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Topological Characterization for Triangular, Regular Triangular Oxides and Silicates Networks

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Abstract. Chemical graph theory can be studied with the aid of mathematical tools called m-polynomials. M-Polynomials offer a potent tool for computing different topological indices associated with vertex degrees and analyzing degree-based structural information in graphs. By counting specific substructure types within them, they are able to encode information about the structure of molecules or networks. In this article, we have developed M-Polynomials with the help of different topological invariants such as first Zagreb ($M_1(\beta)$), second Zagreb ($M_2(\beta)$), second modified Zagreb ($M_2^m(\beta)$), inverse sum ($I(\beta)$), harmonic index ($H(\beta)$) and Randic index ($R_{\alpha_0}(\beta)$) for the molecular structures of Triangular oxide TOX(r), Regular triangular oxide RTOX(r), Triangular silicate TSL(r) & Regular triangular silicate RTSL(r) networks to introduce new closed formulas to get better understanding the applications of M-Polynomials and topological indices in mathematical chemistry especially in the field of QSAR and QSPR study with the help of some software like MATLAB. We have also discussed the graphical behaviors of the above-mentioned structures.

2020 Mathematics Subject Classifications: 05C09, 05C10, 05C12, 05C31, 05C07

Key Words and Phrases: Topological Indices, degree, edge, M-Polynomials, TOX(r), RTOX(r), TSL(r), RTSL(r)

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1. Introduction

A topological invariant in graph theory is a numerical or mathematical property of a graph that does not change while the graph is continuously deformed, provided that the deformation does not cause edges or vertices to break or glue together. As long as no new connections are made or old ones are severed, the graph can be deformed in many ways, such as bending, shrinking, or stretching. Consider a graph as a flexible model. The fundamental characteristics reflected by the topological invariant will not change no matter how you bend and twist it. This is because the connections between the vertices, or nodes, are what hold the structure together. A successful approach for computing closed-form expressions for an assortment of degree-based topological indices is to use M-polynomials. Rather than computing each index independently, the M-polynomial offers a single formula that may be used to generate various topological indices. Because of this, M-Polynomials are an effective tool for researching the connection between chemical characteristics and graph structure. Topological invariants are very effective to calculate the chemical, physical, biological properties of a chemical compound. It has so many uses in chemistry, information, biology, quantitative structure-property relationships, online networking software, industries, electronics and medicines.

Definition 1. *Let β be the graph of the molecular structure of the chemical compound then its M-polynomial can be computed as:*

$$M(\beta, x_0, y_0) = \sum_{\delta_0 \leq i \leq j \leq \Delta_0} m_{ij}(\beta) x_0^i y_0^j \tag{1}$$

Where $\delta_0 = \min\{d_{v_0} : v_0 \in V_0(\beta)\}$, $\Delta_0 = \max\{d_{v_0} : v_0 \in V_0(\beta)\}$, and $m_{ij}(\beta)$ the number of the edges $u_0v_0 \in E_0(\beta)$ such that $d_{u_0}, d_{v_0} = i, j$.

In 1947, Weiner [4–6] developed the formula for the boiling point of alkanes which is given by: $\alpha W(\eth) + \beta P_3 + \gamma$, for empirical constants α, β and γ, Weiner index $W(\eth)$ and path's length P_3. Bollobas and Erdos [8, 9] presented the general Randic index and has been studied by both mathematicians and chemists [11, 24, 26]. For more detail, we can study the book [27].
The general Randic index is computed as

$$R_{\alpha_0}(\beta) = \sum_{u_0v_0 \in E(\beta)} (d_{u_0} d_{v_0})^{\alpha}. \tag{2}$$

The Randic index is a very essential index among all indices such as [27, 28, 30]. Gutman and Trinajstic [16] introduced first Zagreb and second Zagreb indices by

$$M_1(\beta) = \sum_{u_0v_0 \in E(\beta)} (d_{u_0} + d_{v_0}) \tag{3}$$

and

$$M_2(\beta) = \sum_{u_0v_0 \in E(\beta)} (d_{u_0} \times d_{v_0}), \tag{4}$$

respectively. For more detail [2, 14] are referred. The second modified Zagreb index is formulated by

$$^{m}M_2(\beta) = \sum_{u_0v_0\in E(\beta)} \frac{1}{d_{u_0}d_{v_0}} \tag{5}$$

The symmetric division index (SDD) is the one among 148 discrete Adriatic indices and is a good predictor of the total surface area for polychlorobiphenyls, see [1]. The symmetric division index of a connected graph β, is determined as

$$SDD(\beta) = \sum_{u_0v_0\in E(\beta)} \left\{ \frac{\min(d_{u_0}, d_{v_0})}{\max(d_{u_0}, d_{v_0})} + \frac{\max(d_{u_0}, d_{v_0})}{\min(d_{u_0}, d_{v_0})} \right\} \tag{6}$$

Harmonic index is

$$H(\beta) = \sum_{u_0v_0\in E(\beta)} \frac{2}{d_{u_0} + d_{v_0}} \tag{7}$$

The inverse sum index [13, 20] is formulated as

$$I(\beta) = \sum_{u_0v_0\in E(\beta)} \frac{d_{u_0}d_{v_0}}{d_{u_0} + d_{v_0}} \tag{8}$$

The augmented Zagreb index of β presented by Furtula et al. [19] and is computed as

$$A(\beta) = \sum_{u_0v_0\in E(\beta)} \left\{ \frac{d_{u_0}d_{v_0}}{d_{u_0} + d_{v_0} - 2} \right\}^3 \tag{9}$$

The above equation is also known as the minimal augmented Zagreb.

2. Material and Methods

In this study we calculate M-polynomial for Triangular oxide *TOX(r)*, Regular triangular oxide *RTOX(r)*, Triangular silicate *TSL(r)* & Regular triangular silicate *RTSL(r)* networks. M-Polynomial was invented by Klavzar and Deutsch. They also give some operators to find degree based topological indices directly from the M-polynomial [15]. To get different topological indices [17, 21] with their M-Polynomials we use the following table.

Table-1: Shows Topological indices with their corresponding M-Polynomials

Topological indices	M-Polynomials
First Zagreb ($M_1(\beta)$)	$(D_a + D_b)(M(\beta; a, b))\|_{a=b=1}$
Second Zagreb ($M_2(\beta)$)	$(D_aD_b)(M(\beta; a, b))\|_{a=b=1}$
Second Modified Zagreb ($M_2^m(\beta)$)	$(S_aS_b)(M(\beta; a, b))\|_{a=b=1}$
Inverse sum I(β)	$S_aJD_aD_b(M(\beta; a, b))\|_{a=b=1}$
Harmonic index H (β)	$2S_aJ(M(\beta; a, b))\|_{a=b=1}$
Randic index $R_{\alpha_0}(\beta)$	$(D_a^{\alpha_0}D_b^{\alpha_0})(M(\beta); a, b))\|_{a=b=1}$

$$
\begin{aligned}
D_a &= \frac{a\partial f(a,b)}{da},\ D_b = \frac{b\partial f(a,b)}{db},\ S_a = \int_0^a \frac{f(t,b)}{t}dt,\\
S_b &= \int_0^b \frac{f(a,t)}{t}dt,\ J(f(a,b)) = f(a,a).
\end{aligned}
$$

3. Motivation

In this paper, motivated by the regularity notion, we introduce a uniformity notion of graphs conceived depending on the degrees of vertices. It is natural to try to relate the regularity to uniformity of a graph. Some properties and fundamental structural characteristics of these graphs are studied. It is possible that the properties of the graphs, that we are defining in this paper may have some applications in chemistry as well as in other areas. The following results will be useful in the proof of our main results.

4. Main Results

In this section of the article, we derive the closed formulas using M-Polynomials for the molecular structures of Triangular oxide *TOX(r)*, Regular triangular oxide *RTOX(r)*, Triangular silicate *TSL(r)* & Regular triangular silicate *RTSL(r)* networks.

4.1. Triangular oxide network *TOX(r)*

Lemma 1. *The cardinalities of the graph TOX(r) are* $\frac{r^2+3r+2}{2}$ *with respect to node set*
and $\frac{3(r^2+r)}{2}$ *with respect to edge set.*

Theorem 1. *For TOX(r), the M-polynomial is*

$$M(TOX(r);a,b) = 6a^2b^4 + 3(r-1)a^4b^4 + 6(r-2)a^4b^4 + \frac{3((r-3)^2+(r-3))}{2}a^6b^6 \quad (10)$$

Proof : Let *TOX(r)* be a graph. Then we have by above lemma

$$|V(TOX(r))| = \frac{r^2+3r+2}{2}$$

$$|E(TOX(r))| = \frac{3(r^2+r)}{2}$$

Now, the *TOX(r)* has four edge partitions such as:

$$
\begin{aligned}
|E_1(TOX(r))| &= \{e = lm \in E(TOX(r)) : d_l = 2, d_m = 4\}\\
|E_2(TOX(r))| &= \{e = lm \in E(TOX(r)) : d_l = d_m = 4\}
\end{aligned}
$$

$$\begin{aligned}|E_3(TOX(r))| &= \{e = lm \in E(TOX(r)) : d_l = 4, d_m = 6\}\\ |E_4(TOX(r))| &= \{e = lm \in E(TOX(r)) : d_l = d_m = 6\}\end{aligned}$$

Where d_l, d_m are degree of edges l, m respectively.
We get

$$\begin{aligned}|E_1(TOX(r))| &= 6, |E_2(TOX(r))| = 3(r-1), |E_3(TOX(r))| = 6(r-2),\\ |E_4(TOX(r))| &= \frac{3((r-3)^2) + (r-3)}{2}\end{aligned}$$

Now using the definition of M-polynomial

$$\begin{aligned}M(TOX(r); a, b) &= \sum_{r \le s} m_{rs}(TOX(r))x^r y^s\\ &= \sum_{2 \le 4} m_{24}(TOX(r))a^2b^4 + \sum_{4 \le 4} m_{44}(TOX(r))a^4b^4\\ &+ \sum_{4 \le 6} m_{46}(TOX(r))a^4b^6 + \sum_{6 \le 6} m_{66}(TOX(r))a^6b^6\\ &= \sum_{lm \in E_1} m_{24}(TOX(r))a^2b^4 + \sum_{lm \in E_2} m_{44}(TOX(r))a^4b^4\\ &+ \sum_{lm \in E_3} m_{46}(TOX(r))a^4b^6 + \sum_{lm \in E_4} m_{66}(TOX(r))a^6b^6\\ &= |E_1|a^2b^4 + |E_2|a^4b^4 + |E_3|a^4b^6 + |E_4|a^6b^6\\ &= 6a^2b^4 + 3(r-1)a^4b^4 + 6(r-2)a^4b^6 + \frac{3((r-3)^2 + (r-3))}{2}a^6b^6\end{aligned}$$

Theorem 2. *For triangle oxide network TOX(r) some degree based topological indices are*

$$\begin{aligned}M_1(TOX(r)) &= (D_a + D_b)(f(a,b)|_{a=b=1} = 18r^2 - 6r\\ M_2(TOX(r)) &= (D_aD_b)(f(a,b)|_{a=b=1} = 54r^2 - 78r + 36\\ M_2^m(TOX(r)) &= (S_aS_b)(f(a,b)|_{a=b=1} = \frac{r^2}{24} + \frac{11}{48}r + \frac{1}{16}\\ H(TOX(r)) &= (2S_aJ)(f(a,b)|_{a=b=1} = \frac{r^2}{4} + \frac{7}{10}r + \frac{7}{20}\\ I(TOX(r)) &= (S_aJD_aD_b)(f(a,b)|_{a=b=1} = \frac{9}{2}r^2 + \frac{21}{10}r + \frac{1}{5}\\ R_\alpha(TOX(r)) &= (D_a^\alpha D_b^\alpha)(f(a,b)|_{a=b=1} = 6 \times 8^\alpha + 3 \times 16^\alpha(r-1)\\ &+ 6 \times 24^\alpha(r-2) + \frac{3}{2} \times 108^\alpha(r^2 - 5r + 6)\end{aligned}$$

Proof : As the M-polynomial of *TOX(r)* is

$$M(TOX(r); a, b) = 6a^2b^4 + 3(r-1)a^4b^4 + 6(r-2)a^4b^6 + \frac{3((r-3)^2 + (r-3))}{2}a^6b^6$$

$$= \quad f(a,b)$$

then

$$\begin{aligned}
D_a(f(a,b)) &= 12a^2b^4 + 12(r-1)a^4b^4 + 24(r-2)a^4b^6 + 9((r-3)^2+(r-3))a^6b^6 \\
D_b(f(a,b)) &= 24a^2b^4 + 12(r-1)a^4b^4 + 36(r-2)a^4b^6 + 9((r-3)^2+(r-3))a^6b^6 \\
(D_a^{\alpha}D_b^{\alpha}) &= 6\times 8^{\alpha}a^2b^4 + 3\times 16^{\alpha}a^4b^4 + 6\times 24^{\alpha}(r-2)a^4b^6 \\
&+ \frac{3}{2}\times 108^{\alpha}((r-3)^2+(r-3))a^6b^6 \\
S_a(f(a,b)) &= 3a^2b^4 + \frac{3}{4}(r-1)a^4b^4 + \frac{3}{2}(r-2)a^4b^6 + \frac{((r-3)^2+(r-3))}{4}a^6b^6 \\
S_b(f(a,b)) &= \frac{3}{2}a^2b^4 + \frac{3}{4}(r-1)a^4b^4 + (r-2)a^4b^6 + \frac{((r-3)^2+(r-3))}{4}a^6b^6 \\
S_aS_b(f(a,b)) &= \frac{1}{2}a^2b^4 + \frac{3}{16}(r-1)a^4b^4 + \frac{1}{4}(r-2)a^4b^6 + \frac{((r-3)^2+(r-3))}{24}a^6b^6 \\
J(f(a,b)) &= 6a^6 + 3(r-1)a^8 + 6(r-2)a^{10} + \frac{3((r-3)^2+(r-3))}{2}a^{12} \\
S_aJ(f(a,b)) &= a^6 + \frac{3}{8}(r-1)a^8 + \frac{3}{5}(r-2)a^{10} + \frac{1}{8}((r-3)^2+(r-3))a^{12} \\
S_aJD_aD_b(f(a,b)) &= 8a^6 + 6(r-1)a^8 + \frac{72}{5}(r-2)a^{10} + \frac{18}{4}((r-3)^2+(r-3))
\end{aligned}$$

Now, by using the operators of table

(1) First Zagreb index

$$M_1(TOX(r)) = (D_x + D_b)(f(a,b)|_{a=b=1} = 18r^2 - 6r$$

(2) Second Zagreb index

$$M_2(TOX(r)) = (D_aD_b)(f(a,b)|_{a=b=1} = 54r^2 - 78r + 36$$

(3) Second Modified Zagreb index

$$M_2^m(TOX(r)) = (S_aS_b)(f(a,b)|_{a=b=1} = \frac{r^2}{24} + \frac{11}{48}r + \frac{1}{16}$$

(4) Harmonic index

$$H(TOX(r)) = (2S_aJ)(f(a,b)|_{a=b=1} = \frac{r^2}{4} + \frac{7}{10}r + \frac{7}{20}$$

(5) Inverse sum

$$I(TOX(r)) = (S_aJD_aD_b)(f(a,b)|_{a=b=1} = \frac{9}{2}r^2 + \frac{21}{10}r + \frac{1}{5}$$

(6) Randic index

$$R_\alpha(TOX(r)) = (D_a^\alpha D_b^\alpha)(f(a,b)|_{a=b=1} = 6\times 8^\alpha + 3\times 16^\alpha(r-1) + 6\times 24^\alpha(r-2) + \frac{3}{2}\times 108^\alpha(r^2-5r+6)$$

4.2. Regular triangular oxide network *RTOX(r)*

Lemma 2. *The regular triangular oxide network RTOX(r) has* $3r^2+6r$ *edges and* $\frac{3}{2}r^2+\frac{9}{2}r+1$ *vertices.*

Theorem 3. *The M-polynomial for a regular triangular oxide network RTOX(r) is*

$$M(RTOX(r);a,b) = 2a^2b^2 + 6ra^2b^4 + (3r^2-2)a^4b^4 \tag{11}$$

Proof : From the above lemma

$$\begin{aligned} |V(RTOX(r)| &= \frac{3}{2}r^2+\frac{9}{2}r+1 \\ |E(RTOX(r)| &= 3r^2+6r \end{aligned}$$

RTOX(r) has three edge partitions as

$$\begin{aligned} |E_1(RTOX(r))| &= \{e=lm\in E(RTOX(r): d_l=d_m=2\} \\ |E_2(RTOX(r))| &= \{e=lm\in E(RTOX(r): d_l=2, d_m=4\} \\ |E_3(RTOX(r))| &= \{e=lm\in E(RTOX(r): d_l=d_m=4\} \end{aligned}$$

Where,

$$|E_1(RTOX(r))| = 2,\ |E_2(RTOX(r))| = 6r,\ |E_3(RTOX(r))| = 3r^2-2$$

From the definition of M-polynomial

$$\begin{aligned} M(RTOX(r);a,b) &= \sum_{r\le s} m_{rs}(RTOX(r))a^r b^s \\ &= \sum_{2\le 2} m_{22}(RTOX(r))a^2b^2 + \sum_{2\le 4} m_{24}(RTOX(r))a^2b^4 \\ &+ \sum_{4\le 4} m_{44}(RTOX(r))a^4b^4 \\ &= \sum_{lm\in E_1} m_{22}(RTOX(r))a^2b^2 + \sum_{lm\in E_2} m_{24}(RTOX(r))a^2b^4 \\ &+ \sum_{lm\in E_3} m_{44}(RTOX(r))a^4b^4 \end{aligned}$$

$$
\begin{aligned}
&= |E_1|a^2b^2 + |E_2|a^2b^4 + |E_3|a^4b^4 \\
&= 2a^2b^2 + 6ra^2b^4 + (3r^2-2)a^4b^4
\end{aligned}
$$

Theorem 4. *For a regular triangular oxide network RTOX(r) some degree based topological indices are*

$$
\begin{aligned}
M_1(RTOX(r)) &= (D_a + D_b)(f(a,b)|_{a=b=1} = 24r^2 + 36r - 8 \\
M_2(RTOX(r)) &= (D_aD_b)(f(a,b)|_{a=b=1} = 48r^2 + 48r - 24 \\
M_2^m(RTOX(r)) &= (S_aS_b)(f(a,b)|_{a=b=1} = \frac{3}{16}r^2 + \frac{3}{4}r + \frac{3}{8} \\
H(RTOX(r)) &= (2S_aJ)(f(a,b)|_{a=b=1} = \frac{3}{4}r^2 + 2r + \frac{1}{2} \\
I(RTOX(r)) &= S_aJD_aD_b(M(G;a,b))|_{a=b=1} = 6r^2 + 8r - 2 \\
R_\alpha(RTOX(r)) &= (D_a^\alpha D_b^\alpha)(f(a,b))|_{a=b=1} = 2\times 4^\alpha + 6\times 8^\alpha r + (3r^2-2)\times 16^\alpha
\end{aligned}
$$

Proof : From the previous theorem

$$M(RTOX(r);a,b) = f(a,b) = 2a^2b^2 + 6ra^2b^4 + (3r^2-2)a^4b^4$$

then,

$$
\begin{aligned}
D_a(f(a,b)) &= 4a^2b^2 + 12ra^2b^4 + 4(3r^2-2)a^4b^4 \\
D_b(f(a,b)) &= 4a^2b^2 + 24ra^2b^4 + 4(3r^2-2)a^4b^4 \\
D_aD_b(f(a,b)) &= 8a^2b^2 + 48ra^2b^4 + 16(3r^2-2)a^4b^4 \\
S_a(f(a,b)) &= a^2b^2 + 3ra^2b^4 + \frac{(3r^2-2)}{4}a^4b^4 \\
S_b(f(a,b)) &= a^2b^2 + \frac{3}{2}ra^2b^4 + \frac{(3r^2-2)}{4}a^4b^4 \\
S_aS_b(f(a,b)) &= \frac{1}{2}a^2b^2 + \frac{3}{4}ra^2b^4 + \frac{(3r^2-2)}{16}a^4b^4 \\
D_a^\alpha D_b^\alpha(f(a,b)) &= 2\times 4^\alpha + 6\times 8^\alpha r + (3r^2-2)\times 16^\alpha \\
J(f(a,b)) &= f(a,a) = 2a^4 + 6ra^6 + (3r^2-2)a^8 \\
S_aJ(f(a,b)) &= \frac{1}{2}a^4 + ra^6 + \frac{(3r^2-2)}{8}a^8 \\
S_aJD_aD_b(f(a,b)) &= 2a^4 + 8ra^6 + 2(3r^2-2)a^8
\end{aligned}
$$

Now using the operators given in table

(1) First Zagreb index

$$M_1(RTOX(r)) = (D_a + D_b)(f(a,b))|_{a=b=1} = 24r^2 + 36r - 8$$

(2) Second Zagreb index

$$M_2(RTOX(r)) = (D_aD_b)(f(a,b))|_{a=b=1} = 48r^2 + 48r - 24$$

(3) Second Modified Zagreb index

$$M_2^m(RTOX(r)) = (S_aS_b)(f(a,b))|_{a=b=1} = \frac{3}{16}r^2 + \frac{3}{4}r + \frac{3}{8}$$

(4) Harmonic index

$$H(RTOX(r)) = (2S_aJ)(f(a,b))|_{a=b=1} = \frac{3}{4}r^2 + 2r + \frac{1}{2}$$

(5) Inverse sum

$$I(RTOX(r)) = (S_aJD_aD_b)(f(a,b))|_{a=b=1}6r^2 + 8r - 2$$

(6) Randic index

$$R_\alpha(RTOX(r)) = (D_a^\alpha D_b^\alpha)(f(a,b))|_{a=b=1} = 2 \times 4^\alpha + 6 \times 8^\alpha r + (3r^2 - 2) \times 16^\alpha$$

4.3. Triangular silicate network *TSL(r)*

Lemma 3. *The triangular silicate network TSL(r) has* $3(r^2 + r)$ *edges and* $r^2 + 2r + 1$ *vertices.*

Theorem 5. *The M-polynomial of triangular silicate network TSL(r) for* $r \geq 4$ *is:*

$$\begin{aligned} M(TSL(r); a, b) &= 3a^3b^3 + 6ra^3b^6 + 3(r-1)a^6b^6 + \frac{3}{4}(r^2 - 3r + 2)a^3b^9 \\ &\quad +6(r-2)a^6b^9 + \frac{3}{4}(r^2 - 5r + 6)a^9b^9 \end{aligned}$$

Proof From the above lemma we have

$$\begin{aligned} |V(TSL(r))| &= r^2 + 2r + 1 \\ |E(TSL(r))| &= 3(r^2 + r) \end{aligned}$$

We know that *TSL(r)* has six edge partitions

$$\begin{aligned} |E_1(TSL(r))| &= \{e = lm \in E(TSL(r) : d_l = d_m = 3\} \\ |E_2(TSL(r))| &= \{e = lm \in E(TSL(r) : d_l = 3, d_m = 6\} \end{aligned}$$

$$
\begin{aligned}
|E_3(TSL(r))| &= \{e = lm \in E(TSL(r) : d_l = d_m = 6\} \\
|E_4(TSL(r))| &= \{e = lm \in E(TSL(r) : d_l = 3, d_m = 9\} \\
|E_5(TSL(r))| &= \{e = lm \in E(TSL(r) : d_l = 6, d_m = 9\} \\
|E_6(TSL(r))| &= \{e = lm \in E(TSL(r) : d_l = d_m = 9\}
\end{aligned}
$$

$|E_1(TSL(r))| = 3$, $|E_2(TSL(r))| = 6r$, $|E_3(TSL(r))| = 3(r-1)$,
$|E_4(TSL(r))| = \frac{3}{2}(r^2 - 3r + 2)$, $|E_5(TSL(r))| = 6(r-2)$, $|E_6(TSL(r))| = \frac{3}{2}(r^2 - 5r + 6)$
Now putting the values in the definition of M-polynomials as

$$
\begin{aligned}
M(TSL(r); a, b) &= \sum_{r \le s} m_{rs}(TSL(r)) a^r b^s \\
&= \sum_{3 \le 3} m_{33}(TSL(r)) a^3 b^3 + \sum_{3 \le 6} m_{36}(TSL(r)) a^3 b^6 \\
&+ \sum_{6 \le 6} m_{66}(TSL(r)) a^6 b^6 + \sum_{3 \le 9} m_{39}(TSL(r)) a^3 b^9 \\
&+ \sum_{6 \le 9} m_{69}(TSL(r)) a^6 b^9 + \sum_{9 \le 9} m_{99}(TSL(r)) a^9 b^9 \\
&= \sum_{lm \in E_1} m_{33}(TSL(r)) a^3 b^3 + \sum_{lm \in E_2} m_{36}(TSL(r)) a^3 b^6 \\
&+ \sum_{lm \in E_3} m_{66}(TSL(r)) a^6 b^6 + \sum_{lm \in E_4} m_{39}(TSL(r)) a^3 b^9 \\
&+ \sum_{lm \in E_5} m_{69}(TSL(r)) a^6 b^9 + \sum_{lm \in E_6} m_{99}(TSL(r)) a^9 b^9 \\
&= |E_1| a^3 b^3 + |E_2| a^3 b^6 + |E_3| a^6 b^6 + |E_4| a^3 b^9 + |E_5| a^6 b^9 + |E_6| a^9 b^9 \\
&= 3a^3 b^3 + 6r a^3 b^6 + 3(r-1) a^6 b^6 + \frac{3}{2}(r^2 - 3r + 2) a^3 b^9 \\
&+ 6(r-2) a^6 b^9 + \frac{3}{2}(r^2 - 5r + 6) a^9 b^9
\end{aligned}
$$

Theorem 6. *Some degree based topological indices of triangular silicate network TSL(r) are*

$$
\begin{aligned}
M_1(TSL(r)) &= (D_a + D_b)(f(a,b)|_{a=b=1} = 45r^2 - 9r \\
M_2(TSL(r)) &= (D_a D_b)(f(a,b)|_{a=b=1} = 162r^2 - 189r + 81 \\
M_2^m(TSL(r)) &= (S_a S_b)(f(a,b)|_{a=b=1} = \frac{2}{27} r^2 + \frac{29}{108} r + \frac{5}{36} \\
H(TSL(r)) &= (2 S_a J)(f(a,b)|_{a=b=1} = \frac{5}{12} r^2 + \frac{21}{20} r + \frac{2}{5}
\end{aligned}
$$

$$\begin{aligned} I(TSL(r)) &= (S_aJD_aD_b)(f(a,b)|_{a=b=1} = \frac{81}{8}r^2 - \frac{51}{40}r - \frac{9}{20} \\ R_\alpha(TSL(r)) &= (D_a^\alpha D_b^\alpha)(f(a,b)|_{a=b=1} = 3\times 9^\alpha + 6\times 18^\alpha r + 3\times 36^\alpha(r-1) \\ &+ \frac{3}{2}\times 27^\alpha(r^2-3r+2) + 6\times 54^\alpha(r-2) + \frac{3}{2}\times 81^\alpha(r^2-5r+6) \end{aligned}$$

Proof : From the above theorem we have

$$\begin{aligned} M(TSL(r);a,b) &= 3a^3b^3 + 6ra^3b^6 + 3(r-1)a^6b^6 + \frac{3}{2}(r^2-3r+2)a^3b^9 + 6(r-2)a^6b^9 \\ &+\frac{3}{2}(r^2-5r+6)a^9b^9 = f(a,b) \end{aligned}$$

Now,

$$D_a(f(a,b)) = 9a^3b^3 + 18ra^3b^6 + 18(r-1)a^6b^6 + \frac{9}{2}(r^2-3r+2)a^3b^9 + 36(r-2)a^6b^9 + \frac{27}{2}(r^2-5r+6)a^9b^9 \quad (12)$$

$$D_b(f(a,b)) = 9a^3b^3 + 36ra^3b^6 + 18(r-1)a^6b^6 + \frac{27}{2}(r^2-3r+2)a^3b^9 + 54(r-2)a^6b^9 + \frac{27}{2}(r^2-5r+6)a^9b^9 \quad (13)$$

$$D_aD_b(f(a,b)) = 27a^3b^3 + 108ra^3b^6 + 108(r-1)a^6b^6 + \frac{81}{2}(r^2-3r+2)a^3b^9 + 324(r-2)a^6b^9 + \frac{243}{2}(r^2-5r+6)a^9b^9 \quad (14)$$

$$D_a^\alpha D_b^\alpha = 3\times 9^\alpha a^3b^3 + 6\times 18^\alpha ra^3b^6 + 3\times 36^\alpha(r-1)a^6b^6 + \frac{3}{2}\times 27^\alpha(r^2-3r+2)a^3b^9 + 6\times 54^\alpha(r-2)a^6b^9 + \frac{3}{2}\times 81^\alpha(r^2-5r+6)a^9b^9 \quad (15)$$

$$S_a(f(a,b)) = a^3b^3 + 2ra^3b^6 + \frac{(r-1)}{2}a^6b^6 + \frac{(r^2-3r+2)}{2}a^3b^9 + (r-2)a^6b^9\frac{(r^2-5r+6)}{6}a^9b^9 \quad (16)$$

$$S_b(f(a,b)) = a^3b^3 + ra^3b^6 + \frac{(r-1)}{2}a^6b^6 + \frac{(r^2-3r+2)}{6}a^3b^9 + \frac{2}{3}(r-2)a^6b^9 + \frac{(r^2-5r+6)}{6}a^9b^9 \quad (17)$$

$$S_aS_b(f(a,b)) = \frac{1}{3}a^3b^3 + \frac{r}{3}a^3b^6 + \frac{(r-1)}{12}a^6b^6 + \frac{(r^2-3r+2)}{18}a^3b^9 + \frac{(r-2)}{9}a^6b^9 + \frac{(r^2-5r+6)}{54}a^9b^9 \quad (18)$$

$$J(f(a,b)) = 3a^6 + 6ra^9 + \frac{3}{2}(r^2-r)a^{12} + 6(r-2)a^{15} + \frac{3}{2}(r^2-5r+6)a^{18} \quad (19)$$

$$S_aJ(f(a,b)) = \frac{1}{2}a^6 + \frac{2}{3}ra^9 + \frac{(r^2-r)}{8}a^{12} + \frac{6(r-2)}{15}a^{15} + \frac{(r^2-5r+6)}{12}a^{18} \quad (20)$$

$$S_aJD_aD_b(f(a,b)) = \frac{9}{2}a^6 + 12ra^9 + \frac{9}{8}(r^2-3r+2)a^{12} + \frac{108}{5}(r-2)a^{15} + \frac{27}{4}(r^2-5r+6)a^{18} \quad (21)$$

Now, using the formula given in the table

(1) First Zagreb index

$$(1)M_1(TSL(r)) = (D_a + D_b)(f(a,b)|_{a=b=1} = 45r^2 - 9r$$

(2) Second Zagreb index

$$(2)M_2(TSL(r)) = (D_aD_b)(f(a,b)|_{a=b=1} = 162r^2 - 189r + 81$$

(3) Second Modified Zagreb index

$$(3)M_2^m(TSL(r)) = (S_aS_b)(f(a,b)|_{a=b=1} = \frac{2}{27}r^2 + \frac{29}{108}r + \frac{5}{36}$$

(4) Harmonic index

$$(4)H(TSL(r)) = (2S_aJ)(f(a,b)|_{a=b=1} = \frac{5}{12}r^2 + \frac{21}{20}r + \frac{2}{5}$$

(5) Inverse sum

$$(5)I(TSL(r)) = (S_aJD_aD_b)(f(a,b)|_{a=b=1} = \frac{81}{8}r^2 - \frac{51}{40}r - \frac{9}{20}$$

(6) Randic indea

$$(6)R_\alpha(TSL(r)) = (D_a^\alpha D_b^\alpha)(f(a,b)|_{a=b=1} = 3\times 9^\alpha + 6\times 18^\alpha r + 3\times 36^\alpha(r-1) + \frac{3}{2}\times 27^\alpha(r^2-3r+2) + 6\times 54^\alpha(r-2) + \frac{3}{2}\times 81^\alpha(r^2-5r+6)$$

4.4. Regular triangular silicate network *RTSL(r)*

Lemma 4. *The regular triangular silicate network RTSL(r) has* $6r^2+12r$ *edges and* $\frac{5}{2}r^2+\frac{13}{2}r+1$ *vertices.*

Theorem 7. *The M-polynomial of regular triangular silicate network RTSL(r) is:*

$$M(RTSL(r);a,b) = (3r+4)a^3b^3 + (3r^2+9r-2)a^3b^6 + (3r^2-2)a^6b^6 \tag{22}$$

Proof : As lemma we have

$$\begin{aligned}|V(RTSL(r))| &= \frac{5}{2}r^2+\frac{13}{2}r+1\\ |E(RTSL(r))| &= 6r^2+12r\end{aligned}$$

We know *RTSL(r)* has three edge partitions

$$\begin{aligned}|E_1(RTSL(r))| &= \{e=lm\in E(RTSL(r):d_l=d_m=3\}\\ |E_2(RTSL(r)| &= \{e=lm\in E(RTSL(r):d_l=3,d_m=6\}\\ |E_3(RTSL(r))| &= \{e=lm\in E(RTSL(r):d_l=d_m=6\}\end{aligned}$$

Such that:
$|E_1(RTSL(r))|$= 3r+4, $|E_2(RTSL(r))| = 3r^2+9r-2$, $|E_3(RTSL(r))|$=$3r^2-2$
Now using the definition of M-polynomial

$$\begin{aligned}M(RTSL(r);a,b) &= \sum_{r\le s} m_{rs}(RTSL(r))a^rb^s\\ &= \sum_{3\le 3} m_{33}(RTSL(r))a^3b^3 + \sum_{3\le 6} m_{36}(RTSL(r))a^3b^6\\ &+ \sum_{6\le 6} m_{66}(RTSL(r))a^6b^6\end{aligned}$$

$$
\begin{aligned}
&= \sum_{lm\in E_1} m_{33}(RTSL(r))a^3b^3 + \sum_{lm\in E_2} m_{36}(RTSL(r))a^3b^6 \\
&+ \sum_{lm\in E_3} m_{66}(RTSL(r))a^6b^6 \\
&= |E_1|a^3b^3 + |E_2|a^3b^6 + |E_3|a^6b^6 \\
&= (3r+4)a^3b^3 + (3r^2+9r-2)a^3b^6 + (3r^2-2)a^6b^6
\end{aligned}
$$

Theorem 8. *Some well-known degree based topological indices of RTSL(r) are:*

$$
\begin{aligned}
M_1(RTSL(r)) &= (D_a+D_b)(f(a,b))|_{a=b=1} = 36r^2+99r-18 \\
M_2(RTSL(r)) &= (D_aD_b)(f(a,b))|_{a=b=1} = 162r^2+189r-72 \\
M_2^m(RTSL(r)) &= (S_aS_b)(f(a,b))|_{a=b=1} = \frac{r^2}{4}+\frac{5}{6}r-\frac{5}{18} \\
H(RTSL(r)) &= (2S_aJ)(f(a,b))|_{a=b=1} = \frac{7}{6}r^2+3r+\frac{5}{18} \\
I(RTSL(r)) &= (S_aJD_aD_b)(f(a,b))|_{a=b=1} = 15r^2+21r-6 \\
R_\alpha(RTSL(r)) &= (D_a^\alpha D_b^\alpha)(f(a,b))|_{a=b=1} = (3r+4)\times 9^\alpha \\
&+ (3r^2+9r-2)\times 18^\alpha r + (3r^2-2)\times 36^\alpha
\end{aligned}
$$

Proof : From the above theorem we have

$$M(RTSL(r);a,b) = (3r+4)3a^3b^3 + (3r^2+9r-2)a^3b^6 + (3r^2-2)a^6b^6$$

Now,

$$
\begin{aligned}
D_a(f(a,b)) &= 3(3r+4)3a^3b^3 + 3(3r^2+9r-2)a^3b^6 + 6(3r^2-2)a^6b^6 \\
D_b(f(a,b)) &= 3(3r+4)3a^3b^3 + 6(3r^2+9r-2)a^3b^6 + 6(3r^2-2)a^6b^6 \\
D_aD_b(f(a,b)) &= 9(3r+4)3a^3b^3 + 18(3r^2+9r-2)a^3b^6 + 36(3r^2-2)a^6b^6 \\
D_a^\alpha D_b^\alpha &= (3r+4)\times 9^\alpha a^3b^3 + (3r^2+9r-2)\times 18^\alpha a^3b^6 + (3r^2-2)\times 36^\alpha a^6b^6 \\
S_a(f(a,b)) &= \frac{3r+4}{3}a^3b^3 + \frac{3r^2+9r-2}{3}a^3b^6 + \frac{3r^2-2}{6}a^6b^6 \\
S_b(f(a,b)) &= \frac{3r+4}{3}a^3b^3 + \frac{3r^2+9r-2}{6}a^3b^6 + \frac{3r^2-2}{6}a^6b^6 \\
S_aS_b(f(a,b)) &= (3r+4)a^3b^3 + \frac{3r^2+9r-2}{18}a^3b^6 + \frac{3r^2-2}{36}a^6b^6 \\
J(f(a,b)) &= (3r+4)a^6 + (3r^2+9r-2)a^9 + (3r^2-2)a^{12} \\
S_aJ(f(a,b)) &= \frac{(3r+4)}{6}a^6 + \frac{(3r^2+9r-2)}{9}a^9 + \frac{(3r^2-2)}{12}a^{12} \\
S_aJD_aD_b(f(a,b)) &= (3r+4)a^6 + 2(3r^2+9r-2)a^9 + 3(3r^2-2)a^{12}
\end{aligned}
$$

Now by the operators of table

(1) First Zagreb index

$$M_1(RTSL(r)) = (D_a + D_b)(f(a,b))|_{a=b=1} = 36r^2 + 99r - 18$$

(2) Second Zagreb index

$$M_2(RTSL(r)) = (D_a D_b)(f(a,b))|_{a=b=1} = 162r^2 + 189r - 72$$

(3) Second Modified Zagreb index

$$M_2^m(RTSL(r)) = (S_a S_b)(f(a,b))|_{a=b=1} = \frac{r^2}{4} + \frac{5}{6}r - \frac{5}{18}$$

(4) Harmonic index

$$H(RTSL(r)) = (2S_a J)(f(a,b))|_{a=b=1} = \frac{7}{6}r^2 + 3r + \frac{5}{18}$$

(5) Inverse sum

$$I(RTSL(r)) = (S_a J D_a D_b)(f(a,b))|_{a=b=1} = 15r^2 + 21r - 6$$

(6) Randic index

$$R_\alpha(RTSL(r)) = (D_a^\alpha D_b^\alpha)(f(a,b))|_{a=b=1} = (3r+4)\times 9^\alpha + (3r^2+9r-2)\times 18^\alpha r + (3r^2-2)\times 36^\alpha.$$

5. Graphical Representation

M-polynomials' graphical behavior for different networks may provide insight into the structural features they have and how they transform when the size or connectedness of the network varies. Let's examine the M-polynomials' graphical behaviors for the networks given below in Figures (1-4):

- First Zagreb index (FZI).
- Second Zagreb index (SZI).
- Second modified Zagreb indices (SMZI).

5.1. First Zagreb index for *TOX(r)*, *RTOX(r)*, *TSL(r)* & *RTSL(r)*

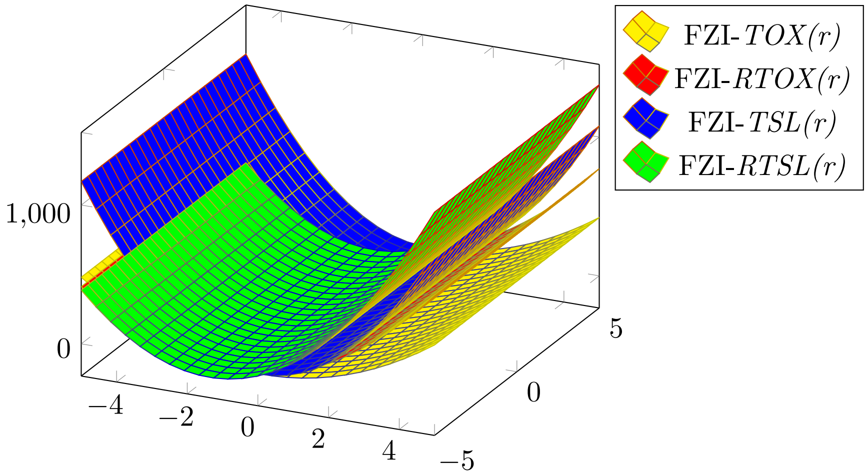

Figure 1: First Zagreb index for TOX(r), RTOX(r), TSL(r) & RTSL(r)

5.2. Second Zagreb index for *TOX(r)*, *RTOX(r)*, *TSL(r)* & *RTSL(r)*

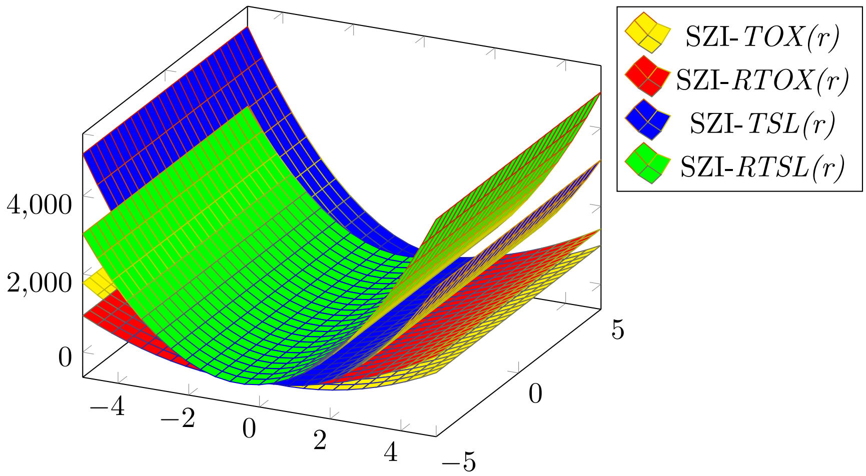

Figure 2: Second Zagreb index for TOX(r), RTOX(r), TSL(r) & RTSL(r)

5.3. Second Modified Zagreb index for *TOX(r)*, *RTOX(r)*, *TSL(r)*

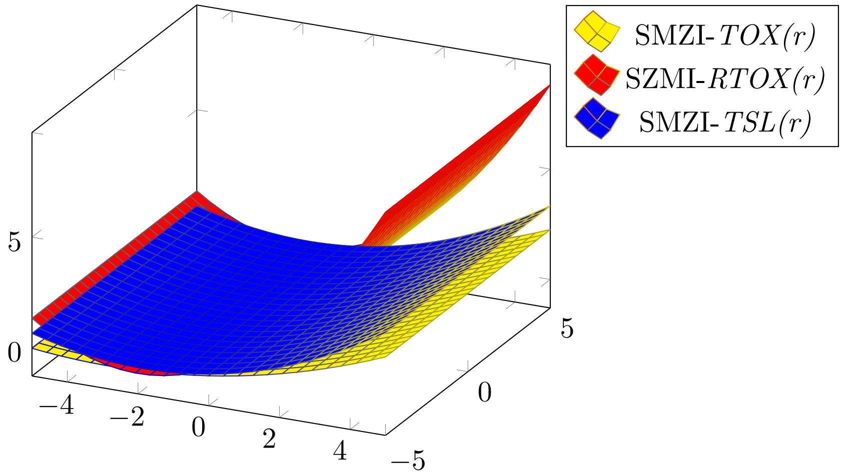

Figure 3: Second Modified Zagreb index for TOX(r), RTOX(r), TSL(r)

5.4. Second Modified Zagreb index for *RTSL(r)*

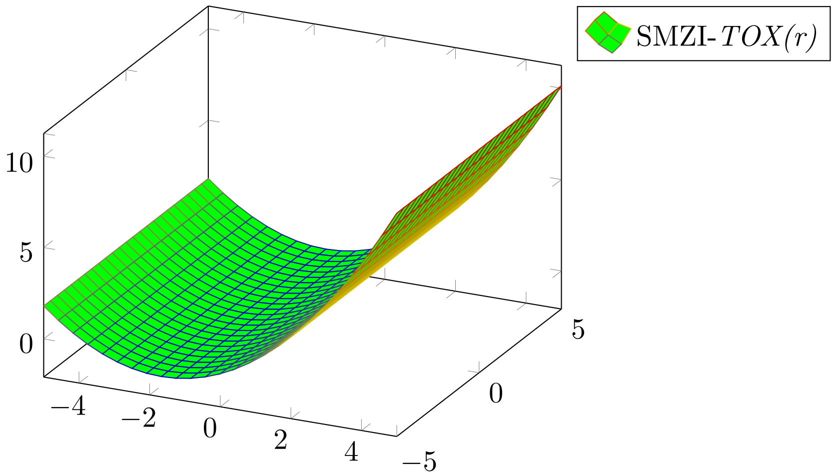

Figure 4: Second Modified Zagreb index for RTSL(r)

6. Applications

M-Polynomials are mostly used in graph theory because of their effectiveness in analysing degree-based topological indices. M-Polynomials provide as a consistent source for the collection of the various topological indices connected with a graph's vertex degrees. These numerical descriptors, known as indices, are particularly helpful in chemical graph theory, where the graph is used to represent a molecule. Chemical Graph theory plays important role in the everyday life applications such as image processing unit, bio sensors, mathematical chemistry, computer science, artificial intelligence, social science and medicine.

With the help of quantitative structure property relationship study (QSPRs) and quantitative structure activity relationship study (QSARs), the topology [23, 29] of the molecular structures Triangular oxide TOX(r), Regular triangular oxide RTOX(r), Triangular silicate TSL(r) and Regular triangular silicate RTSL(r) obtained from the given chemical compound can be correlated and further discussed for the latest research works being used by many pharmacists, chemists and researchers to get better understanding in their fields.

7. Conclusions and Novelty

In conclusion, because of their straightforward counting schemes, the M-polynomials for the networks of triangle oxide and triangle silicate exhibit linear behaviors on the graph. Regular versions of these networks may show more ordered patterns in their M-polynomial graphs, but more specific information about their structures and counting techniques would be needed to create accurate graphical representations. In analysing the relationship between a graph's characteristics and structure (as represented by vertex degrees), M-polynomials are crucial. Researchers can examine the correlation between different topological indices and distinct chemical or physical properties of the molecule represented by the graph, as M-Polynomials provide a practical method for obtaining these indices. For example, research could look into the relationship between a molecule's boiling point and the Zagreb index, which is derived from an M-Polynomial. This may offer insightful information about the relationship between a molecule's structure and behavior. Consideration of the molecular structures of Triangular oxide TOX(r), Regular triangular oxide RTOX(r), Triangular silicate TSL(r) & Regular triangular silicate RTSL(r) networks.

- Association of the molecular structures with their corresponding mathematical graphs.
- Application of M-Polynomials on the above-mentioned molecular graphs to get new and closed generalized formulas.
- The new developed formulas can be applied in mathematical chemistry and can also be used by chemists, pharmacists and researchers for more scientific experiments or lab works.

For the molecular structure of the networks of triangular oxide (TOX(r), regular triangular oxide (RTOX(r), triangular silicate (TSL(r), and regular triangular silicate (RTSL(r)), we have calculated the M-Polynomials [17]. The findings indicate which features influence invariants the most [3, 7, 10, 12, 18, 22, 23, 25, 29], leading one to wonder if networks for administrative structures could be designed to be more efficient in the flow of information. It has also been discussed to compare the graphical behaviors of the chemical compounds indicated above. Furthermore, we can obtain a variety of physicochemical properties-such as boiling point, vaporization, enthalpy, entropy, viscosity, density of material, and many more-without conducting laboratory tests by using linear, quadratic, and logarithmic regression models.

Statement of Contributions

All authors have equally contributed.

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