Research Article

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

Valency-based molecular descriptors of Bakelite network BN_m^n <https://doi.org/10.1515/chem-2019-0081>

received December 12, 2018; accepted February 21, 2019.

Abstract: Bakelite network BN_m^n 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_m^n . These molecular descriptors play a fundamental role in QSPR/QSAR studies in describing the chemical and physical properties of Bakelite network BN_m^n . We computed atom-bond connectivity ABC its fourth version ABC_4 geometric arithmetic GA its fifth version GA_5 Narumi-Katayama, sum-connectivity and Sanskruti indices, first, second, modified and augmented Zagreb indices, inverse and general Randić' indices, symmetric division, harmonic and inverse sum indices of BN_m^n .

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 $\Gamma=(V,E)$ 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 $v \in \Gamma$ is the number of incident edges with v and is denoted by d_v . 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:

$$R_{-1/2}(\Gamma) = \sum_{vw \in E(\Gamma)} \frac{1}{\sqrt{d_v d_w}}$$

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

$$R_\alpha(\Gamma) = \sum_{vw \in E(\Gamma)} (d_v d_w)^\alpha.$$

and inverse Randić' index:

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

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:

*Corresponding author: Chahn Yong Jung, Department of Business Administration, Gyeongsang National University, Jinju, 52828, Korea, E-mail: bb5734@gnu.ac.kr

Maqsood Ahmad, Department of Mathematics, University of Management and Technology, Lahore, Pakistan and Department of Mathematics, COMSATS Institute of Information Technology, Lahore, Pakistan

Muhammad Javaid, Department of Mathematics, University of Management and Technology, Lahore, Pakistan.

Muhammad Saeed, Department of Mathematics, University of Management and Technology, Lahore, Pakistan

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

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 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:

$$^m M_2(\Gamma) = \sum_{vw \in E(\Gamma)} \frac{1}{(d_v d_w)}$$

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

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

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

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

Three prominent and recently developed indices, denoted by $ABC_4(\Gamma)$, $GA_5(\Gamma)$ 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:

$$ABC_4 = \sum_{vw \in E(\Gamma)} \sqrt{\frac{s_v + s_w - 2}{s_v s_w}}$$

$$GA_5 = \sum_{vw \in E(\Gamma)} \frac{2\sqrt{s_v s_w}}{s_v + s_w}$$

$$S = \sum_{vw \in E(\Gamma)} \left(\frac{s_v s_w}{s_v + s_w - 2} \right)^3$$

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

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

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

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

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

$$ISI(\Gamma) = \sum_{vw \in E(\Gamma)} \frac{d_v d_w}{d_v + d_w}$$

$$SDD(\Gamma) = \sum_{vw \in E(\Gamma)} \left[\frac{\min(d_v, d_w)}{\max(d_v, d_w)} + \frac{\max(d_v, d_w)}{\min(d_v, d_w)} \right]$$

To compute topological indices, a huge amount of calculation is required. In 2015, Deutsch and Klavžar [31] introduced M -polynomial to reduce this calculation

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

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

Table 1: Formulae of certain essential topological descriptors in relation with M-polynomial.

Topological indices	Formulae derived from M-polynomial
1st Zagreb index (M_1)	$(D_x + D_y)M(x, y) _{x=y=1}$
2nd Zagreb index (M_2)	$(D_x \cdot D_y)M(x, y) _{x=y=1}$
Modified 2nd Zagreb index (mM_2)	$(S_x \cdot S_y)M(x, y) _{x=y=1}$
General Randić' index R_α	$(D_x^\alpha \cdot D_y^\alpha)M(x, y) _{x=y=1}$
Inverse Randić' index RR_α	$(S_x^\alpha \cdot S_y^\alpha)M(x, y) _{x=y=1}$
Symmetric Division Deg. Index (SDD)	$(D_x S_y + S_x D_y)M(x, y) _{x=y=1}$
Harmonic Index (HI)	$2S_x J M(x, y) _{x=y=1}$
Inverse Sum Index (ISI)	$(S_x J D_x D_y)M(x, y) _{x=y=1}$
Augmented Zagreb Index (AZI)	$(S_x^3 Q_{-2} J D_x^3 D_y^3)M(x, y)$

where $D_x M = x \frac{\partial M}{\partial x}$, $D_y M = y \frac{\partial M}{\partial y}$, $S_x M = \int_0^x \frac{M(t, y)}{t} dt$, $S_y M = \int_0^y \frac{M(x, t)}{t} dt$, $J(M(x, y)) = M(x, x)$, $Q_\alpha M = x^\alpha M$.

$(C_6H_6OCH_2O)_n$ 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 in to 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 BN_m^n . The total number of vertices and edges in the graph of Bakelite network BN_m^n are $8mn - n + m$ and $10mn - 2n$, respectively. In the graph of BN_m^n , 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]

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

$$E_{ij}(\Gamma) = \{uv \in E(\Gamma) \mid (\deg(v), \deg(w)) = (i, j)\}.$$

Figure 1: Structural phases of Bakelite. **Figure 2:** Molecular graph of Bakelite.

Figure 3: Hydrogen depleted molecular graph of Bakelite network BN_m^n .

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 Γ is

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

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,

$$\begin{aligned} V_1 &= \{v \in V(\Gamma) \mid \deg(v) = 1\}, \\ V_2 &= \{v \in V(\Gamma) \mid \deg(v) = 2\}, \\ V_3 &= \{v \in V(\Gamma) \mid \deg(v) = 3\}. \end{aligned}$$

Such that

$$\begin{aligned} |V_1| &= 2m, \\ |V_2| &= 4mn - m + n, \\ |V_3| &= 4mn - 2n. \end{aligned}$$

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:

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

Such that

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

Now,

$$\begin{aligned} M(\Gamma; x, y) &= \sum_{\delta \leq i \leq j \leq \Delta} m_{ij} x^i y^j \\ &= \sum_{1 \leq 3} m_{13} xy^3 + \sum_{2 \leq 2} m_{22} x^2 y^2 + \sum_{2 \leq 3} m_{23} x^2 y^3 + \sum_{3 \leq 3} m_{33} x^3 y^3 \\ &= |E_{13}(\Gamma)| xy^3 + |E_{22}(\Gamma)| x^2 y^2 + |E_{23}(\Gamma)| x^2 y^3 + |E_{33}(\Gamma)| x^3 y^3 \\ &= 2mxy^3 + 2nx^2y^2 + (8mn - 2m - 2n)x^2y^3 + (2mn - 2n)x^3y^3 \end{aligned}$$

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. ${}^m M_2(\Gamma) = \frac{14}{9}mn - \frac{1}{18}n - \frac{1}{3}m$,
4. $R_\alpha(\Gamma) = (2 \times 3^{2\alpha} + 2^{\alpha+3} \times 3^\alpha)mn + (2 \times 3^\alpha - 2^{\alpha+1} \times 3^\alpha)m + (2^{2\alpha+1} - 2 \times 3^{2\alpha} - 2^{\alpha+1} \times 3^\alpha)n$
5. $RR_\alpha(\Gamma) = (8 \times 6^{-\alpha} + 2 \times 9^{-\alpha})mn + (2 \times 3^{-\alpha} - 2 \times 6^{-\alpha})m + (2^{1-2\alpha} - 2 \times 6^{-\alpha} - 2 \times 9^{-\alpha})n$
6. $SDD(\Gamma) = \frac{64}{3}mn - \frac{13}{3}n + \frac{7}{3}m$,
7. $HI(\Gamma) = \frac{58}{15}mn - \frac{7}{15}n + \frac{1}{5}m$,
8. $ISI(\Gamma) = \frac{63}{5}mn - \frac{17}{5}n - \frac{9}{10}m$,
9. $AZI(\Gamma) = \frac{2777}{32}mn - \frac{729}{32}n - \frac{37}{4}m$.

Proof. Consider

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

Then

$$D_x M(\Gamma; x, y) = 2mxy^3 + 4nx^2y^2 + 2(8mn - 2m - 2n)x^2y^3 + 3(2mn - 2n)x^3y^3,$$

$$D_y M(\Gamma; x, y) = 6mxy^3 + 4nx^2y^2 + 3(8mn - 2m - 2n)x^2y^3 + 3(2mn - 2n)x^3y^3,$$

$$(D_x D_y) M(\Gamma; x, y) = 6mxy^3 + 8nx^2y^2 + 12(4mn - m - n)x^2y^3 + 18n(m - 1)x^3y^3,$$

$$(S_x S_y) M(\Gamma; x, y) = \frac{2}{3}mxy^3 + \frac{1}{2}nx^2y^2 + \frac{1}{3}(4mn - m - n)x^2y^3 + \frac{2}{9}n(m - 1)x^3y^3,$$

$$D_x^\alpha D_y^\alpha M(\Gamma; x, y) = 2 \cdot 3^\alpha \cdot mxy^3 + 2 \cdot 4^\alpha \cdot nx^2y^2 + 2 \cdot 9^\alpha \cdot n(m - 1)x^3y^3 + 2 \cdot 6^\alpha \cdot (4mn - m - n)x^2y^3,$$

$$S_x^\alpha S_y^\alpha M(x, y) = \frac{2}{3^\alpha} mxy^3 + 2^{1-2\alpha} nx^2y^2 + \frac{2}{9^\alpha} n(m-1)x^3y^3 + 2^{1-\alpha} 3^{-\alpha} (4mn - m - n)x^2y^3,$$

$$(S_y D_x + S_x D_y)M(x, y) = \frac{20}{3} mxy^3 + 4nx^2y^2 + \frac{13}{3} (4mn - m - n)x^2y^3 + 4n(m-1)x^3y^3,$$

$$JM(x, y) = 2(m+n)x^4 + 2(4mn - m - n)x^5 + 2n(m-1)x^6,$$

$$S_x JM(x, y) = \frac{1}{2} (m+n)x^4 + \frac{2}{5} (4mn - m - n)x^5 + \frac{1}{3} n(m-1)x^6,$$

$$S_x JD_x D_y M(x, y) = \left(\frac{3}{2}m + 2n\right)x^4 + \frac{12}{5} (4mn - m - n)x^5 + 3n(m-1)x^6,$$

$$S_x^3 Q_{-2} JD_x^3 D_y^3 M(x, y) = \frac{1}{4} (27m + 64n)x^2 + 16(4mn - m - n)x^3 + \frac{729}{32} n(m-1)x^4.$$

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

$${}^m M_2(\Gamma) = (S_x S_y)M|_{x=y=1} = \frac{14}{9} mn - \frac{1}{18} n - \frac{1}{3} m.$$

4. Generalized Randić index

$$R_\alpha(\Gamma) = (D_x^\alpha \cdot D_y^\alpha)M|_{x=y=1} = (2 \times 3^{2\alpha} + 2^{\alpha+3} \times 3^\alpha)mn + (2 \times 3^\alpha - 2^{\alpha+1} \times 3^\alpha)m + (2^{2\alpha+1} - 2 \times 3^{2\alpha} - 2^{\alpha+1} \times 3^\alpha)n.$$

5. Inverse Randić index

$$RR_\alpha(\Gamma) = (S_x^\alpha \cdot S_y^\alpha)M|_{x=y=1} = (8 \times 6^{-\alpha} + 2 \times 9^{-\alpha})mn + (2 \times 3^{-\alpha} - 2 \times 6^{-\alpha})m + (2^{1-2\alpha} - 2 \times 6^{-\alpha} - 2 \times 9^{-\alpha})n.$$

6. Symmetric division index

$$SSD(\Gamma) = (D_x S_y + S_x D_y)M|_{x=y=1} = \frac{64}{3} mn - \frac{13}{3} n + \frac{7}{3} m.$$

7. Harmonic index

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

8. Inverse sum index

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

9. Augmented Zagreb index

$$A(\Gamma) = S_x^3 Q_{-2} JD_x^3 D_y^3 M|_{x=1} = \frac{2777}{32} mn - \frac{729}{32} n - \frac{37}{4} m.$$

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

Proof.

$$\begin{aligned} ABC(\Gamma) &= \sum_{vw \in E(\Gamma)} \sqrt{\frac{d_v + d_w - 2}{d_v d_w}} \\ ABC(\Gamma) &= \sum_{vw \in E_{13}(\Gamma)} \sqrt{\frac{d_v + d_w - 2}{d_v d_w}} + \sum_{vw \in E_{22}(\Gamma)} \sqrt{\frac{d_v + d_w - 2}{d_v d_w}} \\ &\quad + \sum_{vw \in E_{23}(\Gamma)} \sqrt{\frac{d_v + d_w - 2}{d_v d_w}} + \sum_{vw \in E_{33}(\Gamma)} \sqrt{\frac{d_v + d_w - 2}{d_v d_w}} \\ &= |E_{13}(\Gamma)| \sqrt{\frac{1+3-2}{3}} + |E_{22}(\Gamma)| \sqrt{\frac{2+2-2}{4}} \\ &\quad + |E_{23}(\Gamma)| \sqrt{\frac{2+3-2}{6}} + |E_{33}(\Gamma)| \sqrt{\frac{3+3-2}{9}} \\ &= \frac{4}{3} [(1 + 3\sqrt{2})mn - n - \frac{1}{2\sqrt{2}}m]. \end{aligned}$$

$$\begin{aligned} GA(\Gamma) &= \sum_{vw \in E(\Gamma)} \frac{2\sqrt{d_v d_w}}{d_v + d_w} \\ GA(\Gamma) &= \sum_{vw \in E_{13}(\Gamma)} \frac{2\sqrt{d_v d_w}}{d_v + d_w} + \sum_{vw \in E_{22}(\Gamma)} \frac{2\sqrt{d_v d_w}}{d_v + d_w} \\ &\quad + \sum_{vw \in E_{23}(\Gamma)} \frac{2\sqrt{d_v d_w}}{d_v + d_w} + \sum_{vw \in E_{33}(\Gamma)} \frac{2\sqrt{d_v d_w}}{d_v + d_w} \\ &= |E_{13}(\Gamma)| \frac{2\sqrt{3}}{1+3} + |E_{22}(\Gamma)| \frac{2\sqrt{4}}{2+2} \\ &\quad + |E_{23}(\Gamma)| \frac{2\sqrt{6}}{2+3} + |E_{33}(\Gamma)| \frac{2\sqrt{9}}{3+3} \end{aligned}$$

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

$$\begin{aligned} SCI(\Gamma) &= \sum_{vw \in E(\Gamma)} \frac{1}{\sqrt{d_v + d_w}} \\ SCI(\Gamma) &= \sum_{vw \in E_{13}(\Gamma)} \frac{1}{\sqrt{d_v + d_w}} + \sum_{vw \in E_{22}(\Gamma)} \frac{1}{\sqrt{d_v + d_w}} \\ &\quad + \sum_{vw \in E_{23}(\Gamma)} \frac{1}{\sqrt{d_v + d_w}} + \sum_{vw \in E_{33}(\Gamma)} \frac{1}{\sqrt{d_v + d_w}} \\ &= |E_{13}(\Gamma)| \frac{1}{\sqrt{1+3}} + |E_{22}(\Gamma)| \frac{1}{\sqrt{2+2}} \\ &\quad + |E_{23}(\Gamma)| \frac{1}{\sqrt{2+3}} + |E_{33}(\Gamma)| \frac{1}{\sqrt{3+3}} \\ &= \left(\sqrt{\frac{2}{3}} + \frac{8}{\sqrt{5}}\right)mn - \left(1 - \sqrt{\frac{2}{3}} + \frac{2}{\sqrt{5}}\right)n - \left(1 - \frac{2}{\sqrt{5}}\right)m. \end{aligned}$$

Theorem 4. Let $\Gamma = BN_m^n$ be the (m, n) -dimensional bakelite network then the fourth atom-bound connectivity index is given by

$$\begin{aligned}
1. \ ABC_4(\Gamma) &= \frac{1}{42}(4\sqrt{462} + 21\sqrt{10} + 3\sqrt{182} + 21)mn + \frac{1}{42}(14\sqrt{14} \\
&\quad + 14\sqrt{10} - 4\sqrt{462} - 3\sqrt{182} + 42)m + \frac{1}{210}(42\sqrt{35} \\
&\quad + 60\sqrt{14} + 105\sqrt{10} - 20\sqrt{462} - 15\sqrt{182} - 105)n + \frac{1}{210} \\
&\quad (126\sqrt{30} + 30\sqrt{462} + 225\sqrt{182} - 130\sqrt{14} - 266\sqrt{10} - 210) \\
2. \ GA_5(\Gamma) &= \frac{1}{1365}(210\sqrt{42} + 780\sqrt{3} + 728\sqrt{14} + 4095)mn + \frac{1}{1365} \\
&\quad (1820\sqrt{2} + 1560\sqrt{3} - 840\sqrt{42} - 728\sqrt{14} + 2730)m + \frac{1}{4095} \\
&\quad (3640\sqrt{5} + 1365\sqrt{35} - 3780\sqrt{42} - 2340\sqrt{3} - 2184\sqrt{14} \\
&\quad + 12285)n + \frac{1}{30030}(15015\sqrt{15} - 40040\sqrt{2} + 32760\sqrt{30} \\
&\quad - 10010\sqrt{35} + 27720\sqrt{42} - 34320\sqrt{3} - 16016\sqrt{14} - 30030) \\
3. \ S(\Gamma) &= \frac{214377473672}{365525875}mn + \frac{10098826628504}{125375375125}m \\
&\quad - \frac{143170728414141}{501501500500}n - \frac{206059154629631}{1354054051350}
\end{aligned}$$

Proof. In order to prove our theorem, we need edge partition of Γ 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.

$$\begin{aligned}
e_{35}(\Gamma) &= \{uv \in E(\Gamma) \mid (s_v, s_w) = (3, 5)\}, \\
e_{36}(\Gamma) &= \{uv \in E(\Gamma) \mid (s_v, s_w) = (3, 6)\}, \\
e_{45}(\Gamma) &= \{uv \in E(\Gamma) \mid (s_v, s_w) = (4, 5)\}, \\
e_{56}(\Gamma) &= \{uv \in E(\Gamma) \mid (s_v, s_w) = (5, 6)\}, \\
e_{57}(\Gamma) &= \{uv \in E(\Gamma) \mid (s_v, s_w) = (5, 7)\}, \\
e_{66}(\Gamma) &= \{uv \in E(\Gamma) \mid (s_v, s_w) = (6, 6)\}, \\
e_{67}(\Gamma) &= \{uv \in E(\Gamma) \mid (s_v, s_w) = (6, 7)\}, \\
e_{68}(\Gamma) &= \{uv \in E(\Gamma) \mid (s_v, s_w) = (6, 8)\}, \\
e_{78}(\Gamma) &= \{uv \in E(\Gamma) \mid (s_v, s_w) = (7, 8)\},
\end{aligned}$$

such that

$$\begin{aligned}
|e_{35}(\Gamma)| &= 2, |e_{36}(\Gamma)| = 2m - 2, |e_{45}(\Gamma)| = 2n, |e_{56}(\Gamma)| = 6, \\
|e_{57}(\Gamma)| &= 2n - 2, |e_{66}(\Gamma)| = 3mn + 3n + 2m - 10, |e_{67}(\Gamma)| = 4mn - 6n - 4m + 6, \\
|e_{68}(\Gamma)| &= mn - n + 2m - 2, |e_{78}(\Gamma)| = 2mn - 2n - 2m + 2.
\end{aligned}$$

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

$$\begin{aligned}
ABC_4(\Gamma) &= \sum_{uv \in E(\Gamma)} \sqrt{\frac{s_u + s_v - 2}{s_u s_v}} \\
&= 2\sqrt{\frac{6}{15}} + (2m - 2)\sqrt{\frac{7}{18}} + 2n\sqrt{\frac{7}{20}} + 6\sqrt{\frac{9}{30}} + (2n - 2)\sqrt{\frac{10}{35}} \\
&\quad + (3mn + 3n + 2m - 10)\sqrt{\frac{10}{36}} + (4mn - 6n - 4m + 6)\sqrt{\frac{11}{42}} \\
&\quad + (mn - n + 2m - 2)\sqrt{\frac{12}{48}} + 2(mn - n - m + 1)\sqrt{\frac{13}{56}} \\
ABC_4(\Gamma) &= \frac{1}{42}(4\sqrt{462} + 21\sqrt{10} + 3\sqrt{182} + 21)mn + \frac{1}{42}(14\sqrt{14} \\
&\quad + 14\sqrt{10} - 4\sqrt{462} - 3\sqrt{182} + 42)m + \frac{1}{210}(42\sqrt{35} \\
&\quad + 60\sqrt{14} + 105\sqrt{10} - 20\sqrt{462} - 15\sqrt{182} - 105)n + \frac{1}{210} \\
&\quad (126\sqrt{30} + 30\sqrt{462} + 225\sqrt{182} - 130\sqrt{14} - 266\sqrt{10} - 210).
\end{aligned}$$

$$\begin{aligned}
GA_5(\Gamma) &= \sum_{uv \in E(\Gamma)} \frac{2\sqrt{s_u s_v}}{(s_u + s_v)} \\
&= \frac{\sqrt{15}}{2} + \frac{4\sqrt{18}}{9}(m - 1) + \frac{4\sqrt{20}}{9}n + \frac{12\sqrt{30}}{11} + \frac{4\sqrt{35}}{12}(n - 1) \\
&\quad + (3mn + 3n + 2m - 10) + \frac{2\sqrt{42}}{13}(4mn - 6n - 4m + 6) \\
&\quad + \frac{2\sqrt{48}}{14}(mn - n + 2m - 2) + 2(mn - n - m + 1)\frac{2\sqrt{56}}{15} \\
&= \frac{1}{1365}(210\sqrt{42} + 780\sqrt{3} + 728\sqrt{14} + 4095)mn \\
&\quad + \frac{1}{1365}(1820\sqrt{2} + 1560\sqrt{3} - 840\sqrt{42} - 728\sqrt{14} + 2730)m \\
&\quad + \frac{1}{4095}(3640\sqrt{5} + 1365\sqrt{35} - 3780\sqrt{42} - 2340\sqrt{3} - 2184\sqrt{14} \\
&\quad + 12285)n + \frac{1}{30030}(15015\sqrt{15} - 40040\sqrt{2} + 32760\sqrt{30} \\
&\quad - 10010\sqrt{35} + 27720\sqrt{42} - 34320\sqrt{3} - 16016\sqrt{14} - 30030).
\end{aligned}$$

$$\begin{aligned}
S(\Gamma) &= \sum_{vw \in E(\Gamma)} \left(\frac{s_v s_w}{s_v + s_w - 2} \right)^3 \\
&= \frac{125}{4} + \frac{5832}{343}(2m - 2) + \frac{16000}{343}n + \frac{1000}{27} + \frac{343}{8}(2n - 2) \\
&\quad + \frac{5832}{125}(3mn + 3n + 2m - 10) + \frac{74088}{1331}(4mn - 6n - 4m + 6) \\
&\quad + 64(mn - n + 2m - 2) + \frac{175616}{2197}(2mn - 2n - 2m + 2) \\
&= \frac{214377473672}{365525875}mn + \frac{10098826628504}{125375375125}m \\
&\quad - \frac{143170728414141}{501501500500}n - \frac{206059154629631}{1354054051350}.
\end{aligned}$$

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 BN_m^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 polyvinyl 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., Jummannavar 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 Graphs, *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 icosahedral 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 $C_k(C_6)$, *Open J. Math. Sci.*, 2017, 1(1), 44-51.
- [9] Sardar M.S., Pan X.-F., Gao W., Farahani, M.R., Computing Sanskruti 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 Om_n , *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, 1(69), 17-20.
- [19] Deza M., Fowler P.W., Rassat A., Rogers, K.M., Fullerenes 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 π -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., Hosseinzadeh M.A., Computing ABC_4 index of nanostar dendrimers. *Optoelectron, Adv. Mater. Rapid Commun.*, 2010, 4, 1419-1422.
- [27] Graovac A., Ghorbani M., Hosseinzadeh M.A., Computing fifth geometric-arithmetic index for nanostar dendrimers, *J. Math. Nanosci.*, 2011, 1, 33-42.
- [28] Hosamani S.M., Computing Sanskruti 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. Math. Chem.*, 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.