M-polynomial-based topological indices of metal-organic networks

1 Introduction

Molecular hydrogen is an odorless, tasteless, colorless, nontoxic, nonmetallic, and nominal molecule in the world with very high flammability scale. On the other hand, it is a next-generation and environmental friendly source of fuel (Petit and Bandosz, 2009). As molecular hydrogen, it is useful in different fuel cells to power engine that is very beneficial for environment. However, hydrogen gas is odorless which makes a little bit leaking identification nearly not possible for humans. The current guiding laws established by the US Energy Department, put the attention on the detecting speed of the tool which must be detect 1 per cent of volume of smell-less molecular hydrogen in air in just 60 seconds.

Koo et al. (2017) prepared a fast molecular hydrogen detecting instrument containing metal nodes and organic ligands recognized as MON with the assistance of palladium (Pd) nanowires. This instrument must sense of hydrogen leaking intensity less than one per cent in only seven seconds. Further, except sensing as well as detecting, the MON shows very useful physico-chemical properties such as changing organic ligands (Yin et al., 2015), grafting active groups (Hwang et al., 2008), post synthetic ligand, preparing composites with different substances (Ahmed and Jhung, 2014), impregnating suitable active material (Thornton et al., 2009), and ion exchange (Kim et al., 2012). Seetharaj et al. (2019) presented the relation among the temperature, solvent, architectures, pH and molar ratio of the metal-organic networks. The MON is also utilized for the separation, purification (Lin et al., 2019), precursor for the formation of different nano-structure (Yap et al., 2017) and energy storage in batteries (Xu et al., 2017). In 2019, Wasson defined the concept of linker competition with the help of MON for topological insights (Wasson et al., 2019).

Graph theory discovered the important tools in the field of chemical graph theory which is utilized to study the several kinds of organic compounds and studied their characteristics. The computed TI of the molecular graph is the numeric value that characteristics chemical reactivates, physical properties and biological
activities (Gonzalez-Diaz et al., 2007) of the organic compounds such as boiling, melting, and flash points; heat of formation; surface tension, pressure, retention time in chromatographic, density, heat of evaporation, temperature, and partition coefficient (Liu et al., 2019a, 2019b). Harry Wiener studied a distance-based TI in chemical graph theory for the paraffin’s boiling point (Wiener, 1947). The most important TIs are degree-based TIs that are derived with the help of degree of nodes of the molecular structure and that is also mentioned in the survey regarding topological indices. In 1972, Gutman and Trinajstić described a degree-based descriptor famous as the first and second Zagreb indices to calculate the total π-electron energy of the chemical compounds (Gutman and Trinajstić, 1972).

Furthermore, topological indices show a vital role in the field of quantitative structures activity relationships or quantitative structures property relationships to describe any structure with a chemical and biological activity or property. The aforesaid relation is denoted as \( P = f(M) \) and \( P \) is a property or activity and \( M \) is a molecular structure (Devillers et al., 1997). The topological indices of various structures such as carbon nanotubes, oxide, icosahedral honeycomb, hexagonal, octahedral, benzenoids, silicate, titania nanotube, hexagonal, and fullerenes are discussed in Javaid et al. (2016). For further details see Chu et al. (2020) and Zhang et al. (2019).

In this paper, we compute the M-polynomials for two different metal-organic networks \( MON_1(n) \) and \( MON_2(n) \) with increasing layers of both organic ligands and metal vertices and with the assistance of these M-polynomials – the various TIs such as first and second Zagreb indices, second modified Zagreb index, general and reciprocal general Randić indices, symmetric division deg, inverse sum, harmonic, and the augmented Zagreb indices are computed. In the end, a comparison among the obtained topological indices with the assistance of graphical presentation is also involved. The rest of the paper is settled as: Section 2 includes the different techniques and definitions that are utilized in various outcomes. Sections 3 and 4 have the major computations in order to M-polynomials that are used in certain TIs related to \( MON_1(n) \) and \( MON_2(n) \) and Section 5 contains the comparison and conclusions.

2 Preliminaries

A molecular graph \( G = (V(G), E(G)) \), \( V(G) = \{x_1, x_2, x_3, ..., x_n\} \) and \( E(G) \) are nodes (metals or organic ligands) and edge-set (bonds among the different atoms) of \( G \), respectively. The \( |V(G)| = v \) and \( |E(G)| = e \) is the order and size of \( G \), respectively. The number of edges which are incident on a vertex is known as degree of \( \varrho(x) \).

In a simple and connected graph, a path is occurring within two nodes and the distance within two nodes \( x \) and \( y \), represented as \( \varrho(x, y) \), in a graph \( G \). In the current discussion, a graph is simple and connected, having no loops and multiple edges.

2.1 First and second Zagreb indices

Let \( G \) be a molecular graph, then its first and second Zagreb indices are:

\[
M_1(G) = \sum_{xy \in E(G)} [\varrho(x) + \varrho(y)],
\]

\[
M_2(G) = \sum_{xy \in E(G)} [\varrho(x) \times \varrho(y)].
\]

2.2 General Randić index

If \( R \) is the set of real numbers and \( G \) be a connected graph, so the general Randić index is given as:

\[
R_u(G) = \sum_{xy \in E(G)} [\varrho(x) \times \varrho(y)]^u.
\]

2.3 Symmetric division deg index

For a molecular graph \( G \), the symmetric division deg index is:

\[
SDD(G) = \sum_{xy \in E(G)} [\min(\varrho(x), \varrho(y)) + \max(\varrho(x), \varrho(y))].
\]

2.4 Harmonic index

For a molecular graph \( G \), the harmonic index is:

\[
H(G) = \sum_{xy \in E(G)} \frac{2}{\varrho(x) + \varrho(y)}.
\]

2.5 Inverse sum index

For a molecular graph \( G \), the inverse sum index is:

\[
IS(G) = \sum_{xy \in E(G)} \frac{\varrho(x) \times \varrho(y)}{\varrho(x) + \varrho(y)}.
\]
2.6 Augmented Zagreb index

For a molecular graph \( G \), the augmented Zagreb index is:

\[
A_{ZG}(G) = \sum_{e \in E(G)} \left\{ \frac{q(x)q(y)}{d(x)+d(y)-2} \right\}^3.
\]

2.7 M-polynomial

Let \( G \) be a molecular graph and \( m_{i,j}(G) \), \( i, j \geq 1 \) be the number of edges \( e = xy \) of \( G \) in such a way \( \{\varrho(x), \varrho(y)\} = \{i, j\} \).

The M-polynomial of \( G \) is:

\[
M(G; a, b) = \sum_{i \leq j} \left( m_{i,j}(G) a^i b^j \right).
\]

In Tables 1 and 2, the relation between the above TIs and M-polynomial is defined.

In Table 1, \( MM_2 \) is the second modified Zagreb index, \( RR_\mu \) is reciprocal general Randić index, \( J(f(a, b)) = (f(a, a)) \), and \( Q_2(f(a, b)) = a^2 \cdot (f(a, b)) \), where \( \alpha \neq 0 \). For further detail discussion, we refer to Javaid and Jung (2017).

In this section, we describe the MON which is a composition of metal nodes as well as organic ligands as presented in Figure 1. The smaller nodes are organic ligands and the bigger nodes are metals that are zinc-based (Hong et al., 2020). In the metal-organic network, all the edges are bonds among the different organic ligands and the metals nodes.

Now we developed the metal-organic networks as shown in Figures 2a,b. The MON\(_n\) is created by introducing the new bonds between the bigger nodes (metals) of the two primary metal-organic networks in such a way two bigger nodes of the upper layer of a primary metal-organic network are linked with a node of the lower layer of the basic MON\(_n\). The MON\(_n\) is shown in Figure 2a, for dimension \( n = 2 \). Also, the MON\(_n\) by introducing the new bonds among the smaller nodes of the two basic metal-organic networks in such a way two smaller nodes of an upper layer of a primary metal-organic network are linked with a smaller node of a lower layer of the second basic metal-organic network. The MON\(_n\) is shown in Figure 2b, where \( n = 2 \). For the aforesaid metal-organic networks, we have \( |V(MON_n)| = 48n \) and \( |E(MON_n)| = 72n - 12 \), where \( n \geq 2 \). For more, see Awais et al. (2019a, 2019b, 2020a, 2020b).

### Table 1: Relation between M-polynomial and TIs

<table>
<thead>
<tr>
<th>Indices</th>
<th>f(a, b)</th>
<th>Derivation from M ( (G, a, b) )</th>
</tr>
</thead>
<tbody>
<tr>
<td>( M_1 )</td>
<td>( a + b )</td>
<td>( (D_a + D_b)(M(G, a, b)) )</td>
</tr>
<tr>
<td>( M_2 )</td>
<td>( ab )</td>
<td>( (D_a D_b)(M(G, a, b)) )</td>
</tr>
<tr>
<td>( MM_2 )</td>
<td>( \frac{1}{ab} )</td>
<td>( (S_a S_b)(M(G, a, b)) )</td>
</tr>
<tr>
<td>( R_\mu )</td>
<td>( (ab)^\alpha, \alpha \in \mathbb{N} )</td>
<td>( (D_a^\mu D_b)(M(G, a, b)) )</td>
</tr>
<tr>
<td>( RR_\mu )</td>
<td>( \left( \frac{ab}{a+b} \right)^\alpha )</td>
<td>( (S_a^\mu S_b^\mu)(M(G, a, b)) )</td>
</tr>
<tr>
<td>( SDD )</td>
<td>( \left( \frac{a+b}{a+b-2} \right)^3 )</td>
<td>( (D_a S_a + D_b S_b)(M(G, a, b)) )</td>
</tr>
</tbody>
</table>

### Table 2: Relation between M-polynomial and TIs

<table>
<thead>
<tr>
<th>Indices</th>
<th>f(a, b)</th>
<th>Derivation from M ( (G, a, b) )</th>
</tr>
</thead>
<tbody>
<tr>
<td>( H )</td>
<td>( \frac{2}{a+b} )</td>
<td>( 2S_a I(M(G, a, b)) )</td>
</tr>
<tr>
<td>( IS )</td>
<td>( \frac{ab}{a+b} )</td>
<td>( S_a Q_2 D_a D_b (M(G, a, b)) )</td>
</tr>
<tr>
<td>( AZI )</td>
<td>( \left( \frac{a+b}{a+b-2} \right)^3 )</td>
<td>( S_a^3 D_a^3 D_b^3 (M(G, a, b)) )</td>
</tr>
</tbody>
</table>

### Figure 1: Basic metal-organic network.

3 Results for first metal-organic network \( MON_1(n) \)

In this section, we computed the different results regarding aforesaid TIs on the MON\(_n\). Before to develop the core computations, we discuss the node-set and edge-set of MON\(_n\) with the help of degrees of nodes.

We have four different kinds of nodes in MON\(_n\) i.e. 2, 3, 4, and 6. Consequently:

- \( V_1 = \{x \in V(MON_n) \mid q(x) = 2\} \),
- \( V_2 = \{x \in V(MON_n) \mid q(x) = 3\} \),
- \( V_3 = \{x \in V(MON_n) \mid q(x) = 4\} \),
- \( V_4 = \{x \in V(MON_n) \mid q(x) = 6\} \),

where \(|V_1| = 30n\), \(|V_2| = 12\), \(|V_3| = 12n - 6\), and \(|V_4| = 6n - 6\). Consequently:

\(|V(MON_1(n))| = u = |V_1| + |V_2| + |V_3| + |V_4| = 48n \).
Therefore, we have four different edges that are degree-based of end nodes in MON\(_1(n)\) that are \(\{2, 3\}\), \(\{2, 6\}\), \(\{2, 4\}\), and \(\{4, 6\}\). Thus, we have:

\[
\begin{align*}
E_1 &= |E\{2,3\}| = \{xy \in E(MON_1(n)) \mid q(x) = 2, q(y) = 3\}, \\
E_2 &= |E\{2,6\}| = \{xy \in E(MON_1(n)) \mid q(x) = 2, q(y) = 6\}, \\
E_3 &= |E\{2,4\}| = \{xy \in E(MON_1(n)) \mid q(x) = 2, q(y) = 4\}, \\
E_4 &= |E\{4,6\}| = \{xy \in E(MON_1(n)) \mid q(x) = 4, q(y) = 6\},
\end{align*}
\]

where \(|E\{2,3\}| = 36\), \(|E\{2,6\}| = 24n - 24\), \(|E\{2,4\}| = 36n - 12\), and \(|E\{4,6\}| = 12n - 12\). Therefore, \(|E(MON_1(n))| = |E_1| + |E_2| + |E_3| + |E_4| = 72n - 12\).

We also define the node-set partition \(V(MON_1(n))\) and edge-set \(E(MON_1(n))\) of \(MON_1(n)\) with addition of degrees of neighbor nodes. So, for \(xy \in E(MON_1(n))\), we got Table 3.

**Theorem 3.1**
Let \(G \cong MON_1(n)\) be the first metal-organic network, where \(n \geq 2\). The M-polynomial of \(G\) is:

\[
M(G, a, b) = 36a^2b^3 + 24(n - 1)a^2b^6 + 12(3n - 1)a^2b^4 + 12(n - 1)a^4b^6
\]

**Proof.** By using the formulae and Table 1, we computed the results as follows:

\[
M(G, a, b) = \sum_{i \leq 3} (m_i, G)a^ib^i
\]

Then, the first Zagreb index \((M_1(G))\), the second Zagreb index \((M_2(G))\), the second modified Zagreb index \((MM_2(G))\), general Randić index \((R_{\alpha}(G))\), and reciprocal General Randić index \((RR_{\alpha}(G))\), where \(\alpha \in \mathbb{N}\) and symmetric division degree index \((SSD(G))\) computed from the M-polynomial, are as follows:

\[
\begin{align*}
M_1(G) &= 528n - 204, \\
M_2(G) &= 864n - 456, \\
MM_2(G) &= 7n + 2, \\
R_{\alpha}(G) &= (6)^{\alpha}36 + (12)^{\alpha}24(n - 1) + (8)^{\alpha}12(3n - 1) + (24)^{\alpha}12(n - 1), \\
RR_{\alpha}(G) &= \frac{36}{(6)^{\alpha}} + \frac{24}{(12)^{\alpha}}(n-1) + \frac{12}{(8)^{\alpha}}(3n-1) + \frac{12}{(24)^{\alpha}}(n-1), \\
SSD(G) &= 196n - 58.
\end{align*}
\]
Proof. Let \( f(a, b) = M(G, a, b) \) be the M-polynomial of the first metal-organic network. We have:

\[
\begin{align*}
&f(a, b) = 36a^2b^3 + 24(n-1)a^2b^6 + 12(3n-1)a^2b^4 + 12(n-1)a^2b^6 \\
&\quad + 48(n-1)ab^8 \\
\end{align*}
\]

The needed partial derivatives and integrals are computed as:

\[
\begin{align*}
D_a(f(a, b)) &= 72ab^3 + 48(n-1)ab^6 + 24(3n-1)ab^4 + 48(n-1)ab^8 \\
D_b(f(a, b)) &= 108a^2b^2 + 144(n-1)a^2b^5 + 48(3n-1)a^2b^3 + 72(n-1)a^4b^6 \\
D_a(D_b(f(a, b))) &= 216ab^7 + 288(n-1)ab^8 + 96(3n-1)ab^6 + 288(n-1)a^8b^6 \\
S_a(f(a, b)) &= 18a^2b^2 + 12(n-1)a^2b^6 + 6(3n-1)a^2b^3 + 3(n-1)a^2b^6 \\
S_b(f(a, b)) &= 12a^6b^3 + 4(n-1)a^6b^5 + 3(3n-1)a^2b^6 + 2(n-1)a^4b^6 \\
S_a(S_b(f(a, b))) &= 6a^2b^2 + 2(n-1)a^2b^6 + \frac{3}{2}(3n-1)a^2b^6 + (n-1)a^4b^6 \\
D_aS_b(f(a, b)) &= 54a^2b^3 + 72(n-1)a^2b^6 + 24(3n-1)ab^5 + 18(n-1)a^2b^6 \\
D_bS_a(f(a, b)) &= 24ab^7 + 8(n-1)ab^8 + 6(3n-1)ab^6 + 8(n-1)a^8b^6 \\
(DDDS)(f(a, b)) &= (6)^236ab^7 + (12)^224(n-1)ab^6 + (8)^212(3n-1)ab^5 + (24)^212(n-1)a^2b^6 \\
(S^{a}S^{a})(f(a, b))) &= \frac{36}{(6)^2}(n-1)a^2b^6 + \frac{24}{(12)^2}(3n-1)a^2b^6 + \frac{12}{(6)^2}(n-1)a^4b^6 \\
(S^{a}S^{b})(f(a, b))) &= \frac{12}{(6)^2}(n-1)a^2b^6 + \frac{12}{(24)^2}(3n-1)a^2b^6 + \frac{12}{(24)^2}(n-1)a^4b^6.
\end{align*}
\]

Now, we obtained:

\[
\begin{align*}
D_a(f(a, b))|_{a^3+b^3} &= 72 + 48(n-1) + 24(3n-1) + 48(n-1) \\
D_b(f(a, b))|_{a^3+b^3} &= 108 + 144(n-1) + 48(3n-1) + 72(n-1) \\
D_a(D_b(f(a, b)))|_{a^3+b^3} &= 216 + 288(n-1) + 96(3n-1) + 288(n-1) \\
S_a(f(a, b))|_{a^3+b^3} &= 18 + 12(n-1) + 6(3n-1) + 3(n-1) \\
S_b(f(a, b))|_{a^3+b^3} &= 12 + 4(n-1) + 3(3n-1) + 2(n-1) \\
S_a(S_b(f(a, b)))|_{a^3+b^3} &= 6 + 2(n-1) + \frac{3}{2}(3n-1) + \frac{1}{2}(n-1).
\end{align*}
\]

Consequently:

(i) \( M_1(G) = (D_a + D_b)(f(a, b)) |_{a^3+b^3} = 528n - 204 \)

(ii) \( M_2(G) = (D_a)(D_b)(f(a, b)) |_{a^2+b^3} = 864n - 456 \)

(iii) \( MM_2(G) = (S_a)(S_b)(f(a, b)) |_{a^2+b^3} = 196n - 58 \)

Theorem 3.3

Let \( G \equiv MON(n) \) be the first metal-organic network, where \( n \geq 2 \). The M-polynomial of \( G \) is:

\[
M(G, a, b) = 36a^2b^3 + 24(n-1)a^2b^6 + 12(3n-1)a^2b^4 + 12(n-1)a^2b^6 + 48(n-1)ab^8.
\]

Then, harmonic \( H(G) \), inverse sum \( IS(G) \), and augmented Zagreb indices \( AZI(G) \) are:

(i) \( H(G) = \left(\frac{102}{5}\right)n + 2 \)

(ii) \( IS(G) = \left(\frac{564}{5}\right)n - \left(\frac{188}{5}\right) \)

(iii) \( AZI(G) = 804n - 324 \)
Proof. Let \( f(a, b) = M(G, a, b) \) be the M-polynomial of the first metal-organic network. We have:

\[
f(a, b) = 36a^2b^3 + 24(n - 1)a^2b^6 + 12(3n - 1)a^2b^4 + 12(n - 1)a^4b^6
\]

The needed partial derivatives and integrals are computed as:

\[
J(f(a, b)) = 36a^5 + 24(n - 1)a^8 + 12(3n - 1)a^6b + 12(n - 1)a^{10}
\]

\[
S_a(J(f(a, b))) = \frac{36}{5}a^5 + 3(n - 1)a^8 + 2(3n - 1)a^6b + \frac{6}{5}(n - 1)a^{10}
\]

\[
J(D_a(D_b(f(a, b)))) = 216a^5 + 288(n - 1)a^8 + 96(3n - 1)a^4 + 288(n - 1)a^{10}
\]

\[
Q_a(J(D_a(D_b(f(a, b)))))) = 216a^5 + 288(n - 1)a^8 + 96(3n - 1)a^4 + 288(n - 1)a^{10}
\]

\[
S_aQ_a(J(D_a(D_b(f(a, b)))))) = \frac{216}{5}a^5 + 36(n - 1)a^8 + 16(3n - 1)a^6 + \frac{144}{5}(n - 1)a^{10}
\]

\[
D_a^3D_b^3 (f(a, b)) = 6^8(36)a^5b^3 + 12^9(24)(n - 1)a^5b^3
\]

\[
+ 8^5(12)(3n - 1)a^5b^3
\]

\[
+ 24^4(12)(n - 1)a^5b^3
\]

\[
J D_a^3D_b^3 (f(a, b)) = 6^8(36)a^5 + 12^9(24)(n - 1)a^6
\]

\[
+ 8^5(12)(3n - 1)a^4 + 24^4(12)(n - 1)a^4
\]

\[
S_a^3J D_a^3D_b^3 (f(a, b)) = 2^3(36)a^5 + 3^3(24)(n - 1)a^6
\]

\[
+ 2^3(12)(3n - 1)a^4 + 3^3(12)(n - 1)a^8
\]

Now we obtained:

\[
S_a(J(f(a, b))) |_{a=b} = \frac{36}{5} + 3(n - 1)
\]

\[
+ 2(3n - 1)
\]

\[
+ \frac{6}{5}(n - 1)
\]

\[
S_aQ_a(J(D_a(D_b(f(a, b)))))) |_{a=b} = \frac{216}{5} + 36(n - 1)
\]

\[
+ 16(3n - 1)
\]

\[
+ \frac{144}{5}(n - 1)
\]

\[
S_a^3J D_a^3D_b^3 (f(a, b)) |_{a=b} = \left(\frac{6}{5}\right)^3(36)
\]

\[
+ \left(\frac{12}{6}\right)^3(24)(n - 1)
\]

\[
+ \left(\frac{24}{6}\right)^3(12)(3n - 1)
\]

\[
+ \left(\frac{24}{6}\right)^3(12)(n - 1)
\]

Consequently:

(i) \( H(G) = 2 \cdot S_a(J(f(a, b))) |_{a=b} = 2 \cdot \frac{36}{5} + 3(n - 1)
\]

\[
+ 2(3n - 1) + \frac{6}{5}(n - 1) = \frac{102}{5}n + 2
\]

(ii) \( IS(G) = S_aQ_a(J(D_a(D_b(f(a, b)))))) |_{a=b} = \frac{216}{5}
\]

\[
+ 36(n - 1) + 16(3n - 1) + \frac{144}{5}(n - 1) = \frac{564}{5}n + \frac{188}{5}
\]

(iii) \( AZ(G) = S_a^3J D_a^3D_b^3 (f(a, b)) |_{a=b} = \left(\frac{6}{5}\right)^3(36)
\]

\[
+ \left(\frac{12}{6}\right)^3(24)(n - 1) + \left(\frac{24}{6}\right)^3(12)(3n - 1)
\]

\[
+ \left(\frac{24}{6}\right)^3(12)(n - 1) = 804n - 324
\]

4 Results for second metal-organic network

In this section, we show the consequences of TIs for the MON\(_n\)\((n)\). So, we define the partitions of node-set and edge-set of MON\(_n\)\((n)\) with respect to degree of nodes. We have three different kinds of nodes in MON\(_n\)\((n)\) with respect to degree of 2, 3, and 4. Thus, we have:

\[
V_1 = |\{x \in MON_n(n) : q(x) = 2\}|
\]

\[
V_2 = |\{x \in MON_n(n) : q(x) = 3\}|
\]

\[
V_3 = |\{x \in MON_n(n) : q(x) = 4\}|
\]

where \(|V_1| = 12n + 18, |V_2| = 24n - 12, \text{ and } |V_3| = 12n - 6.\) Consequently:

\[
|V(MON_n(n))| = u = |V_1| + |V_2| + |V_3| = 48n.
\]

Additionally, we have different kinds of edges that is based on the degree of end nodes in MON\(_n\)\((n)\) that are \{2, 3, 2, 4, 3, 3, 4, 3, 4, 4, 4\}. Hence, we have:

\[
E_1 = |\{xy : E(MON_n(n)) \cap q(x) = 2, q(y) = 3\}|
\]

\[
E_2 = |\{xy : E(MON_n(n)) \cap q(x) = 2, q(y) = 4\}|
\]

\[
E_3 = |\{xy : E(MON_n(n)) \cap q(x) = 3, q(y) = 3\}|
\]

\[
E_4 = |\{xy : E(MON_n(n)) \cap q(x) = 3, q(y) = 4\}|
\]

\[
E_5 = |\{xy : E(MON_n(n)) \cap q(x) = 4, q(y) = 4\}|
\]

where \(|E_{2,3}| = 12(n + 2), |E_{2,4}| = 12(n + 1), |E_{3,3}| = 24(n - 1), |E_{3,4}| = 12(n - 1), \text{ and } |E_{4,4}| = 12(n - 1). \) Consequently, \(|E(MON_n(n))| = e = |E_{2,3}| + |E_{2,4}| + |E_{3,3}| + |E_{3,4}| + |E_{4,4}| = 72n - 12.\)
Therefore, we define the partition of node-set $V(MON_2(n))$ and edge-set $E(MON_2(n))$ of $MON_2(n)$ with respect to addition of degree of neighborhood nodes. Thus, for $xy \in E(MON_2(n))$, we get Table 4.

**Theorem 4.1**
Let $\mathbb{G} \cong MON_2(n)$ be the second metal-organic network, where $n \geq 2$. The $M$-polynomial of $\mathbb{G}$ is:

$$M(\mathbb{G}, a, b) = 12(n + 2)a^2b^3 + 12(n + 1)a^2b^4 + 24(n - 1)a^3b^3 + 12(n - 1)a^3b^4 + 12(n - 1)a^4b^4$$

**Proof**. By using the formulae and Table 2, we computed the results as follows:

$$M(\mathbb{G}, a, b) = \sum_{i=1}^{5} (m_{i,j} \mathbb{G} a^i b^j)$$

$$= \sum_{i=3}^{5} (m_{2,3} \mathbb{G} a^3 b^3) + \sum_{i=4}^{5} (m_{2,4} \mathbb{G} a^4 b^4)$$

$$+ \sum_{i=3}^{5} (m_{3,3} \mathbb{G} a^3 b^3) + \sum_{i=4}^{5} (m_{3,4} \mathbb{G} a^4 b^4)$$

$$+ \sum_{i=4}^{5} (m_{4,4} \mathbb{G} a^4 b^4)$$

$$= |E_1|a^2b^3 + |E_2|a^2b^4 + |E_3|a^3b^3$$

$$+ |E_4|a^3b^4 + |E_5|a^4b^4$$

$$= 12(n + 2)a^2b^3 + 12(n + 1)a^2b^4 + 24(n - 1)a^3b^3 + 12(n - 1)a^3b^4 + 12(n - 1)a^4b^4$$

**Theorem 4.2**
Let $\mathbb{G} \cong MON_2(n)$ be the second metal-organic network, where $n \geq 2$. The $M$-polynomial of $\mathbb{G}$ is:

$$M(\mathbb{G}, a, b) = 24(n + 2)a^2b^3 + 12(n + 1)a^2b^4 + 24(n - 1)a^3b^3 + 12(n - 1)a^3b^4 + 12(n - 1)a^4b^4$$

Then, the first Zagreb index ($M_1(\mathbb{G})$), the second Zagreb index ($M_2(\mathbb{G})$), the second modified Zagreb index ($M_{MM_2}(\mathbb{G})$), general Randić index ($R_\alpha(\mathbb{G})$), and reciprocal general Randić index ($RR_\alpha(\mathbb{G})$), where $\alpha \in N$ and symmetric division degree index ($SSD(\mathbb{G})$) computed from the $M$-polynomial, are as follows:

(i) $M_1(\mathbb{G}) = 456n - 132$,

(ii) $M_2(\mathbb{G}) = 720n - 312$,

(iii) $M_{MM_2}(\mathbb{G}) = \left(\frac{95}{12}\right)n + \frac{13}{12}$,

(iv) $R_\alpha(\mathbb{G}) = (6)\alpha^2(12(n + 2) + (8)\alpha^2(12(n + 1) + (9)\alpha^2(24(n - 1) + (12)\alpha^2(12(n - 1) + (16)\alpha^2(12(n - 1) + (18)\alpha^2(12(n - 1) + (20)\alpha^2)$

(v) $RR_\alpha(\mathbb{G}) = \frac{12}{(6)^\alpha}(n + 2) + \frac{12}{(6)^\alpha}(n + 1) + \frac{24}{(9)^\alpha}(n - 1) + \frac{12}{(12)^\alpha}(n - 1)$,$(n - 1) + \frac{12}{(16)^\alpha}(n - 1)$,$(n - 1)$

(vi) $SSD(\mathbb{G}) = 153n - 15$

**Proof**. Let $f(a, b) = M(\mathbb{G}, a, b)$ be the $M$-polynomial of the second metal-organic network. We have:

$$f(a, b) = 12(n + 2)a^2b^3 + 12(n + 1)a^2b^4 + 24(n - 1)a^3b^3 + 12(n - 1)a^3b^4 + 12(n - 1)a^4b^4$$

The needed partial derivatives and integrals are computed as:

$$D_\alpha(f(a, b)) = 24(n + 2)ab^3 + 24(n + 1)ab^4$$

$$+ 72(n - 1)a^2b^3 + 36(n - 1)a^2b^4 + 48(n - 1)a^3b^4$$

$$D_\alpha(f(a, b)) = 36(n + 1)a^2b^3 + 48(n + 1)a^3b^4 + 72(n - 1)a^2b^3 + 48(n - 1)a^3b^4 + 48(n - 1)a^4b^4$$

$$D_\alpha(D_\alpha(f(a, b))) = 72(n + 2)a^2b^2 + 96(n + 1)a^3b^3$$

$$+ 216(n - 1)a^3b^3 + 144(n - 1)a^2b^4 + 192(n - 1)a^3b^4$$

$$S_\alpha(f(a, b)) = 6(n + 2)a^2b^3 + 6(n + 1)a^2b^4 + 8(n - 1)a^3b^3 + 4(n - 1)a^3b^4 + 3(n - 1)a^4b^4$$

$$S_\alpha(S_\alpha(f(a, b))) = 4(n + 2)a^2b^3 + 3(n + 1)a^2b^4 + 8(n - 1)a^3b^3 + 3(n - 1)a^3b^4 + 3(n - 1)a^4b^4$$

$$D_\alpha S_\alpha(f(a, b)) = 18(n + 2)a^2b^3 + 24(n + 1)a^2b^4 + 24(n - 1)a^3b^3 + 16(n - 1)a^3b^4 + 12(n - 1)a^4b^4.$$
Now, we obtained:

\[ D_a(f(a, b)) \mid_{a=b} = 24(n+2) + 24(n+1) + 72(n-1) + 36(n-1) + 48(n-1), \]

\[ D_b(f(a, b)) \mid_{a=b} = 36(n+2) + 48(n+1) + 72(n-1) + 48(n-1) + 48(n-1), \]

\[ D_a(D_b(f(a, b))) \mid_{a=b} = 72(n+2) + 96(n+1) + 216(n+1) + 144(n-1) + 192(n-1), \]

\[ S_a(f(a, b)) \mid_{a=b} = 6(n+2) + 6(n+1) + 8(n-1) + 4(n-1) + 3(n-1), \]

\[ S_b(f(a, b)) \mid_{a=b} = 4(n+2) + 3(n+1) + 8(n-1) + 3(n-1) + 3(n-1), \]

\[ S_a(S_b(f(a, b))) \mid_{a=b} = 2(n+2) + \frac{3}{2}(n+1) + \frac{8}{3}(n-1) + \frac{1}{3}(n-1), \]

\[ D_bS_a(f(a, b)) \mid_{a=b} = 18(n+2) + 24(n+1) + 24(n-1) + 16(n-1) + 12(n-1), \]

\[ D_aS_b(f(a, b)) \mid_{a=b} = 8(n+2) + 6(n+1) + 24(n-1) + 9(n-1) + 12(n-1), \]

\[ (D_a, D_b) \mid_{a=b} = \frac{12}{(6)^2} (n+2) + \frac{12}{(9)^2} (n+1) + \frac{24}{(9)^2} (n-1) + \frac{12}{(12)^2} (n-1), \]

\[ (S_a, S_b) \mid_{a=b} = \frac{12}{(6)^2} (n+2) + \frac{12}{(9)^2} (n+1) + \frac{24}{(9)^2} (n-1) + \frac{12}{(12)^2} (n-1), \]

Consequently:

(i) \[ M_1(\mathcal{G}) = (D_a + D_b (f(a, b))) \mid_{a=b} \]

\[ = D_a (f(\mathcal{G}, a, b)) \mid_{a=b} + D_b (f(\mathcal{G}, a, b)) \mid_{a=b} \]

\[ = 456n - 132. \]

(ii) \[ M_2(\mathcal{G}) = (D_a D_b (f(a, b))) \mid_{a=b} \]

\[ = (D_a (D_b (f(\mathcal{G}, a, b)))) \mid_{a=b} = 720n - 312. \]

(iii) \[ MM(\mathcal{G}) = (S_a S_b) \mid_{a=b} \]

\[ = S_a(S_b(f(\mathcal{G}, a, b))) \mid_{a=b} = 2(n+2) + \frac{9}{3}(n-1) + \frac{3}{4}(n-1) = \frac{95}{12}n + \frac{13}{12}. \]

(iv) \[ R(\mathcal{G}) = (D_a D_b (f(a, b))) \mid_{a=b} \]

\[ = (6)^2 12(n+2) + (8)^2 12(n+1) + (9)^2 24(n-1) + (12)^2 12(n-1) + (16)^2 12(n-1), \]

\[ + \frac{3}{2}(n+1) + \frac{8}{3}(n-1) + \frac{3}{4}(n-1) = \frac{95}{12}n + \frac{13}{12}. \]

(v) \[ RR(\mathcal{G}) = (S_a S_b) \mid_{a=b} \]

\[ = 12(n+2) + \frac{12}{(6)^2} (n+1) + \frac{24}{(9)^2} (n-1) + \frac{12}{(12)^2} (n-1), \]

\[ + \frac{12}{(16)^2} (n-1), \]

(vi) \[ SDD(\mathcal{G}) = (D_a S_a + D_a S_b) \mid_{a=b} \]

\[ = (D_a S_a (f(a, b))) \mid_{a=b} + (D_a S_b (f(a, b))) \mid_{a=b} \]

\[ = (D_a S_a (f(a, b))) \mid_{a=b} + (D_a S_b (f(a, b))) \mid_{a=b} = 153n - 15 \neq 0. \]

Theorem 4.3

Let \( \mathcal{G} \cong MON(n) \) be the second metal-organic network, where \( n \geq 2 \). The M-polynomial of \( \mathcal{G} \) is:

\[ M(G, a, b) = 12(n+2)a^2b^3 + 12(n+1)a^3b^4 \]

\[ + 24(n-1)a^2b^3 + 24(n-1)a^3b^4 \]

\[ + 12(n-1)a^2b^4, \]

Then, harmonic \( H(\mathcal{G}) \), inverse sum \( IS(\mathcal{G}) \), and augmented Zagreb indices \( AZI(\mathcal{G}) \) are:

(i) \[ H(\mathcal{G}) = 2S_a(\mathcal{J}(f(a, b))) \mid_{a=b} = \frac{813}{35} n - \frac{29}{35}, \]

(ii) \[ IS(\mathcal{G}) = S_aQ_a(\mathcal{J}(D_a(D_a(f(a, b)))) \mid_{a=b} \]

\[ = \frac{3884}{35} n - \frac{1252}{35}, \]

(iii) \[ AZI(\mathcal{G}) = S_a JD_a D_a \mid_{a=b} \]

\[ = 24 \left( \frac{72}{64} \right) (n-1) + 12 \left( \frac{72}{64} \right) (n-1) + 12 \left( \frac{512}{27} \right) (n-1) \]

\[ = \frac{7729367}{9000} n - \left( \frac{3409367}{9000} \right). \]
Proof. Let \( f(a, b) = M(G, a, b) \) be the M-polynomial of the second metal-organic network. We have:

\[
f(a, b) = 12(n + 2)a^2b^3 + 12(n + 1)a^2b^4 + 24(n - 1)a^3b^3 + 12(n - 1)a^3b^4 + 12(n - 1)a^4b^4.
\]

The needed partial derivatives and integrals are computed as:

\[
J(f(a, b)) = 12(n + 2)a^5 + 12(n + 1)a^6 + 24(n - 1)a^6 + 12(n - 1)a^7 + 12(n - 1)a^8,
\]

\[
S_a(J(f(a, b))) = \frac{12}{5} (n+2)a^5 + 2(n+1)a^6 + 4(n-1)a^6 + \frac{12}{7} (n-1)a^7 + \frac{4}{5} (n-1)a^8,
\]

\[
J(D_a(D_b(f(a, b)))) = 72(n + 2)a^5 + 96(n + 1)a^6 + 216(n - 1)a^6 + 144(n - 1)a^7 + 192(n - 1)a^8,
\]

\[
S_aJ(D_a(D_b(f(a, b)))) = \frac{72}{5} (n+2)a^5 + 16(n+1)a^6 + 36(n-1)a^6 + \frac{144}{7} (n-1)a^7 + 24(n-1)a^8,
\]

\[
S_aQ_b(J(D_a(D_b(f(a, b)))))) = 6^4(12)(n+2)ab^2 + 8^3(12)(n+1)ab^3 + 9^3(24)(n-1)ab^2 + 12^2(12)(n-1)a^2b^2 + 16^3(12)(n-1)a^3b^3,
\]

\[
JD_a(D_b(f(a, b))) = 6^3(12)(n+2)a^3 + 8^3(12)(n+1)a^4 + 9^3(24)(n-1)a^4 + 12^2(12)(n-1)a^4 + 16^3(12)(n-1)a^5,
\]

\[
S_aJJD_a(D_b(f(a, b))) = \left(\frac{6}{5}\right)^3(12)(n+2)a^3 + \left(\frac{8}{5}\right)^3 12(n+1)a^4 + \left(\frac{2}{5}\right)^3 24(n-1)a^4 + \left(\frac{12}{5}\right)^3 12(n-1)a^5 + \left(\frac{16}{5}\right)^3 12(n-1)a^6.
\]

Now we obtained:

\[
S_a(J(f(a, b))) \mid_{a=b} = \frac{12}{5} (n+2) + 2(n+1) + 4(n-1) + \left(\frac{12}{7}\right) (n-1) + \frac{4}{5} (n-1),
\]

\[
S_aQ_b(J(D_a(D_b(f(a, b)))))) \mid_{a=b} = \frac{72}{5} (n+2) + 16(n+1) + 36(n-1) + \frac{144}{7} (n-1) + 24(n-1),
\]

\[
S_aJJD_a(D_b(f(a, b))) \mid_{a=b} = 2^3(12)(n+2) + 2^3 12(n+1) + \left(\frac{0}{5}\right) 24(n-1) + \left(\frac{12}{5}\right)^3 12(n-1) + \left(\frac{8}{5}\right)^3 12(n-1).
\]

Consequently:

(i) \( H(G) = \left(\frac{813}{35}\right) n - \frac{29}{35} \),

(ii) \( IS(G) = \left(\frac{3884}{35}\right) n - \left(\frac{1252}{35}\right) \),

(iii) \( AZI(G) = \left(\frac{7729367}{9000}\right) n - \left(\frac{3609367}{9000}\right) \).

5 Conclusions

In this section, a comparison is included among the different topological indices with the assistance of graphical presentation and their numerical values of the
Agha Kashif et al. MON$_1(n)$ and MON$_2(n)$ are presented in Figures 3-8 and Tables 5-10.

In this paper, we computed the M-polynomials of first and second metal-organic networks. Moreover, with the assistance of aforesaid M-polynomials, we calculated the various TIs such as first and second Zagreb indices, second modified Zagreb index, general and reciprocal general Randić indices, symmetric division deg, inverse sum, harmonic, and the augmented Zagreb indices of MON$_1(n)$ and MON$_2(n)$ are presented in Figures 3-8 and Tables 5-10.

Figure 4: Graphical comparison of $R_1(G)$, $RR_1(G)$, and SSD$_1(G)$ are labeled in blue, cyan, and gold graphs, respectively, for MON$_1(n)$.

Figure 5: Graphical comparison of $H(G)$, IS$_1(G)$, and AZI$_1(G)$ are labeled in blue, cyan, and gold graphs, respectively, for MON$_1(n)$.

Figure 6: Graphical comparison of $M_1(G)$, $M_2(G)$, and MM$_1(G)$ are labeled in blue, cyan, and gold graphs, respectively, for MON$_1(n)$.

Figure 7: Graphical comparison of $R_2(G)$, $RR_2(G)$, and SSD$_2(G)$ are labeled in blue, cyan, and gold graphs, respectively, for MON$_2(n)$.

Figure 8: Graphical comparison of $H(G)$, IS$_2(G)$, and AZI$_2(G)$ are labeled in blue, cyan, and gold graphs, respectively, for MON$_2(n)$. 
Table 5: Comparison among \( M(G), M_1(G), \) and \( MM(G) \) of \( MON(n) \)

<table>
<thead>
<tr>
<th>( n )</th>
<th>( M(G) )</th>
<th>( M_1(G) )</th>
<th>( MM(G) )</th>
</tr>
</thead>
<tbody>
<tr>
<td>2</td>
<td>852</td>
<td>1272</td>
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<tr>
<td>3</td>
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<td>6</td>
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<tr>
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<td>3492</td>
<td>5592</td>
<td>51</td>
</tr>
<tr>
<td>8</td>
<td>4020</td>
<td>6456</td>
<td>58</td>
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<tr>
<td>9</td>
<td>4548</td>
<td>7320</td>
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</tr>
<tr>
<td>10</td>
<td>5076</td>
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<td>72</td>
</tr>
</tbody>
</table>

Table 6: Comparison among \( R(G), RR(G), \) and \( SSD(G) \) of \( MON(n) \), where \( \alpha = 1 \)

<table>
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<tr>
<th>( n )</th>
<th>( R(G) )</th>
<th>( RR(G) )</th>
<th>( SSD(G) )</th>
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<tbody>
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<td>10</td>
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<td>72</td>
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</tr>
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Table 7: Comparison among \( H(G), IS(G), \) and \( AZI(G) \) of \( MON(n) \)

<table>
<thead>
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<th>( n )</th>
<th>( H(G) )</th>
<th>( IS(G) )</th>
<th>( AZI(G) )</th>
</tr>
</thead>
<tbody>
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</table>

Table 8: Comparison among \( M(G), M_1(G), \) and \( MM(G) \) of \( MON(n) \)

<table>
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<th>( n )</th>
<th>( M(G) )</th>
<th>( M_1(G) )</th>
<th>( MM(G) )</th>
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</table>

Table 9: Comparison among \( R(G), RR(G), \) and \( SSD(G) \) of \( MON(n) \), where \( \alpha = 1 \)

<table>
<thead>
<tr>
<th>( n )</th>
<th>( R(G) )</th>
<th>( RR(G) )</th>
<th>( SSD(G) )</th>
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</table>

Table 10: Comparison among \( H(G), IS(G), \) and \( AZI(G) \) of \( MON(n) \)

<table>
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<tr>
<th>( N )</th>
<th>( H(G) )</th>
<th>( IS(G) )</th>
<th>( AZI(G) )</th>
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these two networks. Figures 4-6 present that \( M(G), R(G), \) and \( AZI(G) \) are better for both networks discussed in this paper. These M-polynomials and calculated TLs can assist us to understand the various chemical reactivities, physical features, and biological activities of the first and second metal-organic networks. The obtained conclusions can provide a meaningful decision in the pharmaceuticals industries.

Acknowledgement: The authors are indebted to the anonymous referees for their valuable comments to improve the original version of this paper.

Funding information: Authors state no funding involved.

Author contributions: Agha Kashif: writing – review and editing, resources, formal analysis, visualization, methodology; Sumaira Aftab: writing – original draft, methodology; Muhammad Javaid: resources, formal analysis, visualization, methodology. Hafiz Muhammad Awais: writing – original draft, visualization, methodology

Conflict of interest: One of the authors (Muhammad Javaid) is a Guest Editor of the Main Group Metal
Chemistry’s Special Issue “Topological descriptors of chemical networks: Theoretical studies” in which this article is published.

References


