}(G_1) x^i y^j,$$

where $\delta = \min\{d_v \mid v \in V(G_1)\}$, $\Delta = \max\{d_v \mid v \in V(G_1)\}$, and $m_{ij}(G_1)$ is the number of edges $vu \in E(G_1)$, such that $\{d_v, d_u\} = \{i, j\}$.

M-polynomial of many chemical graphs are formulated [2–4,8,19,21] during the last 5 years. In the current study, we formulated M-polynomials of zigzag-edge coronoid fused by starphene $(ZCS(l, m, n))$. With the help of this graph polynomial, we computed various degree-dependent topological indices and presented in Table 1.

The Table 1 narrates few renowned degree-dependent topological indices computed by means of M-polynomial.

| Topological index | Derivation from $M(G_1, x, y)$ |
|-------------------|--------------------------------|
| First Zagreb index | $M_1(G_1) = (D_x + D_y) [f(x, y)]_{x+y=1}$ |
| Second Zagreb index | $M_2(G_1) = (D_x D_y) [f(x, y)]_{x+y=1}$ |
| Modified second Zagreb index | $M_3(G_1) = (D_x D_y) [f(x, y)]_{x+y=1}$ |
| General Randić index | $R_{G_1}(x, y) = D_x D_y [f(x, y)]_{x+y=1}$ |
| Inverse Randić index | $R_{G_1}^{-1}(x, y) = S_x S_y [f(x, y)]_{x+y=1}$ |
| Symmetric division index | $SSD(G_1) = (D_x S_y + S_x D_y) [f(x, y)]_{x+y=1}$ |
| Harmonic index | $H(G_1) = 2S_x [f(x, y)]_{x=1}$ |
| Inverse sum index | $I(G_1) = S_x D_y [f(x, y)]_{x=1}$ |
| Augmented Zagreb index | $A(G_1) = S_x Q_x D_y D_y [f(x, y)]_{x=1}$ |

2 Zigzag-edge coronoid fused by starphene

Benzene is an organic chemical compound with the chemical formula $C_6H_6$. It is used as a solvent in many commercial, research, and industrial operations. Benzene also present in crude oil and is a major component of gasoline. It is used to make dyes, plastics, resins, detergents, synthetic fibrbers, drugs, rubber lubricants and pesticides. Benzene rings joined together to provide larger polycyclics that are aromatic compounds.

A starphene $St(l, m, n)$, shown in Figure 1(a), is a structure obtained by fusing three linear polyacenes of length $l$, $m$, and $n$. The zigzag-edge coronoids $ZC(l, m, n)$, shown in Figure 1(b), can be considered as a structure obtained by fusing six segments of linear polyacenes into

![Figure 1: (a) Starphene $St(l, m, n)$ structure and (b) zigzag-edge coronoid $ZC(l, m, n)$.](image-url)
a closed loop. The formation of ZC is only possible for \( l, m, n \geq 2 \).

Zigzag-edge coronoid fused by starphene, shown in Figure 2, is a composite benzenoid attained by fusing a zigzag-edge coronoid \( ZC(l, m, n) \) by a starphene \( St(l, m, n) \). This system is abbreviated as \( ZCS(l, m, n) \) [9].

### 3 M-Polynomial of zigzag-edge coronoid fused by starphene

#### Theorem 3.1. Let ZCS(l, m, n) be a zigzag-edge coronoid fused by starphene then for \( l, m, n \geq 3 \), and M-polynomial of ZCS(l, m, n) is calculated as follows:

\[
M[ZCS(l, m, n);x, y] = 6x^2y^2 + 12(l + m + n - 7)x^3y^3 + 3(l + m + n + 5)x^3y^3.
\]

**Proof.** Let ZCS(l, m, n) be a zigzag-edge coronoid fused by starphene and then with the help of Table 2 and Figure 2, we find the following vertex sets:

\[
\begin{align*}
V_2 &= \{u \in ZCS(l, m, n) : d_u = 2\} \Rightarrow |V_2| = 6(l + m + n) - 36, \\
V_3 &= \{u \in ZCS(l, m, n) : d_u = 3\} \Rightarrow |V_3| = 6(l + m + n) - 18,
\end{align*}
\]

By using Table 3 and Figure 2, the edge partition of zigzag-edge coronoid fused by starphene is presented as follows:

\[
\begin{align*}
E_{1,2}(ZCS(l, m, n)) &= \{e = uv \in ZCS(l, m, n) : d_u = 2, d_v = 2\} \Rightarrow |E_{1,2}ZCS(l, m, n)| = 6, \\
E_{1,3}(ZCS(l, m, n)) &= \{e = uv \in ZCS(l, m, n) : d_u = 2, d_v = 3\} \Rightarrow |E_{1,3}ZCS(l, m, n)| = 12(l + m + n - 7), \\
E_{3,3}(ZCS(l, m, n)) &= \{e = uv \in ZCS(l, m, n) : d_u = 3, d_v = 3\} \Rightarrow |E_{3,3}ZCS(l, m, n)| = 3(l + m + n + 5).
\end{align*}
\]

Now, with the help of definition of the M-polynomial, we can have

\[
\begin{align*}
M(ZCS(l, m, n);x, y) &= \sum_{\delta \in E_{1,2}} m_{\delta}(ZCS(l, m, n))x^\delta y^{\delta}, \\
M(ZCS(l, m, n);x, y) &= \sum_{\delta \in E_{1,3}} m_{\delta}(ZCS(l, m, n))x^\delta y^{\delta}, \\
M(ZCS(l, m, n);x, y) &= \sum_{\delta \in E_{3,3}} m_{\delta}(ZCS(l, m, n))x^\delta y^{\delta}.
\end{align*}
\]

The graph of M-polynomial of ZCS(l, m, n) is shown in Figure 3.

#### 4 Topological indices of zigzag-edge coronoid fused by starphene

#### Theorem 4.1. Let ZCS(l, m, n) be a zigzag-edge coronoid fused by starphene and

\[
M(ZCS(l, m, n);x, y) = 6x^2y^2 + 12(l + m + n - 7)x^3y^3 + 3(l + m + n + 5)x^3y^3.
\]

Then,

1. \( M_1[ZCS(l, m, n)] = 78(l + m + n) - 306. \)
2. \( M_2[ZCS(l, m, n)] = 99(l + m + n) - 345. \)
3. \( M_3[ZCS(l, m, n)] = \frac{1}{3}(l + m + n) - \frac{65}{6}. \)

#### Table 2: Vertex partition of ZCS(l, m, n)

| \( d_u \) | 2 | 3 | Total vertices |
|---|---|---|---|
| Number of vertices | \( 6(l + m + n) - 36 \) | \( 6(l + m + n) - 18 \) | \( 12(l + m + n) - 54 \) |
4. \(R_4[ZCS(l, m, n)] = 4^a \cdot 6^a \cdot 12(l + m + n - 7) + 9^a \cdot 3(l + m + n + 5).\)

5. \(RR_4[ZCS(l, m, n)] = \frac{6}{a^3} + \frac{12}{a^2}(l + m + n - 7) + \frac{3}{a^2}(l + m + n + 5).\)

6. \(SSD[ZCS(l, m, n)] = 32(l + m + n) - 140.\)

7. \(H[ZCS(l, m, n)] = \frac{29}{3}(l + m + n) - \frac{128}{3}.\)

8. \(I[ZCS(l, m, n)] = \frac{189}{10}(l + m + n) - \frac{723}{10}.\)

9. \(A[ZCS(l, m, n)] = \frac{8331}{64}(l + m + n) - \frac{29001}{64}.\)

**Proof.** Suppose

\(M[ZCS(l, m, n); x, y] = f(x, y) = 6x^2y^2 + 12(l + m + n - 7)x^2y^3 + 3(l + m + n + 5)x^3y^3,\)

\(D_xf(x, y) = 12x^2y^2 + 24(l + m + n - 7)x^2y^3 + 9(l + m + n + 5)x^3y^3,\)

\(D_yf(x, y) = 12x^2y^2 + 36(l + m + n - 7)x^3y^3 + 9(l + m + n + 5)x^4y^3,\)

\((D_x + D_y)f(x, y) = 24x^2y^2 + 60(l + m + n - 7)x^2y^3 + 18(l + m + n + 5)x^3y^3,\)

\(D_xD_yf(x, y) = 24x^2y^2 + 72(l + m + n - 7)x^2y^3 + 27(l + m + n + 5)x^3y^3,\)

\(S_yf(x, y) = 3x^2y^2 + 4(l + m + n - 7)x^2y^3 + (l + m + n + 5)x^3y^3,\)

\(S_xS_yf(x, y) = \frac{3}{2}x^2y^2 + 2(l + m + n - 7)x^2y^3 + \frac{1}{3}(l + m + n + 5)x^3y^3,\)

\(D_x^2D_yf(x, y) = 2^a \cdot 6x^2y^2 + 3^a \cdot 12(l + m + n - 7)x^2y^3 + 3^a \cdot 3(l + m + n + 5)x^3y^3,\)

\(D_x^2S_yf(x, y) = \frac{6}{2^a}x^2y^2 + \frac{12}{3^a}(l + m + n - 7)x^2y^3 + \frac{3}{3^a}(l + m + n + 5)x^3y^3,\)

\(S_x^2S_yf(x, y) = \frac{6}{4^a}x^2y^2 + \frac{12}{6^a}(l + m + n - 7)x^2y^3 + \frac{3}{6^a}(l + m + n + 5)x^3y^3,\)

\(D_xS_yf(x, y) = 6x^2y^2 + 8(l + m + n - 7)x^2y^3 + 3(l + m + n + 5)x^3y^3,\)

\(S_xS_yf(x, y) = 6x^2y^2 + 18(l + m + n - 7)x^2y^3 + 3(l + m + n + 5)x^3y^3,\)

\((D_xS_y + S_xD_y)f(x, y) = 12x^2y^2 + 26(l + m + n - 7)x^2y^3 + 6(l + m + n + 5)x^3y^3,\)

\(Jf(x, y) = 6x^4 + 12(l + m + n - 7)x^5 + 3(l + m + n + 5)x^6,\)

\(S_xJf(x, y) = \frac{3}{2}x^4 + \frac{12}{5}(l + m + n - 7)x^5 + \frac{1}{2}(l + m + n + 5)x^6,\)

\(2S_yJf(x, y) = 3x^4 + \frac{24}{5}(l + m + n - 7)x^5 + (l + m + n + 5)x^6,\)

\(JD_xD_yf(x, y) = 24x^4 + 72(l + m + n - 7)x^5 + 27(l + m + n + 5)x^6,\)

\(S_xJD_xD_yf(x, y) = 6x^4 + \frac{72}{5}(l + m + n - 7)x^5 + \frac{9}{2}(l + m + n + 5)x^6,\)

\(D_x^3f(x, y) = 48x^2y^2 + 324(l + m + n - 7)x^2y^3 + 81(l + m + n + 5)x^3y^3,\)

\(D_x^3Jf(x, y) = 384x^2y^2 + 2592(l + m + n - 7)x^2y^3 + 2187(l + m + n + 5)x^3y^3,\)
The first Zagreb index

\[ M_{\text{ZCS}}(l, m, n) = (D_x + D_y)f(x, y)_{x=1, y=1} \]
\[ = 78 (l + m + n) - 306. \]

2. The second Zagreb index

\[ M_{\text{ZCS}}(l, m, n) = (D_x D_y)f(x, y)_{x=1, y=1} \]
\[ = 99 (l + m + n) - 345. \]
3. The modified second Zagreb index

\[ m^2_{ZCS}(l, m, n) = (S_xS_yf(x, y))_{x \neq y} \]

\[ = \frac{7}{3}(l + m + n) - \frac{65}{6}. \]

4. The general Randić index

\[ R_{a[ZCS]}(l, m, n) = (D_x^aD_y^bf(x, y))_{x \neq y} \]

\[ = 4^a \cdot 6 + 6^a \cdot 12(l + m + n - 7) \]

\[ + 9^a \cdot 3(l + m + n + 5). \]

5. The inverse Randić index

\[ R_{-a[ZCS]}(l, m, n) = (S_xS_y^a[f(x, y)])_{x \neq y} \]

\[ = \frac{6}{4^a} + \frac{12}{6^a}(l + m + n - 7) \]

\[ + \frac{3}{9^a}(l + m + n + 5). \]

6. The symmetric division index

\[ SSD_{ZCS}(l, m, n) = (D_xS_y + S_xD_y)f(x, y)_{x \neq y} \]

\[ = 32(l + m + n) - 140. \]

7. The harmonic index

\[ H[ZCS](l, m, n) = 2S_xJf(x, y)_{x \neq y} \]

\[ = \frac{29}{5}(l + m + n) - \frac{128}{5}. \]

8. The inverse sum index

\[ I[ZCS](l, m, n) = (S_xJD_y + D_xS_y)f(x, y)_{x \neq y} \]

\[ = \frac{189}{10}(l + m + n) - \frac{723}{10}. \]

9. The augmented Zagreb index

\[ A[ZCS](l, m, n) = S_x^2Q_xJD_y^3D_y^3f(x, y)_{x \neq y} \]

\[ = \frac{8331}{64}(l + m + n) - \frac{29001}{64}. \]

Figure 4 shows graphically visualization of topological descriptors of ZCS(l, m, n). These graphs elaborate the trend of the computed topological indices along the parameters involved and provide values of topological indices with respect to the sum of l, m, and n. All graphs have different gradients although graphs are seen to be similar.

5 Conclusion

In this study, we compute M-polynomials of zigzag-edge coronoid fused by starphene (ZCS(l, m, n)). The M-polynomial has improved the procedure to calculate the topological indices values, which depend on the vertex degree for the chemical molecule. So we calculated many indices (Table 1) via M-polynomial. These topological indices can be helpful to know about the physical characteristics, biological functions and chemical behavior. In this perception, topological index can be considered as a key role, which converts the chemical structure into a real number and can be utilized to describe the chemical graph under consideration. We also visualize our result of topological indices. These representations of topological indices with the help of graphs explain that the value of the specific index dependent on the molecular structure.

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

Conflict of interest: Authors declare no conflict of interest.

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