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Comparative Study of Certain Synthetic Polymers via Bond-Additive Invariants

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ABSTRACT Polymers, like vulcanized rubber, bakelite, and poly-methyl methacrylate (PMMA), are widely utilized as denture based materials, and their prominence has been nothing short of excellent. Recently, Ahmad *et al.* [Open Chemistry 17(2019): 663-670] computed bond-additive invariants (BAIs) for the molecular graph of bakelite. In the same paper, they proposed the comparative study of the aforementioned-polymers using BAIs. This paper develops molecular graphs of vulcanized rubber and PMMA to estimate *M-Polynomial* and the generalized Zagreb index. We derive numerous BAIs such as the first and the second Zagreb, Re-defined Zagreb, general Randić, first general Zagreb, and symmetric division degree invariants from the generalized Zagreb index. Moreover, we obtain the modified second Zagreb, inverse Randić, harmonic, inverse sum, and augmented Zagreb invariants from the *M-Polynomials*. Besides, we compute the atom bond connectivity, its fourth version ABC_4, the geometric arithmetic, its fifth version GA_5, and the Sanskruti indices. Finally, we provide insight into the numerical comparison among several BAIs to establish a relation for the underlying polymers' various physicochemical properties.

INDEX TERMS Bond-additive invariants, denture based materials, molecular descriptors, molecular graphs, QSAR/QSPR, synthetic polymers.

I. INTRODUCTION

Polymers (macromolecule) either natural (carbohydrates, proteins, nucleic acids) or synthetic (plastics, elastomers, composites) are crucial for civilized life. Polymers play a vital role in drug delivery and prosthodontic materials, and their prominence has been nothing short of excellent. So, the selection of polymer is of key importance in drug and denture base manufacturing. While selecting polymer care has to be taken regarding its toxicity, drug compatibility, and degradation pattern. The properties of polymeric networks (polymers) rely not only upon the chemical structure but on how the chains of isomers are linked together to develop a network [1]. There are mainly four types of dental materials: metals, polymers, composites, and ceramics. Although complete dentures are formally created with some polymers [2], [3], and expensive metal alloys [4]. However, the advantage of polymeric material over all other materials is due to their cost-effectiveness. The development of polymeric based denture materials, see Figure (1), is the result of the contemporary needs of ideal material and for that matter, the initiation of cutting-edge technologies [5]–[8]. This trend took almost 100 years to reach from vulcanite (vulcanized rubber) to acrylic (poly-methyl methacrylate).

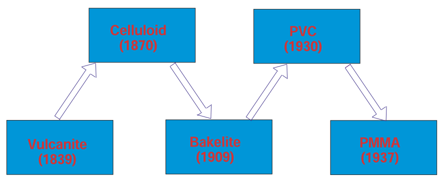

FIGURE 1. **Advancement of polymers as denture base material.**

In the recent past, *graph theory* played a phenomenal role in *mathematical chemistry*, and the resulting field is known as *chemical graph theory* (CGT), which uses graph-theoretic techniques and methods to model and get insights into the properties of a chemical compound. In mathematical chemistry, drugs, polymers, and almost all chemical compounds are often modelled as different ω-cyclic, polygonal structures, bipartite graphs, trees, and nanostructures. In CGT, a topological invariant (TI) is a type of molecular descriptor that is computed from the $2D$ representation (molecular graph) of a molecule. Various types of degree, distance, spectral, and

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counting polynomials based topological invariants of chemical graphs are developed (IUPAC-International Union for Pure and Applied Chemistry) in literature. Numerous studies reveal a correlation between the physicochemical properties such as boiling point, the melting point, similarity, stability, connectivity, and chirality of the chemical compounds and their TIs. TIs, being input in QSAR/QSPR modelling, play a crucial role in developing a better understanding of the complexity of molecules as well as biological, and physicochemical properties of the underlying chemical compound [9]–[16]. Discrete Adriatic indices is a family of 148 BAIs defined by Vukičević [17]. These BAIs were tested on the benchmark datasets provided by the IAMC (International Academy of Mathematical Chemistry), and 20 of them were reported as a significant predictor of physicochemical properties. Among all degree-based TIs, a considerable and most important class of descriptors is bond-additive, i.e., their computation depends upon the sum of edges. Vukičević and Gašperov [18] provide the general expression for bond-additive invariants (BAIs) and is given as:

$$Des(\Gamma) = \sum_{vw\in E(\Gamma)} f(\Gamma, vw) = \theta(d_v, d_w). \tag{1}$$

where $E(\Gamma)$ is the edge set and $\theta : \mathbb{N}\times\mathbb{N} \to \mathbb{R}$ is some function of degrees of vertices.

A *graph* Γ is defined as an ordered pair $(V(\Gamma), E(\Gamma))$ where $V(\Gamma)$ is non-empty set of vertices and $E(\Gamma)$ consists of unordered pairs of distinct elements of $V(\Gamma)$ (connections) called edges. Two vertices u and v belonging to $V(\Gamma)$ are said to be *adjacent* if there is an edge uv between them. Two edges e_1 and e_2 from $E(\Gamma)$ are *incident* if they share a vertex. Moreover, a vertex v and an edge e are incident if v is one of the vertives e connects . The number of adjacent vertices with v, is called *vertex-degree* and is denoted by d_v. The smallest and largest degree of v is denoted by $\delta(v)$ and $\Delta(v)$, respectively. The vertex set and the edge set partition of any graph Γ can generally be defined as:

$$V_d = \{v \in V(\Gamma) \mid d_v = d\}. \tag{2}$$

$$E_{ij}(\Gamma) = \{vw \in E(VR^n_m) \mid (d_v, d_w) = (i, j)\}. \tag{3}$$

Now, we will define some specific and significant BAIs related to our study.

Ivan Gutman and Trinajstić [19] introduced two BAIs called the first and the second Zagreb indices. Soon after, these BAIs were used to study ZE-isomerism, molecular complexity, and the structure-dependency of the total π-electron of molecular graph. First, second, and modified Zagreb indices are defined as follows:

$$M_1(\Gamma) = \sum_{uv\in E(\Gamma)} (d_u + d_v). \tag{4}$$

$$M_2(\Gamma) = \sum_{uv\in E(\Gamma)} (d_u d_v). \tag{5}$$

$$^mM_2(\Gamma) = \sum_{uv\in E(\Gamma)} \frac{1}{(d_u d_v)}. \tag{6}$$

Milan Randić introduced a BAI which is known as Randić index [20]. This index is the most studied vertex degree-based BAI among others [21] and [22]. It is an outstanding BAI in QSPR/QSAR analysis, and suitable for measuring the extent of branching of the carbon atom skeleton of saturated-hydrocarbons. Conventionally the Randić index for a molecular graph Γ is defined as:

$$R(\Gamma) = \sum_{vw\in E(\Gamma)} \frac{1}{\sqrt{d_v d_w}}. \tag{7}$$

Böllöbás and Erdös [23] introduced general Randić index and is defined as:

$$R_\alpha(\Gamma) = \sum_{vw\in E(\Gamma)} \left(d_v d_w\right)^\alpha, \quad \alpha \in \mathbb{R}. \tag{8}$$

In [24], Zhou *et al.* offered an index known as generalized sum-connectivity index which is defined as:

$$\chi_\alpha(\Gamma) = \sum_{vw\in E(\Gamma)} \left(d_v + d_w\right)^\alpha, \quad \alpha \in \mathbb{R}. \tag{9}$$

We get sum-connectivity index (SCI) $\chi_{(\frac{-1}{2})}$ for $\alpha = \frac{-1}{2}$ and "hyper Zagreb index" [25] for $\alpha = 2$. SCI gives high correlation coefficient (0.99) for alkanes.

Li and Zheng [26] instigated the idea of first general Zagrab index and is given by:

$$M_1^\alpha = \sum_{v\in V(\Gamma)} (d_v)^\alpha = \sum_{vw\in E(\Gamma)} \left(d_v^{\alpha-1} + d_w^{\alpha-1}\right). \tag{10}$$

The concept of generalized Zagreb index was established by Azari and Iranmanesh [27] and defined as:

$$Z_{r,s}(\Gamma) = \sum_{vw\in E(\Gamma)} \left(d_v^r d_w^s + d_v^s d_w^r\right), \quad r, s \in Z^+. \tag{11}$$

Estrada *et al.* [28] initiated the famous atom-bond connectivity index $ABC(\Gamma)$ and established its importance during study of thermodynamic properties (stability) of alkanes [29], [30]. Geometric-arithmetic index $GA(\Gamma)$ is an other widely used degree-based BAI offered by Vukičević [31]. The formulas of these indices are given as:

$$ABC(\Gamma) = \sum_{vw\in E(\Gamma)} \sqrt{\frac{d_v + d_w - 2}{d_v d_w}}. \tag{12}$$

$$GA(\Gamma) = \sum_{vw\in E(\Gamma)} \frac{2\sqrt{d_v d_w}}{d_v + d_w}. \tag{13}$$

For the interested reader, we refer survey articles on the Randić index and geometric-arithmetic index of graphs [32] and [33]. The fourth version of atom-bond connectivity index ABC_4 introduced by Ghorbani *et al.* [34], fifth version of geometric-arithmetic index GA_5 introduced by Graovac *et al.* [35] and Sanskruti index proposed by Hosamani [36] are based on sum of degree of vertices at unit distance from the end vertices of each edge. Their formulas are given as:

$$ABC_4(\Gamma) = \sum_{vw \in E(\Gamma)} \sqrt{\frac{S_v + S_w - 2}{S_v S_w}}. \quad (14)$$

$$GA_5(\Gamma) = \sum_{vw \in E(\Gamma)} \frac{2\sqrt{S_v S_w}}{S_v + S_w}. \quad (15)$$

$$SI(\Gamma) = \sum_{vw \in E(\Gamma)} \left(\frac{S_v S_w}{S_v + S_w - 2}\right)^3. \quad (16)$$

Another important BAI of molecular graph is called symmetric division deg index $SDD(\Gamma)$ and is defined as:

$$SDD(\Gamma) = \sum_{vw \in E(\Gamma)} \left(\frac{d_v^2 + d_w^2}{d_v d_w}\right). \quad (17)$$

Few more BAIs of our interest having utmost importance are defined below which include harmonic index (HI), inverse sum index (ISI), and augmented Zagreb index (AZI).

$$HI(\Gamma) = \sum_{vw \in E(\Gamma)} \left(\frac{2}{d_v + d_w}\right). \quad (18)$$

$$ISI(\Gamma) = \sum_{vw \in E(\Gamma)} \left(\frac{d_v d_w}{d_v + d_w}\right). \quad (19)$$

$$AZI(\Gamma) = \sum_{vw \in E(\Gamma)} \left(\frac{d_v d_w}{d_v + d_w - 2}\right)^3. \quad (20)$$

In 2013, Ranjini *et al.*, [37] initiated the concept of first, second, and third Re-defined Zagreb indices and their formulas are as follows:

$$ReZM_1(\Gamma) = \sum_{vw \in E(\Gamma)} \left(\frac{d_v + d_w}{d_v d_w}\right). \quad (21)$$

$$ReZM_2(\Gamma) = \sum_{vw \in E(\Gamma)} \left(\frac{d_v d_w}{d_v + d_w}\right). \quad (22)$$

$$ReZM_3(\Gamma) = \sum_{vw \in E(\Gamma)} (d_v d_w)(d_v + d_w). \quad (23)$$

Clearly, $ReZM_1 = n$ and being constant it does not qualifies the criteria of a TI. Moreover, $ReZM_2$ is identical with previously defined TI called ISI. So, $ReZM_3(\Gamma)$ is the only new TI and we call it Re-defined Zagreb index while using the notation $ReZM(\Gamma)$.

In the Table (1), we sum up the relation of GZI with certain well known BAIs.

Deutsch and Klavžar [38] introduced *M-polynomial* for graph $\Gamma = (V, E)$ as follows:

$$M(\Gamma; x, y) = f(x, y) = \sum_{i \leq j} m_{ij}(\Gamma) x^i y^j. \quad (24)$$

where $m_{ij}(\Gamma)$ represent number of edges $vw \in E(\Gamma)$ such that $\{d_v, d_w\} = \{i, j\}$.

Some promising topological indices are worked out with the help of *M-polynomial* and are depicted in the Table (2).

TABLE 1. Some special cases of generalized-Zagreb index.

Topological index	Corresponding (r, s)-Zagreb index
First Zagreb Index $M_1(\Gamma)$	$Z_{1,0}$
Second Zagreb Index $M_2(\Gamma)$	$\frac{1}{2}Z_{1,1}$
Forgotten Topological Index F(Γ)	$Z_{2,0}$
Re-defined Zagreb Index ReZM(Γ)	$Z_{2,1}$
General first Zagreb Index $M^{\alpha}(\Gamma)$	$Z_{\alpha-1,0}$
General Randić index $R_{\alpha}(\Gamma)$	$\frac{1}{2}Z_{\alpha,\alpha}$
Symmetric division deg index SDD(Γ)	$Z_{1,-1}$

TABLE 2. Formulae of certain essential topological descriptors in relation with *M*-polynomial.

Topological indices	**Formulae derived from M-polynomial**
1st Zagreb index (M_1)	$(D_x + D_y)M(x, y)$
2nd Zagreb index (M_2)	$(D_x.D_y)M(x, y)$
Modified 2nd Zagreb index $(^m M_2)$	$(S_x.S_y)M(x, y)$
General Randić index R_{α}	$D_x^{\alpha}.D_y^{\alpha}M(x, y)$
Inverse Randić index RR_{α}	$S_x^{\alpha}.S_y^{\alpha}M(x, y)$
Symmetric Division Deg Index (SDD)	$(D_x S_y + S_x D_y)M(x, y)$
Harmonic Index (HI)	$2S_x J M(x, y)$
Inverse sum Index (ISI)	$S_x J D_x D_y M(x, y)$
Augmented Zagreb Index (AZI)	$S_x^3 Q_{-2} J D_x^3 D_y^3 M(x, y)$

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

Note: all formulae in Table (2) will be evaluated at $x = y = 1$.

Around 1947, theoretical chemists conceived that TIs obtained from the molecular graph encode information and properties of chemical compounds. Camarda and Maranas [39] employed connectivity indices to design and produce the polymers related to some optimal property. We know that dendrimers are considered the "polymers of the 21st century" and their popularity increased considerably, which was revealed through the scientific publications and patents registered. Wang *et al.* [40], presented the explicit formula of the k-connectivity index for the class of polymeric networks, namely, dendrimer and nanostars. Ali *et al.* [41] computed general formulae of certain degree-based TIs for some conjugated polymers (polyphenylene dendrimer nanostars). Kang *et al.*, Gao *et al.*, and Liu *et al.* [42]–[44] investigated topological properties of 2-D Silicon-Carbons, certain dendrimers, and nanotubes, respectively. Shao *et al.* [45] characterized the chemically oriented graphs with a maximum value of ABC index. Gao *et al.* [46] computed the entropy and enthalpy per unit cell for two types of copper oxides and compared them with ABC and Sanskruti indices. Several mathematical, theoretical, and chemical aspects of diverse TIs for molecular graphs of various chemical structures have been carried out in [47]–[54]. We intend to develop molecular graphs of three pertinent polymers, commonly known as vulcanized rubber, bakelite, and poly-methyl methacrylate (PMMA), to estimate several BAIs to examine their structural properties.

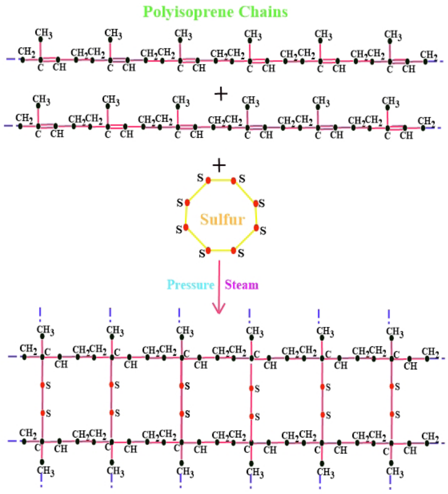

FIGURE 2. Vulcanization of natural rubber.

II. VULCANIZED RUBBER NETWORK

Vulcanite (vulcanized rubbers) is produced by the addition reaction of polyisoprene (natural rubber) with sulfur under steam pressure. The quantity of sulfur alters the hardness of vulcanite by forming cross-links between the polyisoprene chains to form a stiff, thick, and durable solid [55]. Vulcanized rubbers manifest superior physicochemical properties as compared to the natural rubbers. Vulcanite, introduced by Charles Goodyear in 1839, was a pioneer polymer and established to be a successful denture base material for almost 30 years. The vulcanite was acclaimed widely due to its accurate fitting, and affordable cost [56]. Figure (2) illustrates the vulcanization process during which polyisoprene chains ($[C_5H_8]_n$) crosslinked with disulfide atoms [3]. Figure (3) represents the (m, n) dimensional molecular graph of vulcanite, where m is the number of rows having n dodecagons in each row and is denoted by VR_m^n.

A. RESULTS FOR VULCANIZED RUBBER NETWORK VR_m^n

The subsequent lemma exhibit some basic attributes of vulcanized rubber network VR_m^n that are essential rather of key importance for forthcoming results.

Lemma 1: Let VR_m^n be the vulcanized rubber network illustrated in Figure (3) ((m,n)-dimensional molecular graph) then total number of vertices and edges are $8mn+8m+6n+6$ and $10mn + 9m + 6n + 5$, respectively.

Proof: We use the vertex set and edge set partition given by Equations (2) and (3) for molecular graph VR_m^n. Now by inspecting molecular graph VR_m^n, it can easily be observed that there are four type of vertices having valencies 1, 2, 3, and 4 i.e., $\delta(VR_m^n) = 1$ and $\Delta(VR_m^n) = 4$. Now using simple counting technique, we obtain the vertex partition and is given as follows. $|V_1| = 2m + 2n + 4$, $|V_2| = 6mn + 4m + 2n$, $|V_3| = 2n + 2$, $|V_4| = 2mn + 2m$. Consequently, total number of vertices of VR_m^n, denoted by $|V(VR_m^n)| = 8mn + 8m + 6n + 6$.

Likewise, we recognize seven types of edges in VR_m^n relying upon valencies of end vertices of each edge. We employ combinatorial counting technique on network to achieve edge partitioning as $|E_{13}| = 2$, $|E_{14}| = 2m + 2n + 2$, $|E_{22}| = 3mn+2m+2n$, $|E_{23}| = 4n+2$, $|E_{24}| = 6mn+4m-2n-2$, $|E_{34}| = 2n + 2$, $|E_{44}| = mn + m - n - 1$. As a result, total number of edges of vulcanized rubber network, denoted by $|E(VR_m^n)| = 10mn + 9m + 6n + 5$. For the sake of simplicity and further use, edge partition is illustrated in the Table (3).

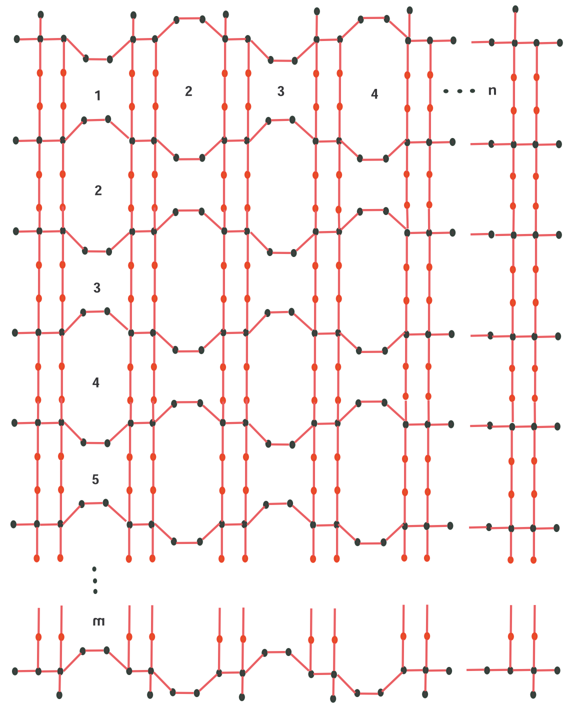

FIGURE 3. Hydrogen depleted molecular graph of VR_m^n.

TABLE 3. Edge partitioning on the basis of end vertex degrees of VR_m^n.

(d_u, d_v)	Number of edges
$(1,3)$	2
$(1,4)$	$2m+2n+2$
$(2,2)$	$3mn+2m+2n$
$(2,3)$	$4n+2$
$(2,4)$	$6mn+4m-2n-2$
$(3,4)$	$2n+2$
$(4,4)$	$mn+m-n-1$

Theorem 1: Let VR_m^n be a (m, n)-dimensional vulcanized rubber network, then the generalized-Zagreb index $Z_{r,s}(VR_m^n)$ is given by the formula:

$$\begin{aligned} Z_{r,s}(VR_m^n) &= (3 + 3 \times 2^s + 3 \times 2^r + 2^{r+s})2^{r+s+1}mn \\ &\quad +\big(2^{2s} + 2^{2r} + 2^{r+s+1} + 2^{2s+r+1} + 2^{2r+s+1} \\ &\quad +2^{2(r+s)}\big)2m + \big(2^{2s}(1 - 2^r + 3^r) \\ &\quad +2^{2r}(1 - 2^s + 3^s) + 2^{r+s}(2 - 2^{r+s}) \\ &\quad +2^{r+1}3^s + 2^{s+1}3^r\big)2n + 2\big(3^s(1 + 2^r + 2^{2r}) \\ &\quad +3^r(1 + 2^s + 2^{2s}) + 2^{2s}(1 - 2^r) \\ &\quad +2^{2r}(1 - 2^s - 2^{2s})\big). \end{aligned}$$

Proof: Using Table (3) and the formula given in Equation (11), we compute the required result as follows:

$$
\begin{aligned}
Z_{r,s}(VR_m^n) &= \sum_{vw\in E(VR_m^n)} (d_v^r d_w^s + d_w^r d_v^s)\\
&= \sum_{vw\in E_{13}} (d_v^r d_w^s + d_w^r d_v^s) + \sum_{vw\in E_{14}} (d_v^r d_w^s + d_w^r d_v^s)\\
&\quad + \sum_{vw\in E_{22}} (d_v^r d_w^s + d_w^r d_v^s) + \sum_{vw\in E_{23}} (d_v^r d_w^s + d_w^r d_v^s)\\
&\quad + \sum_{vw\in E_{24}} (d_v^r d_w^s + d_w^r d_v^s) + \sum_{vw\in E_{34}} (d_v^r d_w^s + d_w^r d_v^s)\\
&\quad + \sum_{vw\in E_{44}} (d_v^r d_w^s + d_w^r d_v^s)\\
&= 2(1^r3^s + 3^r1^s) + (2m+2n+2)(1^r4^s + 4^r1^s)\\
&\quad + (3mn+2m+2n)(2^r2^s + 2^r2^s)\\
&\quad + (4n+2)(2^r3^s + 3^r2^s)\\
&\quad + (6mn+4m-2n-2)(2^r4^s + 4^r2^s)\\
&\quad + (mn+m-n-1)(4^r4^s + 4^r4^s)\\
&\quad + (2n+2)(3^r4^s + 4^r3^s)\\
&= \big(3\times 2^{r+s+1} + 3\times 2^{2s+r+1} + 3\times 2^{2r+s+1}\\
&\quad + 2^{2r+2s+1}\big)mn + \big(2^{2s+1} + 2^{2r+1} + 2^{r+s+2}\\
&\quad + 2^{2s+r+2} + 2^{2r+s+2} + 2^{2r+2s+1}\big)m + \big(2^{2s+1}\\
&\quad + 2^{2r+1} + 2^{r+s+2} + 3^s2^{r+2} + 3^r2^{s+2} - 2^{2s+r+1}\\
&\quad - 2^{2r+s+1} + 3^r2^{2s+1} + 3^s2^{2r+1} - 2^{2r+2s+1}\big)n\\
&\quad + \big(2\times 3^s + 2\times 3^r + 2^{2s+1} + 2^{2r+1} + 2^{r+1}3^s\\
&\quad + 3^r2^{s+1} - 2^{2s+r+1} - 2^{2r+s+1} + 3^r2^{2s+1}\\
&\quad + 3^s2^{2r+1} - 2^{2r+2s+1}\big)\\
&= (3 + 3\times 2^s + 3\times 2^r + 2^{r+s})2^{r+s+1}mn\\
&\quad + \big(2^{2s} + 2^{2r} + 2^{r+s+1} + 2^{2s+r+1} + 2^{2r+s+1}\\
&\quad + 2^{2(r+s)}\big)2m + \big(2^{2s}(1 - 2^r + 3^r)\\
&\quad + 2^{2r}(1 - 2^s + 3^s) + 2^{r+s}(2 - 2^{r+s})\\
&\quad + 2^{r+1}3^s + 2^{s+1}3^r\big)2n + 2\big(3^s(1 + 2^r + 2^{2r})\\
&\quad + 3^r(1 + 2^s + 2^{2s}) + 2^{2s}(1 - 2^r)\\
&\quad + 2^{2r}(1 - 2^s - 2^{2s})\big). \qquad (25)
\end{aligned}
$$

Corollary 1: Using Equation (25) of generalized Zagreb index for VR_m^n and formulae presented in the Table (1), we derived following BAIs as below:

$$
\begin{aligned}
M_1(VR_m^n) &= Z_{1,0}(VR_m^n) = 56mn + 50m + 32n + 22.\\
M_2(VR_m^n) &= \frac{1}{2}Z_{1,1}(VR_m^n) = 76mn + 64m + 32n + 18.\\
F(VR_m^n) &= Z_{2,0}(VR_m^n) = 176mn + 162m + 80n + 58.\\
ReZM(VR_m^n) &= Z_{2,1}(VR_m^n) = 464mn + 392m + 136n + 68.\\
M^\alpha(VR_m^n) &= Z_{\alpha-1,0}(VR_m^n) = (3\times 2^{\alpha+1} + 4\times 2^{2\alpha-1})mn\\
&\quad + (2 + 2^{2\alpha+1} + 2^{2\alpha+2})m\\
&\quad + (2^{2\alpha+2} + 2^{\alpha+2}3^\alpha(1 + 2^{\alpha-1}) - 2^{4\alpha})n\\
&\quad + (2^{2\alpha}(2 - 2^{\alpha+1} - 2^{2\alpha})\\
&\quad + 3^\alpha(2 + 2^{\alpha+1} + 2^{2\alpha+1})).\\
SDD(VR_m^n) &= Z_{1,-1}(VR_m^n) = 23mn + \frac{49}{2}m + \frac{55}{3}n + \frac{50}{3}.
\end{aligned}
$$

Theorem 2: Let VR_m^n be a (m,n)-dimensional vulcanized rubber network, then $ABC(VR_m^n)$ and $GA(VR_m^n)$ are given as:

$$
\begin{aligned}
ABC(VR_m^n) &= \big(6\sqrt{2} + 12\sqrt{2} + \sqrt{6}\big)\frac{mn}{4}\\
&\quad + \big(\sqrt{3} + 3\sqrt{2} + \frac{\sqrt{6}}{4}\big)m\\
&\quad + \big(\sqrt{3} + 2\sqrt{2} + \sqrt{\frac{6}{4}} - \frac{\sqrt{6}}{4}\big)n\\
&\quad + \big(\frac{2\sqrt{2}}{3} + \sqrt{3} + \sqrt{\frac{5}{3}} - \frac{\sqrt{6}}{8}\big).\\
GA(VR_m^n) &= \big(3 + 4\sqrt{2} + \frac{6\sqrt{3}}{7}\big)mn + \big(\frac{23}{5} + \frac{8\sqrt{2}}{3}\big)m\\
&\quad + \big(\frac{13}{5} + \frac{8\sqrt{6}}{5} - \frac{4\sqrt{2}}{3} + \frac{12\sqrt{3}}{7}\big)n\\
&\quad + \big(\frac{3}{5} + \frac{4\sqrt{6}}{5} - \frac{4\sqrt{2}}{3} + \frac{19\sqrt{3}}{7}\big).\\
\chi_{\frac{-1}{2}}(VR_m^n) &= \big(4\sqrt{6} + \sqrt{2} + 6\big)\frac{mn}{4} + \big(24\sqrt{5} + 40\sqrt{6}\\
&\quad + 15\sqrt{2} + 60\big)\frac{m}{60} + \big(504\sqrt{5} - 140\sqrt{6}\\
&\quad + 120\sqrt{7} - 105\sqrt{2} + 420\big)\frac{n}{420} + \big(336\sqrt{5}\\
&\quad - 140\sqrt{6} + 120\sqrt{7} - 105\sqrt{2} + 420\big)\frac{1}{420}.
\end{aligned}
$$

Proof: Using Table (3) and the formulae defined by Equations (12), (13), and (16), respectively. We compute the required result as follows:

$$
\begin{aligned}
&ABC(VR_m^n)\\
&= \sum_{vw\in E(VR_m^n)} \sqrt{\frac{d_v + d_w - 2}{d_v d_w}}\\
&= \sum_{vw\in E_{13}} \sqrt{\frac{d_v + d_w - 2}{d_v d_w}} + \sum_{vw\in E_{14}} \sqrt{\frac{d_v + d_w - 2}{d_v d_w}}\\
&\quad + \sum_{vw\in E_{22}} \sqrt{\frac{d_v + d_w - 2}{d_v d_w}} + \sum_{vw\in E_{23}} \sqrt{\frac{d_v + d_w - 2}{d_v d_w}}\\
&\quad + \sum_{vw\in E_{24}} \sqrt{\frac{d_v + d_w - 2}{d_v d_w}} + \sum_{vw\in E_{34}} \sqrt{\frac{d_v + d_w - 2}{d_v d_w}}\\
&\quad + \sum_{vw\in E_{44}} \sqrt{\frac{d_v + d_w - 2}{d_v d_w}}\\
&= 2\sqrt{\frac{2}{3}} + (2m+2n+2)\sqrt{\frac{3}{4}} + (4n+2)\sqrt{\frac{3}{6}}\\
&\quad + (3mn+2m+2n)\sqrt{\frac{2}{4}} + (6mn+4m-2n-2)\sqrt{\frac{4}{8}}\\
&\quad + (2n+2)\sqrt{\frac{5}{12}} + (mn+m-n-1)\sqrt{\frac{2}{4}}
\end{aligned}
$$

$$= (6\sqrt{2}+12\sqrt{2}+\sqrt{6})\frac{mn}{4}+(\sqrt{3}+3\sqrt{2}+\frac{\sqrt{6}}{4})m + (\sqrt{3}+2\sqrt{2}+\sqrt{\frac{6}{4}}-\frac{\sqrt{6}}{4})n+(\frac{2\sqrt{2}}{3}+\sqrt{3}+\sqrt{\frac{5}{3}}-\frac{\sqrt{6}}{8}).$$

$GA(VR_m^n)$

$$= \sum_{vw\in E(VR_m^n)}\frac{2\sqrt{d_vd_w}}{d_v+d_w} = \sum_{vw\in E_{13}}\frac{2\sqrt{d_vd_w}}{d_v+d_w} + \sum_{vw\in E_{14}}\frac{2\sqrt{d_vd_w}}{d_v+d_w} + \sum_{vw\in E_{22}}\frac{2\sqrt{d_vd_w}}{d_v+d_w} + \sum_{vw\in E_{23}}\frac{2\sqrt{d_vd_w}}{d_v+d_w} + \sum_{vw\in E_{24}}\frac{2\sqrt{d_vd_w}}{d_v+d_w} + \sum_{vw\in E_{34}}\frac{2\sqrt{d_vd_w}}{d_v+d_w} + \sum_{vw\in E_{44}}\frac{2\sqrt{d_vd_w}}{d_v+d_w}$$

$$= 2(\frac{2\sqrt{3}}{4})+(2m+2n+2)(\frac{2\sqrt{4}}{5}) + (3mn+2m+2n)(\frac{2\sqrt{4}}{4})+(4n+2)(\frac{2\sqrt{6}}{5}) + (6mn+4m-2n-2)(\frac{2\sqrt{8}}{6}) + (2n+2)(\frac{2\sqrt{12}}{7})+(mn+m-n-1)(\frac{2\sqrt{4}}{5})$$

$$= (3+4\sqrt{2}+\frac{6\sqrt{3}}{7})mn + (\frac{23}{5}+\frac{8\sqrt{2}}{3})m+(\frac{13}{5}+\frac{8\sqrt{6}}{5}-\frac{4\sqrt{2}}{3} + \frac{12\sqrt{3}}{7})n+(\frac{3}{5}+\frac{4\sqrt{6}}{5}-\frac{4\sqrt{2}}{3}+\frac{19\sqrt{3}}{7}).$$

$\chi_{\frac{-1}{2}}(VR_m^n)$

$$= \sum_{vw\in E(VR_m^n)}\frac{1}{\sqrt{d_v+d_w}} = \sum_{vw\in E_{13}}\frac{1}{\sqrt{d_v+d_w}}+\sum_{vw\in E_{14}}\frac{1}{\sqrt{d_v+d_w}} + \sum_{vw\in E_{22}}\frac{1}{\sqrt{d_v+d_w}}+\sum_{vw\in E_{23}}\frac{1}{\sqrt{d_v+d_w}} + \sum_{vw\in E_{24}}\frac{1}{\sqrt{d_v+d_w}}+\sum_{vw\in E_{34}}\frac{1}{\sqrt{d_v+d_w}} + \sum_{vw\in E_{44}}\frac{1}{\sqrt{d_v+d_w}}$$

$$= 2\frac{1}{\sqrt{4}}+(2m+2n+2)\frac{1}{\sqrt{5}} + (3mn+2m+2n)\frac{1}{\sqrt{4}}+(4n+2)\frac{1}{\sqrt{5}} + (6mn+4m-2n-2)\frac{1}{\sqrt{6}}+(2n+2)\frac{1}{\sqrt{7}} + (mn+m-n-1)\frac{1}{\sqrt{8}}$$

$$= (4\sqrt{6}+\sqrt{2}+6)\frac{mn}{4} + (24\sqrt{5}+40\sqrt{6}+15\sqrt{2}+60)\frac{m}{60} + (504\sqrt{5}-140\sqrt{6}+120\sqrt{7}-105\sqrt{2} + 420)\frac{n}{420}+(336\sqrt{5}-140\sqrt{6} + 120\sqrt{7}-105\sqrt{2}+420)\frac{1}{420}.$$

Theorem 3: Let VR_m^n be the vulcanized rubber network, then *M-polynomial* of VR_m^n is given by:
$M(VR_m^n;x,y) = 2xy^3+(2m+2n+2)xy^4+(3mn+2m+2n)x^2y^2+(4n+2)x^2y^3+(6mn+4m-2n-2)x^2y^4+(2n+2)x^3y^4+(mn+m-n-1)x^4y^4$.

Proof: Degree-based edge partitioning of VR_m^n is given as $E_{ij}(VR_m^n) = \{vw \in E(VR_m^n) : d_v = i, d_w = j\}$,
$|E_{13}| = 2$, $|E_{14}| = (2m+2n+2)$, $|E_{22}| = (3mn+2m+2n)$, $|E_{23}| = (4n+2)$, $|E_{24}| = (6mn+4m-2n-2)$, $|E_{34}| = (2n+2)$, $|E_{44}| = (mn+m-n-1)$.
Using formula of *M-Polynomial* defined by Equation (24), we have

$$M(VR_m^n;x,y) = \sum_{i\le j} m_{ij}x^iy^j = \sum_{1\le 3} m_{13}xy^3 + \sum_{1\le 4} m_{14}xy^4 + \sum_{2\le 2} m_{22}x^2y^2 + \sum_{2\le 3} m_{23}x^2y^3 + \sum_{2\le 4} m_{24}x^2y^4 + \sum_{3\le 4} m_{34}x^3y^4 + \sum_{4\le 4} m_{44}x^4y^4$$

$$= |E_{13}|xy^3+|E_{14}|xy^4+|E_{22}|x^2y^2+|E_{23}|x^2y^3 + |E_{24}|x^2y^4+|E_{34}|x^3y^4+|E_{44}|x^4y^4$$

$$= 2xy^3+(2m+2n+2)xy^4 + (3mn+2m+2n)x^2y^2+(4n+2)x^2y^3 + (6mn+4m-2n-2)x^2y^4 + (2n+2)x^3y^4+(mn+m-n-1)x^4y^4.$$

Theorem 4: For vulcanize rubber network VR_m^n, modified Zagreb index, inverse Randić index, harmonic index, inverse sum index and augmented Zagreb index are:

1) ${}^mM_2(VR_m^n) = \frac{25}{16}m(n+1)+\frac{73}{48}n+\frac{65}{48}$.
2) $RR_\alpha(VR_m^n) = (3\times 2^{2\alpha}+3\times 2^{\alpha+1}+1)\frac{mn}{16^\alpha} +(2^{2\alpha+2}+2^{\alpha+2}+1)\frac{m}{16^\alpha}+(4\times 12^\alpha +4\times 8^\alpha-2\times 6^\alpha+2^{2\alpha-1}-1)\frac{n}{48^\alpha} +(2^{4\alpha+1}+2\times 12^\alpha+2^{3\alpha+1}+2\times 6^\alpha +2^{2\alpha+1}-1)\frac{1}{48^\alpha}$.
3) $HI(VR_m^n) = \frac{15}{4}mn+\frac{203}{60}m+\frac{1283}{420}n+\frac{1367}{420}$.
4) $ISI(VR_m^n) = 13mn+\frac{164}{15}m+\frac{794}{105}n+\frac{179}{42}$.
5) $AZI(VR_m^n) = \frac{2456}{27}mn+\frac{1936}{27}m+\frac{217312}{3375}n+\frac{90791}{4500}$.

Proof: From Theorem 3, we have
$M(VR_m^n;x,y) = 2xy^3+(2m+2n+2)xy^4+(3mn+2m+2n)x^2y^2+(4n+2)x^2y^3+(6mn+4m-2n-2)x^2y^4+(2n+2)x^3y^4+(mn+m-n-1)x^4y^4$.

Now applying specific operators presented in Table (2) on *M-Polynomial*, we get

$$(s_xs_y)M = \frac{2}{3}xy^3 + \frac{1}{2}(m+n+1)xy^4 + \frac{1}{4}(3mn+2m+2n)x^2y^2 + \frac{1}{3}(2n+1)x^2y^3 + \frac{1}{4}(3mn+2m-n-1)x^2y^4 + \frac{1}{6}(n+1)x^3y^4 + \frac{1}{16}(mn+m-n-1)x^4y^4.$$

$$(s_x^\alpha s_y^\alpha)M = \frac{2}{3^\alpha}xy^3 + \frac{2}{4^\alpha}(m+n+1)xy^4 + \frac{1}{4^\alpha}(3mn+2m+2n)x^2y^2 + \frac{2}{6^\alpha}(2n+1)x^2y^3 + \frac{2}{8^\alpha}(3mn+2m-n-1)x^2y^4 + \frac{2}{12^\alpha}(n+1)x^3y^4 + \frac{1}{16^\alpha}(mn+m-n-1)x^4y^4.$$

$$JM(x,y) = M(x) = (3mn+2m+2n+2)x^4 + (2m+6n+4)x^5 + (6mn+4m-2n-2)x^6 + (2n+2)x^7 + (mn+m-n-1)x^8.$$

$$s_xJM(x) = \frac{(3mn+2m+2n+2)}{4}x^4 + \frac{(2m+6n+4)}{5}x^5 + \frac{(6mn+4m-2n-2)}{6}x^6 + \frac{(2n+2)}{7}x^7 + \frac{(mn+m-n-1)}{8}x^8.$$

$$s_xJD_xD_yM = (3mn+2m+2n+\frac{3}{2})x^4 + (8m+32n+14)x^5 + \frac{4}{3}(6mn+4m-2n-2)x^6 + \frac{12}{7}(2n+2)x^7 + 2(mn+m-n-1)x^8.$$

$$s_x^3Q_{-2}JD_x^3D_y^3M = (24mn+16m+16n+\frac{27}{4})x^2 + \frac{1}{27}(128m+992n+560)x^3 + (48mn+32m-16n-16)x^4 + \frac{512}{27}(mn+m-n-1)x^6 + \frac{1728}{125}(2n+2)x^5.$$

By employing formulae of desired BAIs presented in Table (2) over expression derived from *M-Polynomial*, we get our results:

1. $^mM_2(VR_m^n) = s_xs_yM|_{x=y=1} = \frac{25}{16}m(n+1) + \frac{73}{48}n + \frac{65}{48}.$
2. $RR_\alpha(VR_m^n) = (s_x^\alpha s_y^\alpha)(M(x,y))|_{x=y=1}$

$$= (3\times 2^{2\alpha} + 3\times 2^{\alpha+1} + 1)\frac{mn}{16^\alpha} + (2^{2\alpha+2} + 2^{\alpha+2} + 1)\frac{m}{16^\alpha} + (4\times 12^\alpha + 4\times 8^\alpha - 2\times 6^\alpha + 2^{2\alpha-1} - 1)\frac{n}{48^\alpha} + (2^{4\alpha+1} + 2\times 12^\alpha + 2^{3\alpha+1} + 2\times 6^\alpha + 2^{2\alpha+1} - 1)\frac{1}{48^\alpha}.$$

3. $HI(VR_m^n) = 2s_xJM(x)|_{x=1} = \frac{15}{4}mn + \frac{203}{60}m + \frac{1283}{420}n + \frac{1367}{420}.$
4. $ISI(VR_m^n) = s_xJD_xD_yM|_{x=1} = 13mn + \frac{164}{15}m + \frac{794}{105}n + \frac{179}{42}.$
5. $AZI(VR_m^n) = s_x^3Q_{-2}JD_x^3D_y^3M|_{x=1} == \frac{2456}{27}mn + \frac{1936}{27}m + \frac{217312}{3375}n + \frac{90791}{4500}.$

TABLE 4. Edge partitioning based upon neighbor's degree sum of VR_m^n.

(s_v, s_w) : $vw \in E(VR_m^n)$	No. of edges $=\|E_{(i,j)}\|$	(s_v, s_w) : $vw \in E(VR_m^n)$	No. of edges $=\|E_{(i,j)}\|$
(3, 7)	2	(6, 8)	$4n$
(4, 7)	4	(6, 9)	$4m-4$
(4, 8)	$2m-2$	(6, 10)	$6mn-6n$
(5, 6)	$4n+2$	(7, 8)	4
(5, 7)	2	(8, 8)	$2n-2$
(5, 8)	$2n$	(9, 10)	$2m-2$
(6, 6)	$3mn+2m$ $n-2$	(10, 10)	$mn-m$ $-n+1$
(6, 7)	2		

To compute the fourth version of atom-bond connectivity index $ABC_4(VR_m^n)$, Sanskruti index $SI(VR_m^n)$ and the fifth version of geometric-arithmetic index $GA_5(VR_m^n)$, we require the degree sum of vertices at unit distance from end vertices of each edge in vulcanize rubber network. In this scenario, we recognize fifteen types of distinct edges in vulcanize rubber network. By using simple combinatorial counting strategy the partition of the edge set $E(VR_m^n)$, on the basis of neighbor's degree sum, into subsets $E_{(i,j)}(VR_m^n)$, where (i,j) represent edge $vw \in E(VR_m^n)$ such that $(d_v, d_w) = (i,j)$ and is summarized in Table (4).

Theorem 5: Let VR_m^n be vulcanize rubber network, then the fourth version of atom-bond connectivity index ABC_4, the fifth version of geometric arithmetic index GA_5, and the Sanskruti index SI of VR_m^n are given as:

(1) $ABC_4(VR_m^n)$

$$= (5\sqrt{10} + 2\sqrt{210} + 3\sqrt{2})\frac{mn}{10} + (45\sqrt{5} + 30\sqrt{10} + 20\sqrt{78} + 6\sqrt{170} - 27\sqrt{2})\frac{m}{90} + (24\sqrt{30} + 10\sqrt{10} + 6\sqrt{110} - 12\sqrt{210} + 15\sqrt{14} - 18\sqrt{2} + 120)\frac{n}{60} + (2520 - 420\sqrt{10} + 45\sqrt{14} - 84\sqrt{170} + 180\sqrt{182} + 378\sqrt{2} + 252\sqrt{30} + 240\sqrt{42} + 60\sqrt{462} - 630\sqrt{5} + 1080\sqrt{7} - 280\sqrt{78})\frac{1}{1260}.$$

(2) $GA_5(VR_m^n)$

$$= (8+3\sqrt{15})\frac{mn}{2} + (285+380\sqrt{2} + 456\sqrt{6} - 180\sqrt{10})\frac{m}{285} + (4004+1456\sqrt{30} + 1232\sqrt{10} + 4576\sqrt{10} - 3003\sqrt{15})\frac{n}{2002} + (13585\sqrt{13} - 54340\sqrt{2} + 16302\sqrt{21} - 65208\sqrt{6} + 59280\sqrt{7} + 14820\sqrt{30} + 12540\sqrt{42} + 43472\sqrt{14} - 25740\sqrt{10} - 122265)\frac{1}{40755}.$$

(3) $SI(VR_m^n)$

$$= (\frac{24496447312}{31255875})mn + (\frac{561466008516664}{983590583625})m + (\frac{3921718689424}{41601569625})n - (\frac{551233094322072507949}{383182131126674880000}).$$

Proof: Using formula given by Equation (14) and edge partition presented in the Table (4), we proceed as follows:

(1) $ABC_4(VR_m^n)$

$$= \sum_{vw\in E(VR_m^n)} \sqrt{\frac{s_v+s_w-2}{s_vs_w}}$$

$$= |E_{(3,7)}|\sqrt{\frac{8}{21}} + |E_{(4,7)}|\sqrt{\frac{9}{28}} + |E_{(4,8)}|\sqrt{\frac{10}{32}} + |E_{(5,6)}|\sqrt{\frac{9}{30}} + |E_{(5,7)}|\sqrt{\frac{10}{35}} + |E_{(5,8)}|\sqrt{\frac{11}{40}} + |E_{(6,6)}|\sqrt{\frac{10}{36}} + |E_{(6,7)}|\sqrt{\frac{11}{42}} + |E_{(6,8)}|\sqrt{\frac{12}{48}} + |E_{(6,9)}|\sqrt{\frac{13}{54}} + |E_{(6,10)}|\sqrt{\frac{14}{60}} + |E_{(7,8)}|\sqrt{\frac{13}{56}} + |E_{(8,8)}|\sqrt{\frac{14}{64}} + |E_{(9,10)}|\sqrt{\frac{17}{90}} + |E_{(10,10)}|\sqrt{\frac{18}{100}}$$

$$= 2\sqrt{\frac{8}{21}} + 4\sqrt{\frac{9}{28}} + (2m-2)\sqrt{\frac{10}{32}} + (4n+2)\sqrt{\frac{9}{30}} + 2\sqrt{\frac{10}{35}} + 2n\sqrt{\frac{11}{40}} + (3mn+2m+n-2)\sqrt{\frac{10}{36}} + 2\sqrt{\frac{11}{42}} + (4n)\sqrt{\frac{12}{48}} + (4m-4)\sqrt{\frac{13}{54}} + 4\sqrt{\frac{13}{56}} + (6mn-6n)\sqrt{\frac{14}{60}} + (2n-2)\sqrt{\frac{14}{64}} + (2m-2)\sqrt{\frac{17}{90}} + (mn-m-n+1)\sqrt{\frac{18}{100}}$$

$$= (5\sqrt{10}+2\sqrt{210}+3\sqrt{2})\frac{mn}{10} + (45\sqrt{5}+30\sqrt{10}+20\sqrt{78}+6\sqrt{170}-27\sqrt{2})\frac{m}{90} + (24\sqrt{30}+10\sqrt{10}+6\sqrt{110}-12\sqrt{210}+15\sqrt{14} - 18\sqrt{2}+120)\frac{n}{60} + (2520-420\sqrt{10}+45\sqrt{14} - 84\sqrt{170}+180\sqrt{182}+378\sqrt{2}+252\sqrt{30}+240\sqrt{42} + 60\sqrt{462}-630\sqrt{5}+1080\sqrt{7}-280\sqrt{78})\frac{1}{1260}.$$

Employing formula given by Equation (15) and edge partition presented in the Table (4), we compute result in following manner

(2) $GA_5(VR_m^n)$

$$= \sum_{vw\in E(VR_m^n)} \frac{2\sqrt{s_vs_w}}{s_v+s_w}$$

$$= |E_{(3,7)}|(\frac{2\sqrt{21}}{10}) + |E_{(4,7)}|(\frac{2\sqrt{28}}{11}) + |E_{(4,8)}|(\frac{2\sqrt{32}}{12}) + |E_{(5,6)}|(\frac{2\sqrt{30}}{11}) + |E_{(5,7)}|(\frac{2\sqrt{35}}{12}) + |E_{(5,8)}|(\frac{2\sqrt{40}}{13}) + |E_{(6,6)}|(\frac{2\sqrt{36}}{12}) + |E_{(6,7)}|(\frac{2\sqrt{42}}{13}) + |E_{(6,8)}|(\frac{2\sqrt{48}}{14}) + |E_{(6,9)}|(\frac{2\sqrt{54}}{15}) + |E_{(6,10)}|(\frac{2\sqrt{60}}{16}) + |E_{(7,8)}|(\frac{2\sqrt{56}}{15}) + |E_{(8,8)}|(\frac{2\sqrt{64}}{16}) + |E_{(9,10)}|(\frac{2\sqrt{90}}{19}) + |E_{(10,10)}|(\frac{2\sqrt{100}}{20})$$

$$= 2(\frac{\sqrt{21}}{5}) + 4(\frac{2\sqrt{28}}{11}) + (2m-2)(\frac{2\sqrt{2}}{3}) + (4n+2)(\frac{2\sqrt{30}}{11}) + 2(\frac{\sqrt{35}}{6}) + (2n)(\frac{4\sqrt{10}}{13}) + (3mn+2m+n-2) + 2(\frac{2\sqrt{42}}{13}) + (4m-4)(\frac{2\sqrt{6}}{5}) + (4n)(\frac{4\sqrt{3}}{7}) + (6mn-6n)(\frac{\sqrt{15}}{4}) + 4(\frac{4\sqrt{14}}{15}) + (2n-2) + (2m-2)(\frac{6\sqrt{10}}{19}) + (mn-m-n+1)$$

$$= (8+3\sqrt{15})\frac{mn}{2} + (285+380\sqrt{2} + 456\sqrt{6} - 180\sqrt{10})\frac{m}{285} + (4004+1456\sqrt{30} + 1232\sqrt{10} + 4576\sqrt{10} - 3003\sqrt{15})\frac{n}{2002} + (13585\sqrt{13} - 54340\sqrt{2} + 16302\sqrt{21} - 65208\sqrt{6} + 59280\sqrt{7} + 14820\sqrt{30} + 12540\sqrt{42} + 43472\sqrt{14} - 25740\sqrt{10} - 122265)\frac{1}{40755}.$$

Employing formula given by Equation (16) and edge partition presented in the Table (4), the Sanskruti index $SI(VR_m^n)$ can be calculated as:

(3) $SI(VR_m^n)$

$$= \sum_{vw\in E(VR_m^n)} (\frac{s_vs_w}{s_v+s_w-2})^3$$

$$= |E_{(3,7)}|(\frac{21}{8})^3 + |E_{(4,7)}|(\frac{28}{9})^3 + |E_{(4,8)}|(\frac{32}{10})^3 + |E_{(5,6)}|(\frac{30}{9})^3 + |E_{(5,7)}|(\frac{35}{10})^3 + |E_{(5,8)}|(\frac{40}{11})^3 + |E_{(6,6)}|(\frac{36}{10})^3 + |E_{(6,7)}|(\frac{42}{11})^3 + |E_{(6,8)}|(\frac{48}{12})^3 + |E_{(6,9)}|(\frac{54}{13})^3 + |E_{(6,10)}|(\frac{60}{14})^3 + |E_{(7,8)}|(\frac{56}{13})^3 + |E_{(8,8)}|(\frac{64}{14})^3 + |E_{(9,10)}|(\frac{90}{17})^3 + |E_{(10,10)}|(\frac{100}{18})^3$$

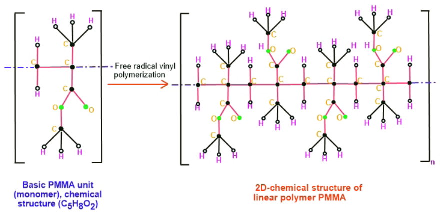

FIGURE 4. Polymerization of Methyl Methacrylate into PMMA with *n* monomers.

$$
\begin{aligned}
&= 2\Big(\frac{9261}{512}\Big) + 4\Big(\frac{21952}{729}\Big) + (2m-2)\Big(\frac{4096}{125}\Big) \\
&\quad + (4n+2)\Big(\frac{1000}{27}\Big) + 2\Big(\frac{343}{8}\Big) + (2n)\Big(\frac{64000}{1331}\Big) \\
&\quad + (3mn+2m+n-2)\Big(\frac{5832}{125}\Big) + 2\Big(\frac{74088}{1331}\Big) \\
&\quad + (4m-4)\Big(\frac{157464}{2197}\Big) + (6mn-6n)\Big(\frac{27000}{343}\Big) \\
&\quad + (4n)(64) + 4\Big(\frac{175616}{2197}\Big) + (2n-2)\Big(\frac{32768}{343}\Big) \\
&\quad + (2m-2)\Big(\frac{729000}{4913}\Big) + (mn-m-n+1)\Big(\frac{125000}{729}\Big) \\
&= \Big(\frac{24496447312}{31255875}\Big)mn + \Big(\frac{561466008516664}{983590583625}\Big)m \\
&\quad + \Big(\frac{3921718689424}{41601569625}\Big)n - \Big(\frac{551233094322072507949}{383182131126674880000}\Big).
\end{aligned}
$$

III. POLY-METHYL METHACRYLATE NETWORK

Although acrylic monomers and their derivatives are familiar to the world since the 1890s, however, the polymer of acrylic monomer started to emerge when Otto Röhm study and explored acrylic chemistry in his PhD thesis (1901) [57]. Poly-methyl methacrylate, a synthetic resin known as acrylic glass, is widely used as an excellent alternate of glass and is often used in products like instrument panels, aircraft canopies, and skylights, and medical technologies [58]. Walter Wright (1937) proposed PMMA, the first replacement for vulcanite, as a denture base material and became the most commonly used fabrication for denture base [59]. The pendent methyl CH_3 groups' presence avoids the close packing of polymer chains like crystalline fashion and prevents them from rotating freely around the carbon-carbon bonds, resulting in transparent and rigid plastic. Now, we provide the self-explanatory construction of the molecular graph of polymer PMMA from its monomer. Figure (4) depicts the bulk free radical polymerization of methyl methacrylate $C_5H_8O_2$ into linear chain polymer poly-methyl methacrylate $[C_5H_8O_2]_n$. Figure (5) represents the n dimensional hydrogen depleted molecular graph of PMMA, where n is the number of monomers in polymer chain and is denoted by $PMMA_n$.

A. RESULTS FOR POLY-METHYL METHACRYLATE NETWORK $PMMA_n$

Following lemma provide some insight in to the poly-methyl methacrylate network $PMMA_n$ and establish an essential result that is of key importance for forthcoming results.

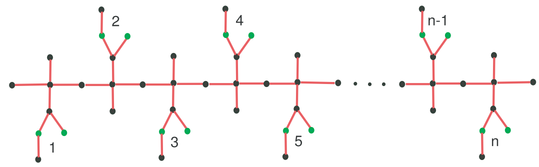

FIGURE 5. Hydrogen depleted molecular graph of $PMMA_n$.

TABLE 5. Valency-based edge partitioning of $PMMA_n$.

$(d_v, d_w) : vw \in E(PMMA_n)$	No. of edges	$(d_v, d_w) : vw \in E(PMMA_n)$	No. of edges
$(1,2)$	$n+1$	$(2,3)$	n
$(1,3)$	n	$(2,4)$	$2n-1$
$(1,4)$	$n+1$	$(3,4)$	n

Lemma 2: Let $PMMA_n$ be the poly-methyl methacrylate network shown in Figure (5) with n monomers, then total number of vertices and edges are $7n+2$ and $7n+1$, respectively.

Proof: Let $PMMA_n$ represent the graph of PMMA network having n monomers. We use the vertex set and edge set partition given by Equations (2) and (3) for molecular graph $PMMA_n$. By examining molecular graph $PMMA_n$, it can easily be observed that there are four type of vertices having valencies 1, 2, 3, and 4 i.e., $\delta(PMMA_n) = 1$ and $\Delta(PMMA_n) = 4$. Now using simple counting technique, we obtain the vertex partition and is given as follows. $|V_1| = 3n+2$, $|V_2| = 2n$, $|V_3| = n$, $|V_4| = n$. Consequently, total number of vertices of $PMMA_n$, denoted by $|V(PMMA_n)| = 7n+2$.
Likewise, we recognize six types of edges in $PMMA_n$ based upon valencies of end vertices of each edge. By using combinatorial counting technique on network to get edge partitioning as $|E_{12}| = n+1$, $|E_{13}| = n$, $|E_{14}| = n+1$, $|E_{23}| = n$, $|E_{24}| = 2n-1$, $|E_{34}| = n$. As a result, total number of edges of PMMA network, denoted by $|E(PMMA_n)| = 10mn + 9m + 6n + 5$. For the sake of simplicity and further use, edge partition is illustrated in the Table (5).

Theorem 6: Let $PMMA_n$ be the poly-methyl methacrylate network with n monomers, then the generalized-Zagreb index $Z_{r,s}(PMMA_n)$ is given by the formula:

$$
\begin{aligned}
Z_{r,s}(PMMA_n) = \big(&2^r + 2^s + 2^{2r}(1 + 2^{s+1} + 3^s) \\
&+ 2^{2s}(1 + 2^{r+1} + 3^r) + 3^r(1 + 2^s) \\
&+ 3^s(1 + 2^r)\big)n + \big(2^r + 2^s + 2^{2r}(1 - 2^s) \\
&+ 2^{2s}(1 - 2^r)\big).
\end{aligned}
$$

Proof: Using Table (5) and the formula stated in the Equation (11), we compute the required result as follows:

$$
\begin{aligned}
&Z_{r,s}(PMMA_n) \\
&\quad = \sum_{vw \in E(PMMA_n)} (d_v^r d_w^s + d_w^r d_v^s) \\
&\quad = \sum_{vw \in E_{12}} (d_v^r d_w^s + d_w^r d_v^s) + \sum_{vw \in E_{13}} (d_v^r d_w^s + d_w^r d_v^s) \\
&\qquad + \sum_{vw \in E_{14}} (d_v^r d_w^s + d_w^r d_v^s) + \sum_{vw \in E_{23}} (d_v^r d_w^s + d_w^r d_v^s) \\
&\qquad + \sum_{vw \in E_{24}} (d_v^r d_w^s + d_w^r d_v^s) + \sum_{vw \in E_{34}} (d_v^r d_w^s + d_w^r d_v^s)
\end{aligned}
$$

$$= (n+1)(1^r2^s+2^r1^s)+n(1^r3^s+3^r1^s) + (n+1)(1^r4^s+4^r1^s)+n(2^r3^s+3^r2^s) + (2n-1)(2^r4^s+4^r2^s)+(2n+2)(3^r4^s+4^r3^s).$$

By performing usual calculation above expressions boils down to the required result.

$$Z_{r,s}(PMMA_n) = \big(2^r+2^s+2^{2r}(1+2^{s+1}+3^s) + 2^{2s}(1+2^{r+1}+3^r)+3^r(1+2^s) + 3^s(1+2^r)\big)n+\big(2^r+2^s+2^{2r}(1-2^s) + 2^{2s}(1-2^r)\big). \quad (26)$$

Corollary 2: Using Equation (26) of generalized Zagreb index of $PMMA_n$, following closed form formulae of certain degree-based topological indices are derived as special cases.

1) $M_1(PMMA_n) = Z_{1,0}(PMMA_n) = 36n+2$.
2) $M_2(PMMA_n) = \frac{1}{2}Z_{1,1}(PMMA_n) = 43n-2$.
3) $F(PMMA_n) = Z_{2,0}(PMMA_n) = 110n+2$.
4) $ReZM(PMMA_n) = Z_{2,1}(PMMA_n) = 248n-22$.
5) $M^\alpha(PMMA_n) = Z_{\alpha-1,0}(PMMA_n) = (3+3^\alpha+2^{\alpha+1}+2^{2\alpha})n+2$.
6) $R_\alpha(PMMA_n) = \frac{1}{2}Z_{\alpha,\alpha}(PMMA_n) = (2^\alpha+2^{2\alpha}(1+3^\alpha+2^{\alpha+1}) + 3^\alpha(1+2^\alpha))n+(2^\alpha+2^{2\alpha}(1-2^\alpha))$.
7) $SDD(PMMA_n) = Z_{1,-1}(PMMA_n) = \frac{58}{3}n+\frac{17}{4}$.

Theorem 7: Let $PMMA_n = \Gamma_3$ be a poly-methyl methacrylate network with n isomers, then ABC and GA indices of Γ_3 are:

1) $ABC(\Gamma_3) = (12\sqrt{2}+2\sqrt{6}+3\sqrt{3}+\sqrt{15})\frac{n}{6} + \frac{\sqrt{3}-\sqrt{2}}{2}$.
2) $GA(\Gamma_3) = (2\sqrt{2}+\frac{15\sqrt{3}}{14}+\frac{2\sqrt{6}}{5}+\frac{4}{5})n+\frac{\sqrt{3}}{2}$.
3) $\chi_{\frac{-1}{2}}(\Gamma_3) = (70\sqrt{3}+84\sqrt{5}+70\sqrt{6}+30\sqrt{7} + 105)\frac{n}{210}+(10\sqrt{3}+6\sqrt{5}-5\sqrt{6})\frac{1}{30}$.

Proof: Using Table (5) and the formulae defined by the Equations (12), (13), and (16), respectively. We compute the required result as follows:

(1) $ABC(\Gamma_3)$

$$= \sum_{vw\in E(\Gamma_3)}\sqrt{\frac{d_v+d_w-2}{d_vd_w}}$$
$$= \sum_{vw\in E_{12}}\sqrt{\frac{d_v+d_w-2}{d_vd_w}}+\sum_{vw\in E_{13}}\sqrt{\frac{d_v+d_w-2}{d_vd_w}} + \sum_{vw\in E_{14}}\sqrt{\frac{d_v+d_w-2}{d_vd_w}}+\sum_{vw\in E_{23}}\sqrt{\frac{d_v+d_w-2}{d_vd_w}} + \sum_{vw\in E_{24}}\sqrt{\frac{d_v+d_w-2}{d_vd_w}}+\sum_{vw\in E_{34}}\sqrt{\frac{d_v+d_w-2}{d_vd_w}}$$
$$= (n+1)\sqrt{\frac{1}{2}}+(n)\sqrt{\frac{2}{3}}+(n+1)\sqrt{\frac{3}{4}} + (n)\sqrt{\frac{3}{6}}+(2n-1)\sqrt{\frac{4}{8}}+(n)\sqrt{\frac{5}{12}}$$
$$= (12\sqrt{2}+2\sqrt{6}+3\sqrt{3}+\sqrt{15})\frac{n}{6}+\frac{\sqrt{3}-\sqrt{2}}{2}.$$

(2) $GA(\Gamma_3)$

$$= \sum_{vw\in E(\Gamma_3)}\frac{2\sqrt{d_vd_w}}{d_v+d_w}$$
$$= \sum_{vw\in E_{12}}\frac{2\sqrt{d_vd_w}}{d_v+d_w}+\sum_{vw\in E_{13}}\frac{2\sqrt{d_vd_w}}{d_v+d_w} + \sum_{vw\in E_{14}}\frac{2\sqrt{d_vd_w}}{d_v+d_w}+\sum_{vw\in E_{23}}\frac{2\sqrt{d_vd_w}}{d_v+d_w} + \sum_{vw\in E_{24}}\frac{2\sqrt{d_vd_w}}{d_v+d_w}+\sum_{vw\in E_{34}}\frac{2\sqrt{d_vd_w}}{d_v+d_w}$$
$$= (n+1)(\frac{2\sqrt{2}}{3})+n(\frac{2\sqrt{3}}{4})+(n+1)(\frac{2\sqrt{4}}{5}) + n(\frac{2\sqrt{6}}{5})+(2n-1)(\frac{2\sqrt{8}}{6})+n(\frac{2\sqrt{12}}{7})$$
$$= (2\sqrt{2}+\frac{15\sqrt{3}}{14}+\frac{2\sqrt{6}}{5}+\frac{4}{5})n+\frac{\sqrt{3}}{2}.$$

(3) $\chi_{\frac{-1}{2}}(\Gamma_3)$

$$= \sum_{vw\in E(\Gamma_3)}\frac{1}{\sqrt{d_v+d_w}}$$
$$= \sum_{vw\in E_{12}}\frac{1}{\sqrt{d_v+d_w}}+\sum_{vw\in E_{13}}\frac{1}{\sqrt{d_v+d_w}} + \sum_{vw\in E_{14}}\frac{1}{\sqrt{d_v+d_w}}+\sum_{vw\in E_{23}}\frac{1}{\sqrt{d_v+d_w}} + \sum_{vw\in E_{24}}\frac{1}{\sqrt{d_v+d_w}}+\sum_{vw\in E_{34}}\frac{1}{\sqrt{d_v+d_w}}$$
$$= (n+1)\frac{1}{\sqrt{3}}+(n)\frac{1}{\sqrt{4}}+(n+1)\frac{1}{\sqrt{5}}+(n)\frac{1}{\sqrt{5}} + (2n-1)\frac{1}{\sqrt{6}}+(n)\frac{1}{\sqrt{7}}$$
$$= (70\sqrt{3}+84\sqrt{5}+70\sqrt{6}+30\sqrt{7}+105)\frac{n}{210} + (10\sqrt{3}+6\sqrt{5}-5\sqrt{6})\frac{1}{30}.$$

Theorem 8: Let $PMMA_n$ be the poly-methyl methacrylate network with n isomers, then *M-polynomial* of $PMMA_n$ is $M(PMMA_n; x, y) = (n+1)xy^2+nxy^3+(n+1)xy^4+nx^2y^3+(2n-1)x^2y^4+nx^3y^4$.

Proof: Using formula of *M-Polynomial* defined by Equation (24) and partition presented in the Table (5), we have

$$M(PMMA_n; x, y) = \sum_{i\le j} m_{ij}x^iy^j$$
$$= \sum_{1\le 2} m_{12}xy^2+\sum_{1\le 3} m_{13}xy^3+\sum_{1\le 4} m_{14}xy^4 + \sum_{2\le 3} m_{23}x^2y^3+\sum_{2\le 4} m_{24}x^2y^4+\sum_{3\le 4} m_{34}x^3y^4$$

$$= |E_{12}|xy^2 + |E_{13}|xy^3 + |E_{14}|xy^4 + |E_{23}|x^2y^3 + |E_{24}|x^2y^4 + |E_{34}|x^3y^4$$
$$= (n+1)xy^2 + nxy^3 + (n+1)xy^4 + nx^2y^3 + (2n-1)x^2y^4 + nx^3y^4.$$

Theorem 9: For poly-methyl methacrylate network $PMMA_n$, modified Zagreb index, inverse Randić index, harmonic index, inverse sum index and augmented Zagreb index are:

$$(1)\ {}^mM_2(PMMA_n) = \frac{19}{12}n + \frac{5}{8}.$$
$$(2)\ RR_\alpha(PMMA_n) = \left(2^\alpha + 2\times 3^\alpha(1+2^\alpha)(4^\alpha+6^\alpha)\right)\frac{n}{24^\alpha} + \left(2^{2\alpha}+2^\alpha-1\right)\frac{1}{8^\alpha}.$$
$$(3)\ HI(PMMA_n) = \frac{613}{210}n + \frac{11}{15}.$$
$$(4)\ ISI(PMMA_n) = \frac{655}{84}n + \frac{2}{15}.$$
$$(5)\ AZI(PMMA_n) = \frac{1392373}{27000}n + \frac{64}{27}.$$

Proof: From Theorem 8, we have $M(PMMA_n; x, y) = (n+1)xy^2 + nxy^3 + (n+1)xy^4 + nx^2y^3 + (2n-1)x^2y^4 + nx^3y^4$.
Now applying specific operators presented in the Table (2) on *M-Polynomial*, we get

$$(s_xs_y)M = \frac{(n+1)}{2}xy^2 + \frac{n}{3}xy^3 + \frac{(n+1)}{4}xy^4 + \frac{n}{6}x^2y^3 + \frac{(2n-1)}{8}x^2y^4 + \frac{n}{12}x^3y^4.$$
$$(s_x^\alpha s_y^\alpha)M = \frac{(n+1)}{2^\alpha}xy^2 + \frac{n}{3^\alpha}xy^3 + \frac{(n+1)}{4^\alpha}xy^4 + \frac{n}{6^\alpha}x^2y^3 + \frac{(2n-1)}{8^\alpha}x^2y^4 \frac{n}{12^\alpha}x^3y^4.$$
$$JM(x,y) = M(x) = (n+1)x^3 + nx^4 + (2n+1)x^5 + (2n-1)x^6 + nx^7.$$
$$s_xJM(x) = \frac{(n+1)}{3}x^3 + \frac{n}{4}nx^4 + \frac{(2n+1)}{5}x^5 + \frac{(2n-1)}{6}x^6 + \frac{n}{7}x^7.$$
$$s_xJD_xD_yM = \frac{2(n+1)}{3}x^3 + \frac{3n}{4}nx^4 + \frac{2(5n+2)}{5}x^5 + \frac{4(2n-1)}{3}x^6 + \frac{12n}{7}x^7.$$
$$s_x^3Q_{-2}JD_x^3D_y^3M = 8(n+1)x + \frac{27n}{8}nx^2 + \frac{8(35n+8)}{27}x^3 + 8(2n-1)x^4 + \frac{1728}{125}x^5.$$

Now employing formulae of desired BAIs presented in Table (2) over expression derived from *M-Polynomial*, we get our results.

Theorem 10: Let $PMMA_n$ be poly-methyl methacrylate network, then ABC_4, GA_5, and SI of $PMMA_n$ are given as:

$$(1)\ ABC_4(PMMA_n) = (105\sqrt{2} + 35\sqrt{42} + 45\sqrt{7} + 21\sqrt{30} + 84\sqrt{5})\frac{n}{210} + (5\sqrt{2} + \sqrt{26} + \sqrt{30} - 4\sqrt{5})\frac{1}{10}.$$
$$(2)\ GA_5(PMMA_n) = (39270\sqrt{2} + 11781\sqrt{21} + 21420\sqrt{7} + 16830\sqrt{10} + 693)\frac{n}{58905} + (36\sqrt{10} + 42\sqrt{2} - 28\sqrt{5})\frac{1}{63}.$$
$$(3)\ SI(PMMA_n) = \left(\frac{166045733}{373248}\right)n - \left(\frac{8783198}{59319}\right).$$

TABLE 6. Edge partitioning based upon neighbor's degree sum of $PMMA_n$.

$(s_v, s_w) : vw \in E(PMMA_n)$	Number of edges=$\lvert E_{(i,j)}\rvert$
$(2,4)$	n
$(2,5)$	1
$(3,7)$	n
$(4,7)$	n
$(4,10)$	$n+1$
$(5,10)$	1
$(7,10)$	n
$(8,10)$	$2n-2$

Proof: In order to compute ABC_4, GA_5, and SI, we need edge partition of $PMMA_n$ based on neighbors' valency-sum of end vertices $\forall\ vw \in PMMA_n$. We identify eight kind of edges on valency based sum of neighbors' vertices of each edge in $PMMA_n$ network. Using formula of invariant ABC_4 given by the Equation (14) and edge partition presented in the Table (6), we proceed as follows:

$$(1)\ ABC_4(PMMA_n) = \sum_{vw\in E(PMMA_n)} \sqrt{\frac{s_v+s_w-2}{s_vs_w}}$$
$$= |E_{(2,4)}|\sqrt{\frac{4}{8}} + |E_{(2,5)}|\sqrt{\frac{5}{10}} + |E_{(3,7)}|\sqrt{\frac{8}{21}} + |E_{(4,7)}|\sqrt{\frac{9}{28}} + |E_{(4,10)}|\sqrt{\frac{12}{40}} + |E_{(5,10)}|\sqrt{\frac{13}{50}} + |E_{(7,10)}|\sqrt{\frac{15}{70}} + |E_{(8,10)}|\sqrt{\frac{16}{80}}$$
$$= n\sqrt{\frac{1}{2}} + \sqrt{\frac{1}{2}} + n\sqrt{\frac{8}{21}} + n\sqrt{\frac{9}{28}} + \sqrt{\frac{13}{50}} + (n+1)\sqrt{\frac{3}{10}} + n\sqrt{\frac{3}{14}} + (2n-2)\sqrt{\frac{1}{5}}$$
$$= \frac{n}{210}(105\sqrt{2} + 35\sqrt{42} + 45\sqrt{7} + 21\sqrt{30} + 84\sqrt{5}) + (5\sqrt{2} + \sqrt{26} + \sqrt{30} - 4\sqrt{5})\frac{1}{10}.$$

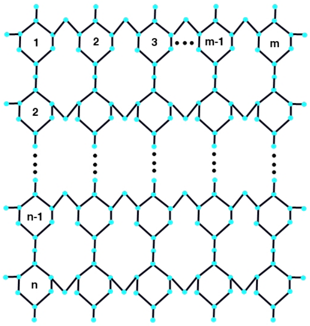

FIGURE 6. Hydrogen suppressed molecular graph of bakelite network BN^n_m.

Now, using formula of invariant GA_5 given in Equation (15) and edge partition presented in the Table (6), we proceed as follows

$$
\begin{aligned}
&(2)\ GA_5(PMMA_n)\\
&= \sum_{vw\in E(PMMA_n)} \frac{2\sqrt{s_v s_w}}{(s_v+s_w)}\\
&= |E_{(2,4)}|(\frac{2\sqrt{8}}{6}) + |E_{(2,5)}|(\frac{2\sqrt{10}}{7}) + |E_{(3,7)}|(\frac{2\sqrt{21}}{10})\\
&\quad + |E_{(4,7)}|(\frac{2\sqrt{28}}{11}) + |E_{(4,10)}|(\frac{2\sqrt{40}}{12}) + |E_{(5,10)}|(\frac{2\sqrt{50}}{15})\\
&\quad + |E_{(7,10)}|(\frac{2\sqrt{70}}{17}) + |E_{(8,10)}|(\frac{2\sqrt{80}}{18})\\
&= n(\frac{2\sqrt{2}}{3}) + (\frac{2\sqrt{10}}{7}) + n(\frac{\sqrt{21}}{5}) + n(\frac{2\sqrt{28}}{11})\\
&\quad + (n+1)(\frac{2\sqrt{10}}{7}) + (\frac{2\sqrt{2}}{3}) + n(\frac{2\sqrt{70}}{17})\\
&\quad + (2n-2)(\frac{4\sqrt{5}}{9})\\
&= (39270\sqrt{2} + 11781\sqrt{21} + 21420\sqrt{7} + 16830\sqrt{10}\\
&\quad + 693)\frac{n}{58905} + (36\sqrt{10} + 42\sqrt{2} - 28\sqrt{5})\frac{1}{63}.
\end{aligned}
$$

Finally, using formula of Sanskruti index given in Equation (16) and edge partition presented in the Table (6), we have

$$
\begin{aligned}
&(3)\ SI(PMMA_n)\\
&= \sum_{vw\in E(PMMA_n)} \left(\frac{s_v s_w}{s_v+s_w-2}\right)^3\\
&= |E_{(2,4)}|\left(\frac{8}{4}\right)^3 + |E_{(2,5)}|\left(\frac{10}{5}\right)^3 + |E_{(3,7)}|\left(\frac{21}{8}\right)^3\\
&\quad + |E_{(4,7)}|\left(\frac{28}{9}\right)^3 + |E_{(4,10)}|\left(\frac{40}{12}\right)^3 + |E_{(5,10)}|\left(\frac{50}{13}\right)^3\\
&\quad + |E_{(7,10)}|\left(\frac{70}{15}\right)^3 + |E_{(8,10)}|\left(\frac{80}{16}\right)^3\\
&= 8n + 8 + \frac{9261n}{512} + \frac{21952n}{729} + \frac{1000(n+1)}{27}\\
&\quad + \frac{125000}{2197} + \frac{2744n}{27} + 125(2n-2)\\
&= \left(\frac{166045733}{373248}\right)n - \left(\frac{8783198}{59319}\right).
\end{aligned}
$$

IV. BAKELITE NETWORK

In an earlier paper [60], we discussed and computed several results regarding bakelite network, see figure (6), that are presented here to use them for comparative analysis.

Corollary 3 [60]: For bakelite network BN^n_m, closed form formulae for first, second, forgotton, redefined Zagreb, general Zagreb, general Randić, and symmetric division degree indices are:

(1) $M_1(BN^n_m) = Z_{1.0}(BN^n_m) = 52mn - 2m - 14n.$

(2) $M_2(BN^n_m) = \frac{1}{2}Z_{1.1}(BN^n_m) = 66mn - 6m - 22n.$

(3) $F(BN^n_m) = Z_{2.0}(BN^n_m) = 140mn - 6m - 46n.$

(4) $ReZM(BN^n_m) = Z_{2.1}(BN^n_m) = 348mn - 36m - 136n.$

(5) $M^\alpha(BN^n_m) = Z_{\alpha-1.0}(BN^n_m) = 4mn(2^\alpha + 3^\alpha) + 2m(1-2^{\alpha-1}) + 2n(2^\alpha - 2^{\alpha-1} - 3^\alpha).$

(6) $R_\alpha(BN^n_m) = \frac{1}{2}Z_{\alpha.\alpha}(BN^n_m) = 2\times 3^\alpha(2^{\alpha+2} + 3^\alpha)mn + 2\times 3^\alpha(1-2^\alpha)m + 2^{\alpha+1}(2-3^\alpha)n.$

(7) $SDD(BN^n_m) = Z_{1,-1}(BN^n_m) = \frac{64}{3}mn + \frac{7}{3}m - \frac{13}{3}n.$

Proposition 1 [60]: For bakelite network BN^n_m, the modified 2nd Zagreb, inverse Randić, harmonic, inverse sum, and augmented Zagreb indices are

(1) ${}^mM_2(BN^n_m) = \frac{14}{9}mn - \frac{1}{18}n - \frac{1}{3}m.$

(2) $RR_\alpha(BN^n_m) = (8\times 6^{-\alpha} + 2\times 9^{-\alpha})mn + (2\times 3^{-\alpha} - 2\times 6^{-\alpha})m + (2^{1-2\alpha} - 2\times 6^{-\alpha} - 2\times 9^{-\alpha})n.$

(3) $HI(BN^n_m) = \frac{58}{15}mn - \frac{7}{15}n + \frac{1}{5}m.$

(4) $ISI(BN^n_m) = \frac{63}{5}mn - \frac{17}{5}n - \frac{9}{10}m.$

(5) $AZI(BN^n_m) = \frac{2777}{32}mn - \frac{729}{32}n - \frac{37}{4}m.$

Theorem 11 [60]: Let BN^n_m be the molecular graph of (m, n)-dimensional bakelite network, then

(1) $ABC(BN^n_m)$
$$= \frac{1}{3}\big((4 + 12\sqrt{2})mn - 4n - (2\sqrt{6} - 3\sqrt{2})m\big).$$

(2) $GA(BN^n_m)$
$$= \frac{1}{5}\big((10 + 16\sqrt{6})mn - 4\sqrt{6}n - (5\sqrt{3} - 4\sqrt{6})m\big).$$

(3) $\chi_{\frac{-1}{2}}(BN^n_m)$
$$= \frac{1}{15}\big(5\sqrt{6} + 24\sqrt{5}\big)mn + \big(15 - 6\sqrt{5} - 5\sqrt{6}\big)n + \big(5 - 2\sqrt{5}\big)\frac{m}{5}.$$

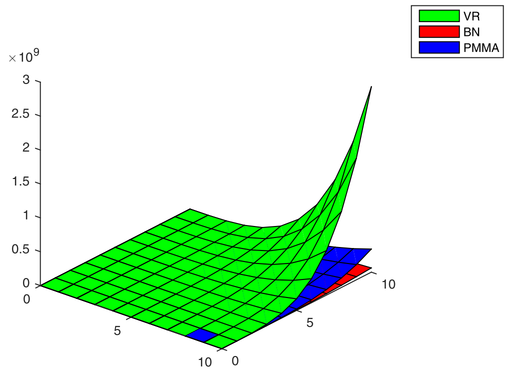

FIGURE 7. 3D graph of *M-polynomial* of VR_4^7, BN_4^7 and $PMMA_{28}$.

Theorem 12 [60]: Let BN_m^n be the (m, n)-dimensional bakelite network then the fourth version of ABC and the fifth geometric arithmetic indices are given by

(1) $ABC_4(BN_m^n)$

$$= \frac{1}{42}\big(4\sqrt{462}+21\sqrt{10}+3\sqrt{182}+21\big)mn + \frac{1}{42}\big(14\sqrt{14}+14\sqrt{10}-4\sqrt{462}-3\sqrt{182}+42\big)m + \frac{1}{210}\big(42\sqrt{35}+60\sqrt{14}+105\sqrt{10}-20\sqrt{462} - 15\sqrt{182}-105\big)n + \frac{1}{210}\big(126\sqrt{30}+30\sqrt{462} + 225\sqrt{182}-130\sqrt{14}-266\sqrt{10}-210\big).$$

(2) $GA_5(BN_m^n)$

$$= \frac{1}{1365}\big(210\sqrt{42}+780\sqrt{3}+728\sqrt{14} + 4095\big)mn + \frac{1}{1365}\big(1820\sqrt{2}+1560\sqrt{3}-840\sqrt{42} - 728\sqrt{14}+2730\big)m + \frac{1}{4095}\big(3640\sqrt{5}+1365\sqrt{35} - 3780\sqrt{42}-2340\sqrt{3}-2184\sqrt{14}+12285\big)n + \frac{1}{30030}\big(15015\sqrt{15}-40040\sqrt{2}+32760\sqrt{30} - 10010\sqrt{35}+27720\sqrt{42}-34320\sqrt{3} - 16016\sqrt{14}-30030\big).$$

V. CONCLUSION AND COMPARATIVE ANALYSIS OF VULCANIZED RUBBER, BAKELITE, AND PMMA NETWORKS

Figure (7) demonstrates a comparison between 3D graphs of *M-polynomial* of vulcanized rubber, bakelite, and PMMA networks (all having the same number of monomers).

The following tables provide an insight into numerical comparison among various BAIs of vulcanized rubber, bakelite, and PMMA networks.

Note: Let us assume $VR_m^n = \Gamma_1$, $BN_m^n = \Gamma_2$, and $PMMA_{mn} = \Gamma_3$ to keep the tables compact.

First Zagreb index M_1, Second Zagreb index M_2, and the Rand ić index $R_{\frac{-1}{2}}$ measure the extent of branching in the carbon-atom skeleton of a molecule. In this regard, Table (7) and (10) reveals the following order of these indices for same values of m and n, $TI(PMMA_{mn}) \leq TI(BN_m^n) \leq TI(VR_m^n)$

TABLE 7. Comparison of Γ_1, Γ_2, and Γ_3 using M_1 and M_2.

			M_1			M_2	
m	n	Γ_1	Γ_2	Γ_3	Γ_1	Γ_2	Γ_3
4	7	2014	1350	1010	2626	1670	1202
7	4	2068	1386	1010	2722	1718	1202
5	12	4016	2942	2162	5282	3666	2578
12	5	4142	3026	2162	5506	3778	2578
10	16	9994	8076	5762	13330	10148	6878
16	10	10102	8148	5762	13522	10244	6878
20	40	47102	41000	28802	63378	51800	34398
40	20	47462	41240	28802	64018	52120	34398

TABLE 8. Comparison of Γ_1, Γ_2, and Γ_3 using ReZM and AZI.

			ReZM			AZI	
m	n	Γ_1	Γ_2	Γ_3	Γ_1	Γ_2	Γ_3
4	7	15580	8648	6922	3304	2274	1446
7	4	16348	8948	6922	3326	2233	1446
5	12	31500	19068	14858	6609	4982	3096
12	5	33292	19768	14858	6660	4887	3096
10	16	80404	53144	39658	16321	13509	8253
16	10	81940	53744	39658	16365	13428	8253
20	40	384548	272240	198378	76800	65599	41258
40	20	389668	274240	198378	76946	68328	41258

TABLE 9. Comparison of Γ_1, Γ_2, and Γ_3 using SDD and ISI.

			SDD			ISI	
m	n	Γ_1	Γ_2	Γ_3	Γ_1	Γ_2	Γ_3
5	8	1205	830	778	639	478	312
8	5	1224	850	778	650	488	312
12	20	6197	5061	4644	3406	2958	1871
20	12	6246	5114	4644	3433	2987	1871
40	65	61988	55278	50270	34733	32547	20274
65	40	62142	55445	50270	34817	32637	20274
70	80	131998	119283	108271	74174	70302	43667
80	70	132060	119350	108271	74208	70338	43667

TABLE 10. Comparison of Γ_1, Γ_2, and Γ_3 using $R_{\frac{-1}{2}}$ and $\chi_{\frac{-1}{2}}$.

			$R_{\frac{-1}{2}}$			$\chi_{\frac{-1}{2}}$	
m	n	Γ_1	Γ_2	Γ_3	Γ_1	Γ_2	Γ_3
5	9	224	174	136	245	192	143
9	5	226	178	136	248	195	143
10	18	795	702	542	874	779	570
18	10	798	709	542	879	785	570
24	40	3937	3764	2890	4357	4192	3040
40	24	3943	3777	2890	4367	4205	3040
50	90	17899	17670	13543	19854	19715	14249
90	50	17916	17703	13543	19878	19747	14249

TABLE 11. Comparison of Γ_1, Γ_2, and Γ_3 using ABC and GA.

			ABC			GA	
m	n	Γ_1	Γ_2	Γ_3	Γ_1	Γ_2	Γ_3
5	9	437	364	258	630	472	324
9	5	444	358	258	634	484	324
10	18	5194	4944	3610	7538	6823	4525
18	10	5221	4927	3610	7549	6855	4525
24	40	18032	17553	12891	26157	24509	16160
40	24	35731	35095	25782	51891	49007	32320
50	90	35802	35039	25782	51930	49116	32320

TABLE 12. Comparison of Γ_1, Γ_2, and Γ_3 viz a viz ABC_4.

			ABC_4	
m	n	Γ_1	Γ_2	Γ_3
5	10	307	403	191
10	5	313	403	191
20	35	3648	3725	2658
35	20	3666	3725	2658
50	50	12662	12904	9492
50	100	25090	25648	18983
100	50	25150	25648	18983
100	500	247336	254926	189817
500	100	247816	254926	189817

TABLE 13. Comparison of Γ_1, Γ_2, and Γ_3 viz a viz GA_5.

			GA_5	
m	n	Γ_1	Γ_2	Γ_3
5	10	612	332	189
10	5	589	342	189
20	35	7294	4818	2617
35	20	7226	4847	2617
50	50	25236	17353	9343
50	100	50226	34709	18685
100	50	49999	34803	18685
100	500	495632	348105	186836
500	100	493816	348860	186836

where $TI \in \{M_1, M_2, R_{\frac{-1}{2}}\}$. The densities of these polymers support this fact, e.g., the density of vulcanized rubber is 1.522 g/cm^3, the density of bakelite is 1.3 g/cm^3, and density of PMMA is 1.18 g/cm^3. We further anticipate that the extensive branching may be associated with the melting temperature of polymers. The melting temperature of vulcanized rubber and PMMA is 873 K and 433 K, respectively. We don't have the melting temperature of bakelite as it catches fire at excessive heat. We know that the sum-connectivity index and the product-connectivity index correlate well among themselves, and the Table (10) reflects this fact. Since the SDD index is a good predictor of total surface area for poly-chlorobiphenyls, ISI index is a significant predictor of total surface area for octane isomers. Based upon comparison of Table (9), we conjecture the order in which surface area (SA) of vulcanized rubber (elastomer), bakelite (thermosetting polymer), and PMMA (thermoplastic polymer) would have been arranged and is given as $SA(PMMA_{mn}) \leq SA(BN_m^n) \leq SA(VR_m^n)$, having same values of parameters m and n. Besides, the results obtained in Tables (7 - 13) could further be effective in the models of QSPR/QSAR relationships for assessing the thermodynamic and the mechanical properties of underlying polymeric structures. Although synthetic and natural polymers are appropriate for the pharmaceutical industry, natural polymers are attractive as they are economical, biocompatible, have no side effects, non-toxic, and suitable for drug delivery systems. A similar study could have been performed on natural polymers like cellulose, glycogen, and amylopectin to predict their behavior, nature, and biological properties.

VI. DECLARATIONS

A. COMPETING INTERESTS

The authors declare that they have no competing interests.

B. AUTHORS' CONTRIBUTIONS

All the authors contributed equally and significantly in preparation of final manuscript of this article. Moreover, all authors read and approved the final manuscript.

LIST OF ABBREVIATIONS

Abbreviation	Meaning
TI	Topological Index/Invariant
BAIs	Bond-Additive Invariants
CGT	Chemical Graph Theory
QSAR	Quantitative Structure Activity Relationships
QSPR	Quantitative Structure Property Relationships
IAMC	International Academy of Mathematical Chemistry
IUPAC	International Union for Pure and Applied Chemistry
ABC	Atom-Bond Connectivity Index
ABC_4	Fourth Version of ABC
GA	Geometric-Arithmetic Index
GA_5	Fifth Version of GA
SI	Sanskruti Index
SDD	symmetric division deg Index
ISI	Inverse Sum Index
SCI	Sum Connectivity Index
AZI	Augmented Zagreb Index
GZI	Generalized Zagreb Index
ReZM	Re-defined Zagreb Index
SA	Surface Area
K	Kelvin
PMMA	Poly-methyl Methacrylate

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