Research Article

Topological Properties of Degree-Based Invariants via M-Polynomial Approach

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Abstract

Chemical graph theory provides a link between molecular properties and a molecular graph. The M-polynomial is emerging as an efficient tool to recover the degree-based topological indices in chemical graph theory. In this work, we give the closed formulas of redefined first and second Zagreb indices, modified first Zagreb index, nano-Zagreb index, second hyper-Zagreb index, Randić index, reciprocal Randić index, first Gourava index, and product connectivity Gourava index via M-polynomial. We also present the M-polynomial of silicate network and then closed formulas of topological indices are applied on the silicate network.

1. Introduction

Chemical graph theory (CGT) provides a connection between chemical structure and discrete mathematics. The ordered pair between the vertex set and edge set is considered a graph. In CGT, a graph is the replacement of molecular structure in which vertices are replaced by atoms and edges are considered as bonds. A topological index or invariant is an important tool of CGT that can guess the properties of the chemical species [1]. A mapping \( I: Y \rightarrow \mathbb{R} \) is called a topological invariant if \( Y, G, H \in \mathbb{Y} \) and \( G \) and \( H \) are isomorphic to each other if and only if \( I(G) = I(H) \), where \( \mathbb{Y} \) is the collection of molecular structure. Topological indices are a very useful application in structure-activity and structure-property modeling [2]. These are the best predictor to determine the physical, chemical, and biological behavior of the chemical substances [3].

Without performing any testing, topological indices analyze many physicochemical properties of chemical compounds. Topological indices analyze the physical characteristics such as molar volume, melting point, surface tension, boiling point, molar refraction, and heats of vaporization.

Topological indices also represent the biological behavior of compounds such as pH regulation, stimulation of cell growth, lipophilicity, toxicity, and nutrition. Hence, these topological indices may be helpful to know the chemical and physical characteristics and biological behaviors.

The first topological index is the Wiener index which was initiated by Wiener in 1947 [4]. After that, thousands of indices have been designed till now [5]. A degree-dependent topological index for the graph \( G \) is defined as

\[
I(G) = \sum_{e=xy, e \in E_G} f(d_x, d_y).
\]  

(1)

In the chemical graph, by counting the same end-degree edges, then equation (1) can be rewritten as
where \( \{d_x, d_y\} = \{j, k\} \) and the total number of edges \( xy \) is denoted by \( m_{jk} \).

In 2013, Ranjini et al. introduced the new version of Zagreb indices known as redefined second and third Zagreb indices defined as [6]

\[
\text{ReZG}_1 = \sum_{xy \in E(G)} \frac{d_x + d_y}{d_x d_y},
\]

\[
\text{ReZG}_2 = \sum_{xy \in E(G)} \frac{d_x d_y}{d_x + d_y}.
\]

In 2003, the theory of Zagreb indices was reviewed in [7] written by Nikolić et al. and the new index was named as the modified first Zagreb index defined as

\[
mM_1(G) = \sum_{xy \in E(G)} \frac{1}{d_x + d_y}.
\]

In 2019, Jahanbani and Shooshtary [8] presented the nano-Zagreb index stated as:

\[
NZ(G) = \sum_{xy \in E(G)} |d^2_x - d^2_y|.
\]

Alameri [9] proposed the second hyper Zagreb index in 2021 and defined as

\[
HM_2(G) = \sum_{xy \in E(G)} d^2_x d^2_y.
\]

A bond-additive topological index was proposed by Randić in 1975 [10]. This index is a frequently examined index among all previously topological descriptors:

\[
R_{(1/2)}(G) = \sum_{xy \in E(G)} \frac{1}{\sqrt{d^2_x d^2_y}}.
\]

In 2014, Gutman et al. [11] presented the reciprocal Randić index defined as

\[
RR(G) = \sum_{xy \in E(G)} \sqrt{d^2_x d^2_y}.
\]

In 2014, Kulli [12] presented the first Gourava index defined as

\[
G_1O(G) = \sum_{xy \in E(G)} (d_x + d_y + d_x d_y).
\]

In 2017, Kulli [13] presented the product connectivity Gourava index and defined as

\[
PGO(G) = \sum_{xy \in E(G)} \frac{1}{(d_x + d_y)(d_x d_y)}.
\]

By using different tools, we convert the molecular graph into some algebraic polynomial. Using these polynomials, the structural properties are determined easily [14].

### 2. Main Results

In the present section, proofs of closed formulas mentioned in Table 1 are provided.
Theorem 1. If $M_G(u, v)$ represents the $M$-polynomial for the graph $G$, then the redefined first Zagreb index is also calculated as $\text{Re}ZG_1(G) = S_uS_v(D_u + D_v)M_G(u, v)|_{u=v=1}$.

Proof. By taking

$$S_uS_v(D_u + D_v)M_G(u, v) = S_uS_v(D_u + D_v) \sum_{\psi \leq j \leq k \leq \Psi} m_{jk}u^jv^k$$

$$= S_uS_v(D_u \sum_{\psi \leq j \leq k \leq \Psi} m_{jk}u^jv^k + D_v \sum_{\psi \leq j \leq k \leq \Psi} m_{jk}u^jv^k)$$

$$= S_uS_v \left( \sum_{\psi \leq j \leq k \leq \Psi} jm_{jk}u^jv^k + \sum_{\psi \leq j \leq k \leq \Psi} km_{jk}u^jv^k \right)$$

$$= S_u \sum_{\psi \leq j \leq k \leq \Psi} (j + k)m_{jk}u^jv^k$$

$$= S_u \sum_{\psi \leq j \leq k \leq \Psi} \frac{(j + k)}{k}m_{jk}u^jv^k$$

$$= \sum_{\psi \leq j \leq k \leq \Psi} \frac{(j + k)}{jk}m_{jk}u^jv^k,$$

now $S_uS_v(D_u + D_v)M_G(u, v)|_{u=v=1} = \sum_{\psi \leq j \leq k \leq \Psi} \frac{(j + k)}{jk}m_{jk}$

$$= \sum_{x,y \in E_G} d_x + d_y.$$

Hence, $\text{Re}ZG_1(G) = S_uS_v(D_u + D_v)M_G(u, v)|_{u=v=1}$.

Theorem 2. If $M_G(u, v)$ represents the $M$-polynomial of the graph $G$, then the redefined second Zagreb index is given by $\text{Re}ZG_2(G) = S_uJD_uD_vM_G(u, v)|_{u=1}$.

Proof. By taking

$$S_uJD_uD_vM_G(u, v) = S_uJD_uD_v \sum_{\psi \leq j \leq k \leq \Psi} m_{jk}u^jv^k$$

$$= S_uJD_u \sum_{\psi \leq j \leq k \leq \Psi} km_{jk}u^jv^k$$

$$= S_uJ \sum_{\psi \leq j \leq k \leq \Psi} jkm_{jk}u^jv^k$$

$$= S_u \sum_{\psi \leq j \leq k \leq \Psi} jkm_{jk}u^{j+k}$$

$$= \sum_{\psi \leq j \leq k \leq \Psi} \frac{j}{j + k}m_{jk}u^{j+k},$$

now $S_uJD_uD_vM_G(u, v)|_{u=1} = \sum_{\psi \leq j \leq k \leq \Psi} \frac{j}{j + k}m_{jk}$

$$= \sum_{\psi \leq j \leq k \leq \Psi} \frac{d_x + d_y}{d_x + d_y}.$$
Hence, \( m_1(G) = S_u J_{M_G}(u, v)|_{u=1} \).

**Theorem 3.** If \( M_G(u, v) \) represents the \( M \)-polynomial of the graph \( G \), then the modified first Zagreb index is computed by

\[
m_M^1(G) = SuJ_{M_G}(u, v)|_{u=1}.
\]

**Proof.** By taking

\[
S_u J_{M_G}(u, v) = \sum_{v \in S_u \cup S_v} m_{jk} u^j v^k
\]

\[
= \sum_{v \in S_u \cup S_v} \frac{1}{j + k} m_{jk} u^j v^k,
\]

now \( S_u J_{M_G}(u, v)|_{u=1} = \sum_{v \in S_u \cup S_v} \frac{1}{j + k} m_{jk} \)

\[
= \sum_{x \in E_G} \frac{1}{d_x^2 + d_y^2} \tag{15}
\]

\[
(D_v^2 - D_u^2)M_G(u, v) = (D_v^2 - D_u^2) = \sum_{v \in S_u \cup S_v} m_{jk} u^j v^k
\]

\[
= D_v^2 \sum_{v \in S_u \cup S_v} m_{jk} u^j v^k - D_u^2 \sum_{v \in S_u \cup S_v} m_{jk} u^j v^k
\]

\[
= \sum_{v \in S_u \cup S_v} j^2 m_{jk} u^j v^k - \sum_{v \in S_u \cup S_v} j^2 m_{jk} u^j v^k
\]

\[
= \sum_{v \in S_u \cup S_v} (k^2 - j^2) m_{jk} u^j v^k, \tag{16}
\]

now \( (D_v^2 - D_u^2)M_G(u, v)|_{u=1} = \sum_{v \in S_u \cup S_v} (k^2 - j^2) m_{jk} \)

\[
= \sum_{x \in E_G} |d_x^2 - d_y^2|.
\]

Hence, \( NZ(G) = (D_v^2 - D_u^2)M_G(u, v)|_{u=1} \).

**Proof.** By taking

\[
D_u^2 D_v^2 M_G(u, v) = D_u^2 D_v^2 = \sum_{v \in S_u \cup S_v} m_{jk} u^j v^k
\]

\[
= D_u^2 \sum_{v \in S_u \cup S_v} k^2 m_{jk} u^j v^k
\]

\[
= \sum_{v \in S_u \cup S_v} j^2 k^2 m_{jk} u^j v^k.
\]
Proof. By taking
\[ S_u^{1/2} S^G_{v}(u, v) = S_u^{1/2} S_v^{1/2} = \sum_{\psi \leq j \leq k} m_{jk} u^{1/2} v^{k} \]
\[ = S_u^{1/2} \sum_{\psi \leq j \leq k} \frac{1}{\sqrt{k}} m_{jk} u^{1/2} v^{k} \]
\[ = \sum_{\psi \leq j \leq k} \frac{1}{\sqrt{k}} m_{jk} u^{1/2} v^{k}, \]
then the Randić index is computed as
\[ \text{Randić index} = \sum_{\psi \leq j \leq k} \frac{1}{\sqrt{k}} m_{jk} u^{1/2} v^{k}. \]

Hence, \( HM_2(G) = D_u^{1/2} D_v^{1/2} M_G(u, v) \)|_{u=v=1}. □

**Theorem 6.** If \( M_G(u, v) \) represents the M-polynomial of the graph \( G \), then the Randić index is computed as
\[ R_{-(1/2)}(G) = S_u^{1/2} S^G_{v}(u, v) |_{u=v=1}. \]

**Proof.** By taking
\[ S_u^{1/2} S^G_{v}(u, v) = S_u^{1/2} S_v^{1/2} = \sum_{\psi \leq j \leq k} m_{jk} u^{1/2} v^{k} \]
\[ = \sum_{\psi \leq j \leq k} \frac{1}{\sqrt{k}} m_{jk} u^{1/2} v^{k}, \]
then the reciprocal Randić index is given by
\[ RR(G) = D_u^{1/2} D_v^{1/2} M_G(u, v) |_{u=v=1}. \]

**Theorem 7.** If \( M_G(u, v) \) represents the M-polynomial for the graph \( G \), then the reciprocal Randić index is given by
\[ RR(G) = D_u^{1/2} D_v^{1/2} M_G(u, v) |_{u=v=1}. \]

**Proof.** By taking
\[ D_u^{1/2} D_v^{1/2} M_G(u, v) = D_u^{1/2} D_v^{1/2} \sum_{x \in E(G)} m_{jk} u^{\psi} v^{\psi} \]
\[ = D_u^{1/2} \sum_{\psi \leq j \leq k} \sqrt{k} m_{jk} u^{\psi} v^{\psi} \]
\[ = \sum_{\psi \leq j \leq k} \sqrt{j k} m_{jk} u^{\psi} v^{\psi}, \]
now \( D_u^{1/2} D_v^{1/2} M_G(u, v) |_{u=v=1} = \sum_{x \in E(G)} m_{jk} u^{\psi} v^{\psi} \)
\[ = \sum_{x \in E(G)} m_{jk} u^{\psi} v^{\psi}, \]

Hence, \( RR(G) = D_u^{1/2} D_v^{1/2} M_G(u, v) |_{u=v=1}. \) □

**Theorem 8.** If \( M_G(u, v) \) represents the M-polynomial of the graph \( G \), then the first Gourava index is computed as
\[ G_1(G) = (D_u + D_v + D_u D_v)M_G(u, v) |_{u=v=1}. \]

**Proof.** By taking
\[ (D_u + D_v + D_u D_v)M_G(u, v) = (D_u + D_v + D_u D_v) \sum_{\psi \leq j \leq k} m_{jk} u^{\psi} v^{\psi} \]
\[ = D_u \sum_{\psi \leq j \leq k} m_{jk} u^{\psi} v^{\psi} + D_v \sum_{\psi \leq j \leq k} m_{jk} u^{\psi} v^{\psi} + D_u D_v \sum_{\psi \leq j \leq k} m_{jk} u^{\psi} v^{\psi} \]
\[ = \sum_{\psi \leq j \leq k} j m_{jk} u^{\psi} v^{\psi} + \sum_{\psi \leq j \leq k} k m_{jk} u^{\psi} v^{\psi} + D_u \sum_{\psi \leq j \leq k} k m_{jk} u^{\psi} v^{\psi} \]
\[ = \sum_{\psi \leq j \leq k} j k m_{jk} u^{\psi} v^{\psi} + \sum_{\psi \leq j \leq k} j k m_{jk} u^{\psi} v^{\psi} \]
\[ = \sum_{\psi \leq j \leq k} (j + k) m_{jk} u^{\psi} v^{\psi}, \]
now \( (D_u + D_v + D_u D_v)M_G(u, v) |_{u=v=1} = \sum_{\psi \leq j \leq k} (j + k) m_{jk} u^{\psi} v^{\psi} \)
\[ = \sum_{\psi \leq j \leq k} (d_x + d_y + d_x d_y). \]
Hence, 
\[ G_1O(G) = (D_u + D_v + D_uD_v)M_G \]
\[(u, v)\big|_{u=v=1}. \]

**Theorem 9.** If \( M_G(u, v) \) represents the \( M \)-polynomial for the graph \( G \), then the product connective Gourava index is computed as
\[ PGO(G) = S_u^{1/2}S_v^{1/2}M_G(u, v)\big|_{u=1}. \]

**Proof.** By taking
\[ S_u^{1/2}J_{1/2}S_v^{1/2}M_G(u, v) = S_u^{1/2}J_{1/2}S_v^{1/2} \sum_{\psi \leq j \leq k \leq \Psi} m_{jk}u^jv^k, \]
\[ = S_u^{1/2}J_{1/2} \sum_{\psi \leq j \leq k \leq \Psi} \frac{1}{\sqrt{k}}m_{jk}u^jv^k, \]
\[ = S_u^{1/2}J_{1/2} \sum_{\psi \leq j \leq k \leq \Psi} \frac{1}{\sqrt{k}}m_{jk}u^{j+k}, \]
\[ = \sum_{\psi \leq j \leq k \leq \Psi} \frac{1}{\sqrt{(j+k)k}}m_{jk}, \]
\[ \text{now} S_u^{1/2}J_{1/2}S_v^{1/2}M_G(u, v)\big|_{u=1}, \]
\[ = \sum_{\psi \leq j \leq k \leq \Psi} \frac{1}{\sqrt{(j+k)k}}m_{jk}, \]
\[ = \sum_{x,y \in E_G} \frac{1}{(d_x + d_y)(d_x d_y)} \]
\[ \text{Hence,} \quad PGO(G) = S_u^{1/2}J_{1/2}S_v^{1/2}M_G(u, v)\big|_{u=1}. \]

**3. Chemical Graph of Silicate Network**

The chemical graph of the silicate network (\( SL_n \)) is shown in Figure 1, where \( n \) is the total number of hexagons present between the center of the network and the boundary of \( SL_n \). In Figure 1, blue and red dots represent the vertices having degrees 3 and 6, respectively. The edges having end-degrees (3, 3), (3, 6), and (6, 6) are represented with yellow, green, and brown lines, respectively. Table 2 shows the vertex partitions, and Table 3 represents the edge partitions of \( SL_n \). In this present work, we extract some topological indices via \( M \)-polynomial of \( SL_n \).

**4. M-Polynomial and Topological Invariants of Silicate Network**

**Theorem 10.** If \( SL_n \) represent a silicate network, then \( M \)-polynomial of \( SL_n \) is
\[ M_{SL_n}(u, v) = 6n\; u^3v^3 + 6n(3n + 1)u^3v^6 + 6n(3n - 2)u^6v^6 \] [22].

The surface plot of \( M \)-polynomial of silicate network is shown in Figure 2.
Proof

(1) The redefined first Zagreb index:

\[ D_uM_G(u, v) = 18n u^3 v^3 + 18n(3n + 1) u^3 v^6 + 36n (3n - 2) u^6 v^6 \]

(2) The redefined second Zagreb index:

\[ D_uD_vM_G(u, v) = 54n u^3 v^3 + 108n (3n + 1) u^3 v^6 + 216n (3n - 2) u^6 v^6 \]

(3) The modified first Zagreb index:

\[ J_M_G(u, v) = nu^3 + 2/3n(3n + 1) u^3 v^6 + 1/2n(3n - 2) u^6 v^6 \]

(4) The modified second Zagreb index:

\[ S_{p}S_j(u, v) = 12nu^3 + 18n(3n + 1) u^3 v^6 + 72n (3n - 2) u^6 v^6 \]
\[ D_v M_G(u, v) = 18nu^3v^3 + 36n(3n + 1)u^3v^6 + 36n(3n - 2)u^6v^3 \]
\[ D_u D_v M_G(u, v) = 54nu^3v^3 + 108n(3n + 1)u^3v^6 + 216n(3n - 2)u^6v^3 \]
\[ (D_u + D_v + D_u D_v) M_G(u, v) = 90nu^3v^3 + 162n(3n + 1)u^3v^6 + 288n(3n - 2)u^6v^3 \]
\[ G_1[SL_n] = (D_u + D_v + D_u D_v) M_G(u, v)|_{u=v=1} = 1350n^7 - 324n \]

(9) The product connective Gourava index:
\[ S_{1/2}^{u} M_G(u, v) = 2\sqrt{3}nu^3v^3 + \sqrt{6n(3n + 1)}u^3v^6 + \sqrt{6n(3n - 2)}u^6v^3 \]
\[ S_{1/2}^{u} S_{1/2}^{v} M_G(u, v) = 2nu^3v^3 + \sqrt{3n(3n + 1)}u^3v^6 + n(3n - 2)u^6v^3 \]
\[ J_{S_{1/2}^{u}} S_{1/2}^{v} M_G(u, v) = 2nu^3v^3 + \sqrt{3n(3n + 1)}u^3v^6 + n(3n - 2)u^6v^3 \]
\[ J_{S_{1/2}^{u}} S_{1/2}^{v} M_G(u, v) = \sqrt{6/3nu^3v^3 + \sqrt{2/3n(3n + 1)u^3v^6 + 3/6n(3n - 2)u^6v^3}} \]
\[ GPO[SL_n] = S_{1/2}^{u} J_{S_{1/2}^{u}} S_{1/2}^{v} M_G(u, v)|_{u=v=1} = 1/2(2\sqrt{3} + \sqrt{3} \sqrt{n + 3/\sqrt{3} + \sqrt{6}n}) \]

The plot of topological indices of \( SL_n \) is shown in Figure 3. According to the figure, product connective Gourava index, modified first Zagreb index, and redefined first Zagreb index have low values as compared to others. \( \square \)

5. Conclusion
In the paper, we gave some new formulas to find the vertex degree-dependent topological indices via M-polynomial. These formulas were then applied to the silicate network. These indices have valuable information about the molecular structure. The proposed new technique gave vast application in QSAR/QSPR to analyze the chemical structure. The results obtained are also plotted.

Data Availability
No data were used to support the study.

Conflicts of Interest
The authors declare that they have no conflicts of interest.

References