Research Article

Maqsood Ahmad, Muhammad Javaid, Muhammad Saeed, Chahn Yong Jung*

Valency-based molecular descriptors of Bakelite network BN<sub>n</sub><sup>m</sup>

https://doi.org/10.1515/chem-2019-0081
received December 12, 2018; accepted February 21, 2019.

Abstract: Bakelite network BN<sub>n</sub><sup>m</sup> is a molecular graph of bakelite, a pioneering and revolutionary synthetic polymer (Thermosetting Plastic) and regarded as the material of a thousand uses. In this paper, we aim to compute various degree-based topological indices of a molecular graph of bakelite network BN<sub>n</sub><sup>m</sup>. These molecular descriptors play a fundamental role in QSPR/QSAR studies in describing the chemical and physical properties of Bakelite network BN<sub>n</sub><sup>m</sup>. We computed atom-bond connectivity ABC its fourth version ABC<sub>4</sub>, geometric arithmetic GA its fifth version GA<sub>5</sub>, Narumi-Katayama, sum-connectivity and Sanskruti indices, first, second, modified and augmented Zagreb indices, inverse and general Randic indices, symmetric division, harmonic and inverse sum indices of BN<sub>n</sub><sup>m</sup>.

Keywords: Molecular graph; Bakelite network; Zagreb index; Chemical properties.

1 Introduction

In Chemical graph theory, chemical compounds are represented by graphs and mathematical techniques are used to solve problems arising in chemistry. A molecular graph is a simple connected graph in which atoms are taken as vertices and chemical bonds are taken as the edges of the graph. Topological indices are numerical numbers associated with molecular graphs of chemical compounds and help us to predict the properties of chemical compounds without performing experiments and save money and time [1, 2]. Some applications related to topological indices of molecular graphs are given in [3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15, 16, 17].

Throughout this paper, Γ is an ordered pair Γ=(V,E) where V is the set of vertices, and E is the set of edges. The order and size of a graph Γ is the cardinality of vertex set V and edge set E denoted by |V| and |E| respectively. Two vertices u and v are adjacent if e=uv is an edge in graph and e is said to be incident with u and v. The valency of a vertex v∈Γ is the number of incident edges with v and is denoted by dv. The minimum and maximum valency of Γ is denoted by δ and Δ, respectively. The first topological index was introduced by Harold Wiener [18], when he was investigating the boiling point of alkane. Initially, this index was named as path number and now it is known as the Wiener index/number [19]. In 1975, after Wiener index, Milan Randić [20], introduced a prominent index known as Randić index and is defined as:

\[ R_1(\Gamma) = \frac{1}{2} \sum_{uv \in \Gamma} \frac{1}{\sqrt{d_u d_w}} \]

This simple graph invariant has found many applications in chemistry. Böllöbás and Erdös [21], extended the idea of Randić and proposed the general Randić index:

\[ R_u(\Gamma) = \sum_{uv \in \Gamma} (d_u d_w)^u, \]

and inverse Randić index:

\[ RR_u(\Gamma) = \sum_{uv \in \Gamma} \frac{1}{(d_u d_w)^u}. \]

The additive version of Randić’ index is known as the sum-connectivity index (SCI) [22] and it gives a high correlation coefficient (0.99) for alkanes. The formula for SCI is given by:

\[ K = \frac{1}{N} \sum_{uv \in \Gamma} (d_u d_w)^{1/2}. \]
Ivan Gutman and Trinajstić [23] proposed two topological indices named as the first and the second Zagreb indices which were denoted by $M_1$ and $M_2$ and got an immense attraction of researchers due to the applications in chemistry. First and second and Zagreb indices are defined as follows:

$$M_1(\Gamma) = \sum_{vw \in E(\Gamma)} (d_v + d_w)$$
$$M_2(\Gamma) = \sum_{vw \in E(\Gamma)} d_v d_w$$

The modified second Zagreb index is defined as:

$$mM_2(\Gamma) = \sum_{vw \in E(\Gamma)} \frac{1}{d_v d_w}$$

In 1998, Estrada et al. [24] established an important index named as the $\text{ABC}(\Gamma)$ index, which is a good model to test the stability of linear and branched alkanes and is defined below:

$$\text{ABC}(\Gamma) = \sum_{vw \in E(\Gamma)} \frac{d_v + d_w - 2}{d_v d_w}$$

In 2009, Vukićević et al. [25] introduced another remarkable index known as the geometric-arithmetic index $\text{GA}(\Gamma)$ and is given by the formula:

$$\text{GA}(\Gamma) = \sum_{vw \in E(\Gamma)} \frac{2\sqrt{d_v d_w}}{d_v + d_w}$$

Three prominent and recently developed indices, denoted by $\text{ABC}_4(\Gamma)$, $\text{GA}_5(\Gamma)$ and $S(\Gamma)$ are proposed by Ghorbani et al. [26], Graovac et al. [27], and Hosamani [28], respectively. These indices are different as compared to other vertex valency-based indices in the sense that they require partitioning of the edges of the network on the basis of neighbors’ valency-sum of end vertices for every edge in an interconnected network. Their formulae are given as:

$$\text{ABC}_4(\Gamma) = \sum_{vw \in E(\Gamma)} \frac{s_v + s_w - 2}{s_v s_w}$$
$$\text{GA}_5(\Gamma) = \sum_{vw \in E(\Gamma)} \frac{2\sqrt{s_v s_w}}{s_v + s_w}$$

where $s_v = \sum_{w \in N(v)} d_w$ and $N(\Gamma) = \{v \in V(\Gamma) \mid vw \in E(\Gamma)\}$.

Motivated by the $\text{ABC}$ index, Furtula et al. [29] offered the so called Augmented Zagreb index ($\text{AZI}$) which proved to have a better correlation coefficient as compared to $\text{ABC}$ [30] and is defined as:

$$\text{AZI}(\Gamma) = \sum_{vw \in E(\Gamma)} \left( \frac{d_v d_w}{d_v + d_w - 2} \right)^3$$

A few more topological indices that have key importance are defined below which include harmonic index ($\text{HI}$), inverse sum index ($\text{ISI}$), and symmetric division index ($\text{SDD}$):

$$\text{HI}(\Gamma) = \sum_{vw \in E(\Gamma)} \frac{2}{d_v + d_w}$$
$$\text{ISI}(\Gamma) = \sum_{vw \in E(\Gamma)} \frac{d_v d_w}{d_v + d_w}$$
$$\text{SDD}(\Gamma) = \sum_{vw \in E(\Gamma)} \frac{\min(d_v, d_w)}{\max(d_v, d_w)}$$

To compute topological indices, a huge amount of calculation is required. In 2015, Deutsch and Klavžar introduced $M$-polynomial to reduce this calculation

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

where $m_{ij}(\Gamma)$ represent number of edges $vw \in E(\Gamma)$ such that $(d_v(\Gamma), d_w(\Gamma)) = (i, j)$. The other polynomials are Hosoya polynomial [32], matching polynomial [33], the Zhang-Zhang polynomial [34], the Schultz polynomial [35] and the Tutte polynomial [36]. Some promising topological indices are worked out in [31] with the help of $M$-polynomial and are depicted in the table 1 below.

In this paper, we computed all the above defined topological indices for Bakelite Network $BN_{m}^n$.

## 2 Bakelite Network $BN_{m}^n$

Synthetic polymers, such as Teflon, Bakelite, Polyvinyl chloride (PVC) and High-density polyethylene (HDPE) have been studied for a long time and are of industrial interest for diverse potential applications. For example, Bakelite
Valency-based molecular descriptors of Bakelite network BN

(C₆H₆OCH₂O)n is very attractive and had immense influence on the development of technology. Since time immemorial natural materials like gum, amber, shellac, tortoise-shell, and horn have been used to make various type of tools and objects. Bakelite, invented by Belgian-American chemist Leo Hendrik Arthur Baekeland (1863-1944), was the very first synthetic material that brought mankind into the plastic-age. Bakelite, being phenolic resin, possesses several desirable properties like water, heat, organic solvent and scratch resistant, hard, insoluble, rigid, and low-conductivity [37]. This revolutionary thermosetting plastic has enormous engineering applications and is used as an electric insulator, propellers, automotive accessories, and medical as well as sports equipment [38, 39].

### 3 Methodology

To compute our results, we count the number of vertices and number of edges of the graph of the Bakelite Network BNₚⁿ. The total number of vertices and edges in the graph of Bakelite network BNₚⁿ are 8mn+n+m and 10mn-2n, respectively. In the graph of BNₚⁿ, figure 3, n represent number of hexagons in one row and m represent number of hexagons in one column. The vertex set and edge set partition of any graph Γ can generally be defined as [3]

\[ V_d = \{ v \in V(\Gamma) \mid \deg(v) = d \} \]

\[ E_{ij}(\Gamma) = \{ uv \in E(\Gamma) \mid (\deg(\nu), \deg(\nu w)) = (i, j) \}. \]
We divide the edge set of graph of Bakelite Network \(BN_m^n\) into classes depending on the degrees of end vertices of each edge. Then using this edge partition, we compute our desired results.

## 4 Computational Results

In this section, we compute various topological indices of bakelite network \(BN_m^n\). In subsequent theorems, we provide the M-polynomial of a bakelite network which will be a core component of the forthcoming theorems.

**Theorem 1.** Let \(\Gamma = BN_m^n\) be the \((m,n)\)-dimensional bakelite network then M-polynomial of \(\Gamma\) is

\[
M(\Gamma; x, y) = 2mxy^3 + 2nx^2y^3 + (8mn - 2m - 2n)x^2y^3 +
+ (2mn - 2n)x^3y^3.
\]

**Proof.** By analyzing the molecular graph of bakelite network \(BN_m^n\) it can readily be observed that there are following three kind of vertices based on the degrees,

\[
\begin{align*}
V_1 &= \{v \in V(\Gamma) \mid \deg(v) = 1\}, \\
V_2 &= \{v \in V(\Gamma) \mid \deg(v) = 2\}, \\
V_3 &= \{v \in V(\Gamma) \mid \deg(v) = 3\}.
\end{align*}
\]

Such that

\[
\begin{align*}
|V_1| &= 2m, \\
|V_2| &= 4mn - m + n, \\
|V_3| &= 4mn - 2n.
\end{align*}
\]

Now based on the degree of end vertices, the edge set of the molecular graph of bakelite network \(BN_m^n\) can be divided into following classes:

\[
\begin{align*}
E_{13}(\Gamma) &= \{uv \in E(\Gamma) \mid (\deg(v), \deg(w)) = (1,3)\}, \\
E_{22}(\Gamma) &= \{uv \in E(\Gamma) \mid (\deg(v), \deg(w)) = (2,2)\}, \\
E_{23}(\Gamma) &= \{uv \in E(\Gamma) \mid (\deg(v), \deg(w)) = (2,3)\}, \\
E_{33}(\Gamma) &= \{uv \in E(\Gamma) \mid (\deg(v), \deg(w)) = (3,3)\}.
\end{align*}
\]

Such that

\[
|E_{13}| = 2m, |E_{22}| = 2n, |E_{23}| = 8mn - 2m - 2n, |E_{33}| = 2n(m - 1).
\]

Now,

\[
M(\Gamma; x, y) = \sum_{\deg(v) = 1} m_{ij} x^i y^j = \sum_{\deg(v) = 2} m_{ij} x^i y^j + \sum_{\deg(v) = 3} m_{ij} x^i y^j = |E_{13}(\Gamma)| x^1 y^3 + |E_{22}(\Gamma)| x^2 y^2 + |E_{23}(\Gamma)| x^2 y^3 + |E_{33}(\Gamma)| x^3 y^3 = 2mxy^3 + 2nx^2y^3 + (8mn - 2m - 2n)x^2y^3 + (2mn - 2n)x^3y^3
\]

The next theorem is about the computation of nine indices from the M-polynomial.

**Theorem 2.** For bakelite network \(\Gamma = BN_m^n\) closed form formulae for first, second, modified and augmented Zagreb indices, Randić indices, symmetric division degree, harmonic and inverse sum indices are:

1. \(M_1(\Gamma) = 52mn - 14n - 2m\),
2. \(M_2(\Gamma) = 66mn - 22n - 6m\),
3. \(mM_2(\Gamma) = \frac{14}{9}mn - \frac{1}{9}n - 1\frac{1}{9}m\),
4. \(R_4(\Gamma) = (2 \times 3^2 + 2 \times 3^3 \times 3^1)m + (2 \times 3^2 - 2 \times 3^3 \times 3^1)n + (2^1 \times 2^1 - 2 \times 2^2 \times 2^1)n\),
5. \(RR_4(\Gamma) = (8 \times 6^n + 2 \times 9^n)m + (2 \times 3^2 - 2 \times 6^n)m + (2^{1-2n} - 2 \times 9^n)n\),
6. \(SDD(\Gamma) = \frac{64}{3}mn - 13n + \frac{13}{3}m\),
7. \(H(\Gamma) = \frac{58}{5}mn - \frac{7}{5}n - \frac{7}{5}m\),
8. \(ISI(\Gamma) = \frac{17}{5}mn - \frac{17}{5}n - \frac{17}{5}m\),
9. \( AZI(\Gamma) = \frac{2777}{32}mn - \frac{2779}{32}n - \frac{37}{4}m\).

**Proof.** Consider

\[
M(\Gamma; x, y) = 2mxy^3 + 2nx^2y^3 + (8mn - 2m - 2n)x^2y^3 + (2mn - 2n)x^3y^3
\]

Then

\[
\begin{align*}
D_1M(\Gamma; x, y) &= 2mxy^3 + 4nx^2y^3 + 2(8mn - 2m - 2n)x^2y^3 + (2mn - 2n)x^3y^3, \\
D_2M(\Gamma; x, y) &= 6mxy^3 + 4nx^2y^3 + 3(8mn - 2m - 2n)x^2y^3 + (2mn - 2n)x^3y^3, \\
(D_1, D_2)M(x, y) &= 6mxy^3 + 8nx^2y^3 + 12(4mn - m - n)x^2y^3 + 8(mn)(-1)x^3y^3, \\
(S_1, S_2)M(x, y) &= \left(\frac{2}{3}mxy^3 + \frac{1}{3}nx^2y^3 + \frac{1}{3}(4mn - m - n)x^2y^3 + \frac{2}{3}(m - 1)x^3y^3, \\
D_1D_2M(x, y) &= 2.3mxy^3 + 2.4nx^2y^3 + 2.9n(m - 1)x^2y^3 + 2.6(4mn - m - n)x^3y^3.
\end{align*}
\]
Valency-based molecular descriptors of Bakelite network BN\textsuperscript{n}_m

1. First Zagreb index

\[ M_1(\Gamma) = (D_x + D_y)M|_{x=y=1} = 52mn - 14n - 2m. \]

2. Second Zagreb index

\[ M_2(\Gamma) = (D_y D_x)M|_{x=y=1} = 66mn - 22n - 6m. \]

3. Modified second Zagreb index

\[ m^2 M_2(\Gamma) = (S_x S_y)M|_{x=y=1} = \frac{14}{9}mn - \frac{1}{3}n - \frac{1}{3}m. \]

4. Generalized Randić index

\[ R_\alpha(\Gamma) = (D_\alpha S_{\alpha})M|_{x=y=1} = (2 \times 3^2 \alpha + 2 \times 3 \alpha \times 3 \alpha)mn + (2 \times 3^2 \alpha - 2 \times 3 \alpha \times 3 \alpha)m + (2^2 \alpha + 2 \times 2^2 \alpha - 2 \times 2 \alpha \times 2 \alpha)n. \]

5. Inverse Randić index

\[ R_{R_\alpha}(\Gamma) = (S_{R_\alpha} S_{R_\alpha})M|_{x=y=1} = (8 \times 6^2 \alpha - 2 \times 9 \alpha)mn + (2 \times 3 \alpha \times 2 \times 6 \alpha)m + (2 \times 1 \alpha - 2 \times 6 \alpha - 2 \times 9 \alpha)n. \]

6. Symmetric division index

\[ SSD(\Gamma) = (D_0 S_0 + S_0 D_0)M|_{x=y=1} = \frac{64}{3}mn - \frac{13}{3}n + \frac{7}{3}m. \]

7. Harmonic index

\[ H(\Gamma) = 2S_y JM(x)|_{x=1} = \frac{58}{15}mn - \frac{7}{5}n + \frac{1}{5}m. \]

8. Inverse sum index

\[ I(\Gamma) = S_x D_x D_y M|_{x=1} = \frac{63}{5}mn - \frac{17}{5}n + \frac{9}{10}m. \]

9. Augmented Zagreb index

\[ A(\Gamma) = S_2^2 Q - 2D_2^2 D_2^2 M|_{x=1} = \frac{2777}{32}mn - \frac{729}{32}n - \frac{37}{4}m. \]

Theorem 3. Let \( \Gamma = BN^m_n \) be the molecular graph of \((m, n)\)-dimensional bakelite network, then

1. \( ABC(\Gamma) = \frac{4}{3}(1 + 3\sqrt{2})mn - n - \frac{1}{2\sqrt{2}}m. \)
2. \( GA(\Gamma) = \frac{1}{5}((10 + 16\sqrt{6})mn - 4\sqrt{6}n - (5\sqrt{3} - 4\sqrt{6})m. \)
3. \( SCI(\Gamma) = \left( \frac{2}{3} + \frac{8}{\sqrt{5}} \right)mn - \left( 1 - \frac{2}{\sqrt{3}} + \frac{2}{\sqrt{5}} \right)n - \left( 1 - \frac{2}{\sqrt{3}} \right)m. \)

Proof.

\[ ABC(\Gamma) = \sum_{v \in \Xi(\Gamma)} \left( \frac{d_v + d_w - 2}{d_v d_w} \right) + \sum_{w \in \Xi(\Gamma)} \left( \frac{d_v + d_w - 2}{d_v d_w} \right) \]

\[ + \left( \sum_{v \in \Xi(\Gamma)} \frac{d_v + d_w - 2}{d_v d_w} \right) \left( \sum_{w \in \Xi(\Gamma)} \frac{d_v + d_w - 2}{d_v d_w} \right) \]

\[ = |E_{E_3}(\Gamma)| \cdot \left( \frac{1}{3} - 2 \right) + |E_{E_2}(\Gamma)| \cdot \left( \frac{2}{3} + 2 \right) \]

\[ + |E_{E_3}(\Gamma)| \cdot \left( \frac{2}{3} + 3 \right) - \left( \frac{3}{3} - 2 \right) \]

\[ = \frac{4}{3}((1 + 3\sqrt{2})mn - n - \frac{1}{2\sqrt{2}}m). \]

\[ GA(\Gamma) = \sum_{v \in \Xi(\Gamma)} \left( \frac{2\sqrt{d_v + d_w}}{d_v + d_w} \right) \]

\[ + \sum_{w \in \Xi(\Gamma)} \left( \frac{2\sqrt{d_v + d_w}}{d_v + d_w} \right) \]

\[ + \sum_{v \in \Xi(\Gamma)} \left( \frac{2\sqrt{d_v + d_w}}{d_v + d_w} \right) \]

\[ = |E_{E_3}(\Gamma)| \cdot \left( \frac{2\sqrt{3}}{1 + 3} \right) + |E_{E_2}(\Gamma)| \cdot \left( \frac{2\sqrt{2}}{1 + 3} \right) \]

\[ + |E_{E_3}(\Gamma)| \cdot \left( \frac{2\sqrt{6}}{2 + 3} \right) + |E_{E_3}(\Gamma)| \cdot \left( \frac{2\sqrt{9}}{3 + 3} \right) \]

\[ = \frac{1}{5}((10 + 16\sqrt{6})mn - 4\sqrt{6}n - (5\sqrt{3} - 4\sqrt{6})m). \]

\[ SCI(\Gamma) = \sum_{v \in \Xi(\Gamma)} \left( \frac{1}{d_v + d_w} \right) \]

\[ + \sum_{w \in \Xi(\Gamma)} \left( \frac{1}{d_v + d_w} \right) \]

\[ + \sum_{v \in \Xi(\Gamma)} \left( \frac{1}{d_v + d_w} \right) \]

\[ = |E_{E_3}(\Gamma)| \cdot \left( \frac{1}{\sqrt{1 + 3}} \right) + |E_{E_2}(\Gamma)| \cdot \left( \frac{1}{\sqrt{2 + 2}} \right) \]

\[ + |E_{E_3}(\Gamma)| \cdot \left( \frac{1}{\sqrt{3 + 3}} \right) \]

\[ = \left( \frac{2}{3} + \frac{8}{\sqrt{5}} \right)mn - \left( 1 - \frac{2}{\sqrt{3}} + \frac{2}{\sqrt{5}} \right)n - \left( 1 - \frac{2}{\sqrt{3}} \right)m. \]

Theorem 4. Let \( \Gamma = BN^m_n \) be the \((m, n)\)-dimensional bakelite network then the fourth atom-bound connectivity index is given by
Proof. In order to prove our theorem, we need edge partition of \( \Gamma \) based on neighbors’ valency-sum of end vertices \( \forall uv \in \Gamma \). We identify following nine categories of edges on valency based sum of neighbors’ vertices of each edge in the bakelite network.

\[
\begin{align*}
\epsilon_{35}(\Gamma) & = \{ uv \in E(\Gamma) \mid (s_u, s_v) = (3, 5) \}, \\
\epsilon_{36}(\Gamma) & = \{ uv \in E(\Gamma) \mid (s_u, s_v) = (3, 6) \}, \\
\epsilon_{45}(\Gamma) & = \{ uv \in E(\Gamma) \mid (s_u, s_v) = (4, 5) \}, \\
\epsilon_{55}(\Gamma) & = \{ uv \in E(\Gamma) \mid (s_u, s_v) = (5, 5) \}, \\
\epsilon_{57}(\Gamma) & = \{ uv \in E(\Gamma) \mid (s_u, s_v) = (5, 7) \}, \\
\epsilon_{66}(\Gamma) & = \{ uv \in E(\Gamma) \mid (s_u, s_v) = (6, 6) \}, \\
\epsilon_{67}(\Gamma) & = \{ uv \in E(\Gamma) \mid (s_u, s_v) = (6, 7) \}, \\
\epsilon_{68}(\Gamma) & = \{ uv \in E(\Gamma) \mid (s_u, s_v) = (6, 8) \}, \\
\epsilon_{78}(\Gamma) & = \{ uv \in E(\Gamma) \mid (s_u, s_v) = (7, 8) \},
\end{align*}
\]

such that

\[
|\epsilon_{35}(\Gamma)| = 2, |\epsilon_{36}(\Gamma)| = 2n - 2, |\epsilon_{45}(\Gamma)| = 2n, |\epsilon_{55}(\Gamma)| = 6, \\
|\epsilon_{57}(\Gamma)| = 2n - 2, |\epsilon_{66}(\Gamma)| = 3n + 3m + 2n - 10, |\epsilon_{67}(\Gamma)| = 4mn - 6n - 4m + 6, \\
|\epsilon_{68}(\Gamma)| = mn - n + 2m - 2, |\epsilon_{78}(\Gamma)| = 2mn - 2n - 2m + 2.
\]

Now, the fourth version of ABC can be calculated as follows:

\[
ABC_4(\Gamma) = \sum_{uv \in E(\Gamma)} \sqrt{{s_u}^2 + {s_v}^2 - 2s_us_v}
\]

\[
\begin{align*}
&= \frac{2}{\sqrt{15}} \left( \frac{6}{15} \right)^{2m - 2} \left( \frac{7}{18} \right)^{2n} \left( \frac{2}{20} \right)^{6} \left( \frac{2}{30} \right)^{2} \left( \frac{2}{35} \right)^{2n - 2m - 2} \left( \frac{3}{42} \right)^{m} \left( \frac{11}{42} \right)^{n - m} \\
&+ (3mn + 3n + 2m - 10) \left( \frac{10}{35} \right)^{n} \left( \frac{4mn - 6n - 4m + 6}{42} \right)^{n} \\
&+ (mn - n + 2m - 2) \left( \frac{12}{48} \right)^{m} \left( \frac{2}{48} \right)^{n - m - 1} \left( \frac{13}{48} \right)^{m} \left( \frac{15}{48} \right)^{n}
\end{align*}
\]

\[
ABC_4(\Gamma) = \frac{1}{42} \left( 4\sqrt{462} + 21\sqrt{10} + 3\sqrt{182} + 21 \right) mn + \frac{1}{42} \left( 4\sqrt{14} + 14\sqrt{10} - 4\sqrt{462} - 3\sqrt{182} + 42 \right) m + \frac{1}{210} \left( 4\sqrt{35} + 60\sqrt{14} + 105\sqrt{10} - 20\sqrt{462} - 15\sqrt{182} - 105 \right) n + \frac{1}{210} \left( 4\sqrt{35} + 60\sqrt{14} + 105\sqrt{10} - 20\sqrt{462} - 15\sqrt{182} - 105 \right) n
\]

\[
G_A(\Gamma) = \sum_{uv \in E(\Gamma)} \left( \frac{2}{s_u s_v} \right)
\]

\[
= \frac{\sqrt{15}}{2} + \frac{\sqrt{18}}{9} \left( m - 1 \right) + \frac{\sqrt{20}}{9} \left( n - 1 \right) + \frac{\sqrt{210}}{n} \left( n - 1 \right) + \frac{\sqrt{247}}{4} \left( 4mn - 6n - 4m + 6 \right)
\]

\[
S(\Gamma) = \sum_{uv \in E(\Gamma)} \left( \frac{s_u + s_v - 2}{s_u + s_v} \right)^3
\]

\[
= \frac{125}{4} \left( \frac{3432}{343} \right)^{2m - 2} + \frac{1009}{343} \left( \frac{3433}{343} \right)^{2n - 2} \left( \frac{3433}{343} \right)^{n} \left( \frac{3433}{343} \right)^{m}
\]

\[
+ \frac{125}{1331} \left( \frac{40040}{1331} \right)^{2n - 2} \left( \frac{3433}{343} \right)^{n} \left( \frac{3433}{343} \right)^{m} \left( \frac{3433}{343} \right)^{n}
\]

\[
+ \frac{125}{1331} \left( \frac{40040}{1331} \right)^{2n - 2} \left( \frac{3433}{343} \right)^{n} \left( \frac{3433}{343} \right)^{m} \left( \frac{3433}{343} \right)^{n}
\]

5 Conclusions

QSARs represent predictive models derived from the application of statistical tools correlating to the biological activity (including desirable therapeutic effect and undesirable side effects) of chemicals (drugs/toxicants/environmental pollutants) with descriptors representative of molecular structure and/or properties. QSARs are being applied in many disciplines like risk assessment, toxicity prediction, and regulatory decisions in addition to drug discovery and lead optimization. In this article, we obtained numerous molecular descriptors for a molecular graph of a pioneer synthetic polymer called bakelite. We employed edge partitioning procedures on the molecular graph on the basis of valency of vertices \( d_v \) and sum of valency \( s_v \) of vertices at unit distance from each other. In addition, we computed M-polynomial of bakelite network \( B_n \) along with closed form formulae of various valency-based topological descriptors of substantial significance. Moreover, we took advantage of Matlab and Maple for the simplification and plotting of results. For a future prospect, we propose to develop molecular graphs of certain synthetic polymers (plastics) like polystyrene chloride (PVC) and Polyethylene terephthalate (PETE), and work out their topological descriptors which will eventually take part in determining a relation as well as comparison between the physical and chemical properties of these synthetic polymers with bakelite.
**Data Availability Statement:** All data required for this research is available in this paper.

**Author Contribution:** All authors contributed equally in this paper.

**Funding Statement:** This research is partially funded by University of Management and Technology, Lahore, Pakistan.

**Acknowledgment:** Authors are thankful to reviewers for valuable suggestions that improve the quality of this paper.

**Completing Interest:** The authors do not have any competing interests.

**References**

[1] Brückler F.M., Došlić T., Graovac A., Gutman I., On a class of distance-based molecular structure descriptors, Chem. Phys. Lett., 2011, 503, 336-338.

[2] Rücker G., Rücker C., On topological indices, boiling points, and cycloalkanes, J. Chem. Inf. Comput. Sci., 1999, 39, 788-802.

[3] Ramane H. S., Jummannaver R. B., Note on forgotten topological index of chemical structure in drugs, AMNS, 2016, 1(2), 369-374.

[4] De N., Hyper Zagreb Index of Bridge and Chain Grpahs, Open J. Math. Sci., 2018, 2(1), 1-17.

[5] Tang Z., Liang L., Gao W., Wiener polarity index of quasi-tree molecular structures, Open J. Math. Sci., 2018, 2(1), 73-83.

[6] Baig A.Q., Naeem M., Gao W., Revan and hyper-Revan indices of Octahedral and icosaahedral networks, AMNS, 2018, 3(1), 33-40.

[7] Liu G., Jia Z., Gao W., Ontology similarity computing based on stochastic primal dual coordinate technique, Open J. Math. Sci., 2018, 2(1), 221-227.

[8] Sardar M.S., Zafar S., Farahani M.R., The Generalized Zagreb Index of Capra-Designed Planar Benzenoid Series C a k ( C 6 ), Open J. Math. Sci., 2017, 1(1), 44-51.

[9] Sardar M.S., Pan X.-F., Gao W., Farahani, M.R., Computing Sanskriti Index of Titania Nanotubes, Open J. Math. Sci., 2017, 1(1), 126-131.

[10] Naeem M., Siddiqui M.K., Guirao J. L. G., Gao W., New and Modified Eccentric Indices of Octagonal Grid Omn, AMNS, 2018, 3(1), 209-228.

[11] Siddiqui H., Farahani M.R., Forgotten Polynomial and Forgotten Index of Certain Interconnection Networks, Open J. Math. Anal., 2017, 1(1), 45-60.

[12] Gao W., Muzaffar B., Nazeer W., K-Banhatti and K-hyper Banhatti Indices of Dominating David Derived Network, Open J. Math. Anal., 2017, 1(1), 13-24.

[13] Noreen S., Mahmood A., Zagreb Polynomials and Redefined Zagreb Indices for the line graph of Carbon Nanocones, Open J. Math. Anal., 2018, 2(1), 67-76.

[14] Fath-Tabar G. H., Old and new Zagreb indices of graphs. MATCH Commun. Math. Comput. Chem., 2011, 65(1), 79-84.

[15] Gao W., Asif M., Nazeer W., The Study of Honey Comb Derived Network via Topological Indices, Open J. Math. Anal., 2018, 2(2), 10-26.

[16] Rehman H. M., Sardar R., Raza A., Computing topological indices of hex board and its line graph, Open J. Math. Sci., 2017, 1, 62-71.

[17] Gao W., Farahani M.R., Shi L., Forgotten topological index of some drug structures, Acta Medica Mediterranea, 2016, 32, 579-585.

[18] Wiener H., Structural determination of paraffin boiling points, J. Am. Chem. Soc., 1947, 1169, 17-20.

[19] Deza M., Fowler P.W., Rassat A., Rogers, K.M., Fullerene as tiling of surfaces, J. Chem. Inf. Comput. Sci., 2000, 40, 550-558.

[20] Randić M., Characterization of molecular branching, J. Am. Chem. Soc., 97(23), 6609-6615.

[21] Bollobás B., Erdős P., Graphs of extremal weights, Ars Combin., 1998, 50, 225-233.

[22] Zhou B., Trinajstić N., On a novel connectivity index, J. Math. Chem., 2009, 46, 1252-1270.

[23] Gutman I, Trinajstić N., Graph theory and molecular orbitals. Total n-electron energy of alternant hydrocarbons, Chem. Phys. Lett., 1972, 17, 535-538.

[24] Estrada E., Torres L., Rodríguez L., Gutman I., An atom-bond connectivity index: modelling the enthalpy of formation of alkanes, Indian J. Chem., 1998, 37A, 849-855.

[25] Vukičević D., Furtula B., Topological index based on the ratios of geometrical and arithmetical means of end-vertex degrees of edges, J. Math. Chem., 2009, 46, 1369-1376.

[26] Ghorbani M., Hosseinizadeh M.A., Computing ABC index of nanostar dendrimers. Optoelectron, Adv. Mater. Rapid Commun., 2010, 4, 1419-1422.

[27] Graovac A., Ghorbani M., Hosseinizadeh M.A., Computing fifth geometric-arithmetic index for nanostar dendrimers, J. Math. Nanosci., 2011, 1, 33-42.

[28] Hosamani S.M., Computing Sanskriti Index of Certain Nanostructures, J. Appl. Math. Comput., 2016, 54, 425-433.

[29] Furtula B., Graovac A., Vukičević D., Augmented Zagreb index, J. Math. Chem., 2010, 48, 370-380.

[30] Wang D., Huang Y., Liu B., Bounds on augmented Zagreb index, MATCH Commun. Math. Comput. Chem., 2012, 68, 209-216.

[31] Deutsch E., Klavžar S., M-Polynomial and degree-based topological indices. Iran. J. Math. Chem., 2015, 6, 93-102.

[32] Hosoya H., On some counting polynomials in chemistry, Discrete Appl. Math., 1988, 19, 239-257.

[33] Farrell E.J., An introduction to matching polynomials, J. Combin. Theory Ser., 1979, B 27, 75-86.

[34] Chou C.P., Witek H.A., Closed-form formulas for the Zhang-Zhang polynomials of benzenoid structures: chevrons and generalized chevrons, MATCH Commun., Math. Comput. Chem., 2014, 72, 105-124.

[35] Hassani F., Iranmanesh A., Mirzaie S., Schultz and modified Schultz polynomials of C100 fullerene, MATCH Commun. Math. Comput. Chem., 2013, 69, 87-92.

[36] Došlić T., Planar polycyclic graphs and their Tutte polynomials, J. Chem. Inf. Comput. Sci., 2013, 51, 1599-1607.
[37] Dong Y., Xiaofeng L., Yue J., Hao-Bin Z., Bing-Bing J., Hui-Ling M., et al., Thermally conductive phenol formaldehyde composites filled with carbon fillers, Materials Letters, 2014, 118, 212-216.

[38] Cheng L., Jizhi Z., Zhao Y., Hua Y., Bin Z., Wei Z., et al., Preparation and characterization of a novel environmentally friendly phenol-formaldehyde adhesive modified with tannin and urea, Int. J. Adhes. Adhes., 2016, 66, 26-32.

[39] Foyer G., Chanfi B., Boutevin B., Caillol S., David G., New method for the Synthesis of formaldehyde-free phenolic resins from lignin-based aldehyde precursors, Eur. Polym. J., 2016, 74, 296-309.