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

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Abstract: Topological index (TI) is a numerical invariant that helps to understand the natural relationship of the physicochemical properties of a compound in its primary structure. George Polya introduced the idea of counting polynomials in chemical graph theory and Winer made the use of TI in chemical compounds working on the paraffin's boiling point. The literature of the topological indices and counting polynomials of different graphs has grown extremely since that time. Metal-organic network (MON) is a group of different chemical compounds that consist of metal ions and organic ligands to represent unique morphology, excellent chemical stability, large pore volume, and very high surface area. Working on structures, characteristics, and synthesis of various MONs show the importance of these networks with useful applications, such as sensing of different gases, assessment of chemicals, environmental hazard, heterogeneous catalysis, gas and energy storage devices of excellent material, conducting solids, super-capacitors and catalysis for the purification, and separation of different gases. The above-mentioned properties and physical stability of these MONs become a most discussed topic nowadays. In this paper, we calculate the M-polynomials and various TIs based on these polynomials for two different MONs. A comparison among the aforesaid topological indices is also included to represent the better one.

Keywords: M-polynomial, chemical compounds, topological indices, metal-organic network

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 reactivities, physical properties and biological

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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 $\mathbb{G} = (V(\mathbb{G}), E(\mathbb{G}))$, $V(\mathbb{G}) = \{x_1, x_2, x_3, \dots, x_n\}$ and $E(\mathbb{G})$ are nodes (metals or organic ligands)

and edge-set (bonds among the different atoms) of $\mathbb{G}$, respectively. The $|V(\mathbb{G})| = v$ and $|E(\mathbb{G})| = e$ is the order and size of $\mathbb{G}$, 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 $\mathbb{G}$. In the current discussion, a graph is simple and connected, having no loops and multiple edges.

2.1 First and second Zagreb indices

Let $\mathbb{G}$ be a molecular graph, then its first and second Zagreb indices are:

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

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

2.2 General Randić index

If R is the set of real numbers and $\mathbb{G}$ be a connected graph, so the general Randić index is given as:

$$R_\alpha(\mathbb{G}) = \sum_{xy \in E(\mathbb{G})} [\varrho(x) \times \varrho(y)]^\alpha.$$

2.3 Symmetric division deg index

For a molecular graph $\mathbb{G}$, the symmetric division deg index is:

$$SDD(\mathbb{G}) = \sum_{xy \in E(\mathbb{G})} \left[\frac{\min(\varrho(x), \varrho(y))}{\max(\varrho(x), \varrho(y))} + \frac{\max(\varrho(x), \varrho(y))}{\min(\varrho(x), \varrho(y))} \right]$$

2.4 Harmonic index

For a molecular graph $\mathbb{G}$, the harmonic index is:

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

2.5 Inverse sum index

For a molecular graph $\mathbb{G}$, the inverse sum index is:

$$IS(\mathbb{G}) = \sum_{xy \in E(\mathbb{G})} \left[\frac{\varrho(x)\varrho(y)}{\varrho(x) + \varrho(y)} \right].$$

2.6 Augmented Zagreb index

For a molecular graph $\mathbb{G}$, the augmented Zagreb index is:

$$AZI(\mathbb{G}) = \sum_{xy \in E(\mathbb{G})} \left[\frac{q(x)q(y)}{q(x)+q(y)-2} \right]^3.$$

2.7 M-polynomial

Let $\mathbb{G}$ be a molecular graph and $m_{ij}(\mathbb{G})$; $i, j \geq 1$ be the number of edges $e = xy$ of $\mathbb{G}$ in such a way $\{q(x), q(y)\} = \{i, j\}$. The M-polynomial of G is:

$$M(\mathbb{G}, a, b) = \sum_{i \leq j} [m_{ij}(\mathbb{G}) a^i b^j].$$

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_α is reciprocal general Randić index, $D_a = \frac{\varphi(f(a,b))}{\varphi(a)}$, $D_b = \frac{\varphi(f(a,b))}{\varphi(b)}$, $S_a = \int_0^a \frac{f(t,b)}{t} dt$, $S_b = \int_0^b \frac{f(a,t)}{t} dt$. Also $J(f(a, b)) = (f(a, a))$, and $Q_\alpha(f(a, b)) = a^\alpha (f(a, b))$, 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 $MON_1(n)$ 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 $MON_1(n)$. The $MON_1(n)$ is shown in Figure 2a, for dimension $n = 2$. Also, the $MON_2(n)$ 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 $MON_2(n)$ is shown in Figure 2b, where $n = 2$. For the aforesaid metal-organic networks, we have $|V(MON_1(n))| = |V(MON_2(n))| = 48n$ and $|E(MON_1(n))| = |E(MON_2(n))| = 72n - 12$, where $n \geq 2$. For more, see Awais et al. (2019a, 2019b, 2020a, 2020b).

Table 1: Relation between M-polynomial and TIs

Indices	$f(a, b)$	Derivation from $M(\mathbb{G}, a, b)$
M_1	$a + b$	$(D_a + D_b)(M(\mathbb{G}, a, b)) _{a=1=b}$
M_2	ab	$(D_a D_b)(M(\mathbb{G}, a, b)) _{a=1=b}$
MM_2	$\frac{1}{ab}$	$(S_a S_b)(M(\mathbb{G}, a, b)) _{a=1=b}$
R_α	$(ab)^\alpha, \alpha \in \mathbb{N}$	$(D_a^\alpha D_b^\alpha)(M(\mathbb{G}, a, b)) _{a=1=b}$
RR_α	$\frac{1}{(ab)^\alpha}$	$(S_a^\alpha S_b^\alpha)(M(\mathbb{G}, a, b)) _{a=1=b}$
SDD	$\left(\frac{a^2+b^2}{ab}\right)$	$(D_a S_b + D_b S_a)(M(\mathbb{G}, a, b)) _{a=1=b}$

Table 2: Relation between M-polynomial and TIs

Indices	$f(a, b)$	Derivation from $M(\mathbb{G}, a, b)$
H	$\frac{2}{a+b}$	$2S_a J(M(\mathbb{G}, a, b)) _{a=1}$
IS	$\frac{ab}{a+b}$	$S_a Q_2 J D_a D_b (M(\mathbb{G}, a, b)) _{a=1=b}$
AZI	$\left(\frac{ab}{a+b-2}\right)^3$	$S_a^3 J D_a^3 D_b^3 (M(\mathbb{G}, a, b)) _{a=1=b}$

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 $MON_1(n)$. Before to develop the core computations, we discuss the node-set and edge-set of $MON_1(n)$ with the help of degrees of nodes.

We have four different kinds of nodes in $MON_1(n)$ i.e. 2, 3, 4, and 6. Consequently:

$$\begin{aligned} V_1 &= \{x \in V(MON_1(n)) \mid q(x) = 2\}, \\ V_2 &= \{x \in V(MON_1(n)) \mid q(x) = 3\}, \\ V_3 &= \{x \in V(MON_1(n)) \mid q(x) = 4\}, \\ V_4 &= \{x \in V(MON_1(n)) \mid q(x) = 6\}, \end{aligned}$$

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

$$|V(MON_1(n))| = u = |V_1| + |V_2| + |V_3| + |V_4| = 48n.$$

Figure 2: (a) First metal-organic network ($\text{MON}_1(n)$ for $n = 2$). (b) Second metal-organic network ($\text{MON}_2(n)$ for $n = 2$).

Therefore, we have four different edges that are degree-based of end nodes in $\text{MON}_1(n)$ that are $\{2, 3\}$, $\{2, 6\}$, $\{2, 4\}$, and $\{4, 6\}$. Thus, we have:

$$E_1 = E\{2, 3\} = \{xy \in E(\text{MON}_1(n)) \mid \varrho(x) = 2, \varrho(y) = 3\},$$

$$E_2 = E\{2, 6\} = \{xy \in E(\text{MON}_1(n)) \mid \varrho(x) = 2, \varrho(y) = 6\},$$

$$E_3 = E\{2, 4\} = \{xy \in E(\text{MON}_1(n)) \mid \varrho(x) = 2, \varrho(y) = 4\},$$

$$E_4 = E\{4, 6\} = \{xy \in E(\text{MON}_1(n)) \mid \varrho(x) = 4, \varrho(y) = 6\},$$

where $|E\{2, 3\}| = 36$, $|E\{2, 6\}| = 24n - 24$, $|E\{2, 4\}| = 36n - 12$, and $|E\{4, 6\}| = 12n - 12$. Therefore, $|E(\text{MON}_1(n))| = e = |E_1| + |E_2| + |E_3| + |E_4| = 72n - 12$.

We also define the node-set partition $V(\text{MON}_1(n))$ and edge-set $E(\text{MON}_2(n))$ of $\text{MON}_1(n)$ with addition of degrees of neighbor nodes. So, for $xy \in E(\text{MON}_1(n))$, we got Table 3.

Theorem 3.1

Let $\mathbb{G} \cong \text{MON}_1(n)$ be the first metal-organic network, where $n \geq 2$. The M-polynomial of $\mathbb{G}$ is:

$$M(\mathbb{G}, a, b) = 36a^2b^3 + 24(n-1)a^2b^6 + 12(3n-1)a^2b^4 + 12(n-1)a^4b^6$$

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

$$\begin{aligned} M(\mathbb{G}, a, b) &= \sum_{i \leq j} (m_{i,j} \mathbb{G} a^i b^j) \\ &= \sum_{2 \leq 3} (m_{2,3} \mathbb{G} a^2 b^3) + \sum_{2 \leq 6} (m_{2,6} \mathbb{G} a^2 b^6) \\ &\quad + \sum_{2 \leq 4} (m_{2,4} \mathbb{G} a^2 b^4) + \sum_{4 \leq 6} (m_{4,6} \mathbb{G} a^4 b^6) \end{aligned}$$

Table 3: Partitions of edges of $\text{MON}_1(n)$

$E\{\varrho(x), \varrho(y)\}$ $ E\{\varrho(x), \varrho(y)\} $	$E\{2, 3\}$	$E\{2, 6\}$	$E\{2, 4\}$	$E\{4, 6\}$
	36	$24(n-1)$	$12(3n-1)$	$12(n-1)$

$$\begin{aligned} &= |E_1|a^2b^3 + |E_2|a^2b^6 + |E_3|a^2b^4 + |E_4|a^4b^6 \\ &= 36a^2b^3 + 24(n-1)a^2b^6 \\ &\quad + 12(3n-1)a^2b^4 + 12(n-1)a^4b^6 \end{aligned}$$

Theorem 3.2

Let $\mathbb{G} \cong \text{MON}_1(n)$ be the first metal-organic network, where $n \geq 2$. The M-polynomial of $\mathbb{G}$ is:

$$M(\mathbb{G}, a, b) = 36a^2b^3 + 24(n-1)a^2b^6 + 12(3n-1)a^2b^4 + 12(n-1)a^4b^6$$

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

- (i) $M_1(\mathbb{G}) = 528n - 204$,
- (ii) $M_2(\mathbb{G}) = 864n - 456$,
- (iii) $MM_2(\mathbb{G}) = 7n + 2$,
- (iv) $R_\alpha(\mathbb{G}) = (6)^\alpha 36 + (12)^\alpha 24(n-1) + (8)^\alpha 12(3n-1) + (24)^\alpha 12(n-1)$,
- (v) $RR_\alpha(\mathbb{G}) = \frac{36}{(6)^\alpha} + \frac{24}{(12)^\alpha} (n-1) + \frac{12}{(8)^\alpha} (3n-1) + \frac{12}{(24)^\alpha} (n-1)$,
- (vi) $SDD(\mathbb{G}) = 196n - 58$.

Proof. Let $f(a, b) = M(\mathbb{G}, a, b)$ 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:

$$D_a(f(a, b)) = 72ab^3 + 48(n-1)ab^6 + 24(3n-1)ab^4 + 48(n-1)a^3b^6$$

$$D_b(f(a, b)) = 108a^2b^2 + 144(n-1)a^2b^5 + 48(3n-1)a^2b^3 + 72(n-1)a^4b^5,$$

$$D_a(D_b(f(a, b))) = 216ab^2 + 288(n-1)ab^5 + 96(3n-1)ab^3 + 288(n-1)a^3b^5$$

$$S_a(f(a, b)) = 18a^2b^3 + 12(n-1)a^2b^6 + 6(3n-1)a^2b^4 + 3(n-1)a^4b^6$$

$$S_b(f(a, b)) = 12a^2b^3 + 4(n-1)a^2b^6 + 3(3n-1)a^2b^4 + 2(n-1)a^4b^6$$

$$S_a(S_b(f(a, b))) = 6a^2b^3 + 2(n-1)a^2b^6 + \frac{3}{2}(3n-1)a^2b^4 + (n-1)a^4b^6,$$

$$D_bS_a(f(a, b)) = 54a^2b^2 + 72(n-1)a^2b^5 + 24(3n-1)a^2b^3 + 18(n-1)a^4b^5$$

$$D_aS_b(f(a, b)) = 24ab^3 + 8(n-1)ab^6 + 6(3n-1)ab^4 + 8(n-1)a^3b^6$$

$$(D_a^\alpha D_b^\alpha)(f(a, b)) = (6)^\alpha 36ab^2 + (12)^\alpha 24(n-1)ab^5 + (8)^\alpha 12(3n-1)ab^3 + (24)^\alpha 12(n-1)a^3b^5$$

$$(S_a^\alpha S_b^\alpha)(f(a, b)) = \frac{36}{(6)^\alpha} a^2b^3 + \frac{24}{(12)^\alpha} (n-1) a^2b^6 + \frac{12}{(8)^\alpha} (3n-1) a^2b^4 + \frac{12}{(24)^\alpha} (n-1) a^4b^6,$$

Now, we obtained:

$$D_a(f(a, b))|_{a=1=b} = 72 + 48(n-1) + 24(3n-1) + 48(n-1),$$

$$D_b(f(a, b))|_{a=1=b} = 108 + 144(n-1) + 48(3n-1) + 72(n-1),$$

$$D_a(D_b(f(a, b)))|_{a=1=b} = 216 + 288(n-1) + 96(3n-1) + 288(n-1),$$

$$S_a(f(a, b))|_{a=1=b} = 18 + 12(n-1) + 6(3n-1) + 3(n-1),$$

$$S_b(f(a, b))|_{a=1=b} = 12 + 4(n-1) + 3(3n-1) + 2(n-1),$$

$$S_a(S_b(f(a, b)))|_{a=1=b} = 6 + 2(n-1) + \frac{3}{2}(3n-1) + \frac{2}{4}(n-1),$$

$$D_bS_a(f(a, b))|_{a=1=b} = 54 + 72(n-1) + 24(3n-1) + 18(n-1),$$

$$D_aS_b(f(a, b))|_{a=1=b} = 24 + 8(n-1) + 6(3n-1) + 8(n-1),$$

$$(D_a^\alpha D_b^\alpha)(f(a, b))|_{a=1=b} = (6)^\alpha 36 + (12)^\alpha 24(n-1) + (8)^\alpha 12(3n-1) + (24)^\alpha 12(n-1),$$

$$(S_a^\alpha S_b^\alpha)(f(a, b))|_{a=1=b} = \frac{36}{(6)^\alpha} + \frac{24}{(12)^\alpha} (n-1) + \frac{12}{(8)^\alpha} (3n-1) + \frac{12}{(24)^\alpha} (n-1),$$

Consequently:

$$(i) \quad M_1(\mathbb{G}) = (D_a + D_b)(f(a, b))|_{a=1=b} = D_a(f(\mathbb{G}, a, b))|_{a=1=b} + D_b(f(\mathbb{G}, a, b))|_{a=1=b} = 528n - 204$$

$$(ii) \quad M_2(\mathbb{G}) = (D_a D_b)(f(a, b))|_{a=1=b} = (D_a(D_b(f(\mathbb{G}, a, b))))|_{a=1=b} = 864n - 456$$

$$(iii) \quad MM_2(\mathbb{G}) = (S_a S_b)(f(a, b))|_{a=1=b} = S_a(S_b(f(\mathbb{G}, a, b)))|_{a=1=b} = 6 + 2(n-1) + \frac{3}{2}(3n-1) + \frac{2}{4}(n-1) = 7n + 2$$

$$(iv) \quad R_\alpha(\mathbb{G}) = (D_a^\alpha D_b^\alpha)(f(a, b))|_{a=1=b} = (6)^\alpha 36 + (12)^\alpha 24(n-1) + (8)^\alpha 12(3n-1) + (24)^\alpha 12(n-1)$$

$$(v) \quad RR_\alpha(\mathbb{G}) = (D_a^\alpha D_b^\alpha)(f(a, b))|_{a=1=b} = \frac{36}{(6)^\alpha} + \frac{24}{(12)^\alpha} (n-1) + \frac{12}{(8)^\alpha} (3n-1) + \frac{12}{(24)^\alpha} (n-1),$$

$$(vi) \quad SDD(\mathbb{G}) = (D_a S_b + D_b S_a)(f(a, b))|_{a=1=b} = (D_a S_b)(f(a, b))|_{a=1=b} + (D_b S_a)(f(a, b))|_{a=1=b} = (D_a(S_b(f(a, b))))|_{a=1=b} + (D_b(S_a(f(a, b))))|_{a=1=b} = 196n - 58$$

Theorem 3.3

Let $\mathbb{G} \cong \text{MON}_1(n)$ be the first metal-organic network, where $n \geq 2$. The M-polynomial of $\mathbb{G}$ is:

$$M(\mathbb{G}, a, b) = 36a^2b^3 + 24(n-1)a^2b^6 + 12(3n-1)a^2b^4 + 12(n-1)a^4b^6$$

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

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

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

$$(iii) \quad AZI(\mathbb{G}) = 804n - 324.$$

Proof. Let $f(a, b) = M(\mathbb{G}, a, b)$ 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:

$$\begin{aligned} J(f(a, b)) &= 36a^5 + 24(n-1)a^8 \\ &\quad + 12(3n-1)a^6 + 12(n-1)a^{10} \\ S_a(J(f(a, b))) &= \frac{36}{5}a^5 + 3(n-1)a^8 \\ &\quad + 2(3n-1)a^6 + \frac{6}{5}(n-1)a^{10} \\ J(D_a(D_b(f(a, b)))) &= 216a^3 + 288(n-1)a^6 \\ &\quad + 96(3n-1)a^4 + 288(n-1)a^8 \\ Q_2(J(D_a(D_b(f(a, b)))))) &= 216a^5 + 288(n-1)a^8 \\ &\quad + 96(3n-1)a^6 + 288(n-1)a^{10} \\ S_aQ_2(J(D_a(D_b(f(a, b)))))) &= \frac{216}{5}a^5 + 36(n-1)a^8 \\ &\quad + 16(3n-1)a^6 + \frac{144}{5}(n-1)a^{10} \\ D_a^3 D_b^3(f(a, b)) &= 6^3(36)ab^2 + 12^3(24)(n-1)ab^5 \\ &\quad + 8^3(12)(3n-1)ab^3 \\ &\quad + 24^3(12)(n-1)a^3b^5, \\ J D_a^3 D_b^3(f(a, b)) &= 6^3(36)a^3 + 12^3(24)(n-1)a^6 \\ &\quad + 8^3(12)(3n-1)a^4 \\ &\quad + 24^3(12)(n-1)a^8, \\ S_a^3 J D_a^3 D_b^3(f(a, b)) &= 2^3(36)a^3 + 2^3(24)(n-1)a^6 \\ &\quad + 2^3(12)(3n-1)a^4 \\ &\quad + 3^3(12)(n-1)a^8. \end{aligned}$$

Now we obtained:

$$\begin{aligned} S_a(J(f(a, b)))|_{a=1=b} &= \frac{36}{5} + 3(n-1) \\ &\quad + 2(3n-1) \\ &\quad + \frac{6}{5}(n-1) \\ S_aQ_2(J(D_a(D_b(f(a, b))))))|_{a=1=b} &= \frac{216}{5} + 36(n-1) \\ &\quad + 16(3n-1) \\ &\quad + \frac{144}{5}(n-1) \\ S_a^3 J D_a^3 D_b^3(f(a, b))|_{a=1=b} &= \left(\frac{6}{3}\right)^3(36) \\ &\quad + \left(\frac{12}{6}\right)^3(24)(n-1) \\ &\quad + \left(\frac{8}{4}\right)^3(12)(3n-1) \\ &\quad + \left(\frac{24}{8}\right)^3(12)(n-1). \end{aligned}$$

Consequently:

$$\begin{aligned} \text{(i)} \quad H(\mathbb{G}) &= 2 S_a(J(f(a, b)))|_{a=1=b} = 2\left[\frac{36}{5} + 3(n-1) \right. \\ &\quad \left. + 2(3n-1) + \frac{6}{5}(n-1)\right] = \left(\frac{102}{5}\right)n + 2 \\ \text{(ii)} \quad IS(\mathbb{G}) &= S_aQ_2(J(D_a(D_b(f(a, b))))))|_{a=1=b} = \frac{216}{5} \\ &\quad + 36(n-1) + 16(3n-1) + \frac{144}{5}(n-1) = \left(\frac{564}{5}\right)n - \frac{188}{5} \\ \text{(iii)} \quad AZI(\mathbb{G}) &= S_a^3 J D_a^3 D_b^3(f(a, b))|_{a=1=b} = \left(\frac{6}{3}\right)^3(36) \\ &\quad + \left(\frac{12}{6}\right)^3(24)(n-1) + \left(\frac{8}{4}\right)^3(12)(3n-1) \\ &\quad + \left(\frac{24}{8}\right)^3(12)(n-1) = 804n - 324 \end{aligned}$$

4 Results for second metal-organic network

In this section, we show the consequences of TIs for the $MON_2(n)$. So, we define the partitions of node-set and edge-set of $MON_2(n)$ with respect to degree of nodes. We have three different kinds of nodes in $MON_2(n)$ with respect to degree of 2, 3, and 4. Thus, we have:

$$\begin{aligned} V_1 &= \{x \in V(MON_2(n)) \mid \deg(x)=2\}, \\ V_2 &= \{x \in V(MON_2(n)) \mid \deg(x)=3\}, \\ V_3 &= \{x \in V(MON_2(n)) \mid \deg(x)=4\}, \end{aligned}$$

where $|V_1| = 12n + 18$, $|V_2| = 24n - 12$, and $|V_3| = 12n - 6$. Consequently:

$$|V(MON_2(n))| = u = |V_1| + |V_2| + |V_3| = 48n.$$

Additionally, we have different kinds of edges that is based on the degree of end nodes in $MON_2(n)$ that are $\{2, 3\}$, $\{2, 4\}$, $\{3, 3\}$, $\{3, 4\}$, and $\{4, 4\}$.

Hence, we have:

$$\begin{aligned} E_1 &= E_{\{2,3\}} = \{xy \in E(MON_2(n)) \mid \deg(x)=2, \deg(y)=3\}, \\ E_2 &= E_{\{2,4\}} = \{xy \in E(MON_2(n)) \mid \deg(x)=2, \deg(y)=4\}, \\ E_3 &= E_{\{3,3\}} = \{xy \in E(MON_2(n)) \mid \deg(x)=3, \deg(y)=3\}, \\ E_4 &= E_{\{3,4\}} = \{xy \in E(MON_2(n)) \mid \deg(x)=3, \deg(y)=4\}, \\ E_5 &= E_{\{4,4\}} = \{xy \in E(MON_2(n)) \mid \deg(x)=4, \deg(y)=4\}, \end{aligned}$$

where $|E_{\{2,3\}}| = 12(n+2)$, $|E_{\{2,4\}}| = 12(n+1)$, $|E_{\{3,3\}}| = 24(n-1)$, $|E_{\{3,4\}}| = 12(n-1)$, and $|E_{\{4,4\}}| = 12(n-1)$. Consequently, $|E(MON_2(n))| = e = |E_{\{2,3\}}| + |E_{\{2,4\}}| + |E_{\{3,3\}}| + |E_{\{3,4\}}| + |E_{\{4,4\}}| = 72n - 12$.

Table 4: Partitions of edges of $\text{MON}_2(n)$

$E_{\{e(x), e(y)\}}$	$E_{\{2,3\}}$	$E_{\{2,4\}}$	$E_{\{3,3\}}$	$E_{\{3,4\}}$	$E_{\{4,4\}}$
$ E_{\{e(x), e(y)\}} $	$12(n+2)$	$12(n+1)$	$24(n-1)$	$12(n-1)$	$12(n-1)$

Therefore, we define the partition of node-set $V(\text{MON}_2(n))$ and edge-set $E(\text{MON}_2(n))$ of $\text{MON}_2(n)$ with respect to addition of degree of neighborhood nodes.

Thus, for $x, y \in E(\text{MON}_2(n))$, we get Table 4.

Theorem 4.1.

Let $\mathbb{G} \cong \text{MON}_2(n)$ be the second metal-organic network, where $n \geq 2$. The M-polynomial of $\mathbb{G}$ is:

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

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

$$\begin{aligned} M(\mathbb{G}, a, b) &= \sum_{i \leq j} (m_{i,j} \mathbb{G} a^i b^j) \\ &= \sum_{2 \leq 3} (m_{2,3} \mathbb{G} a^2 b^3) + \sum_{2 \leq 4} (m_{2,4} \mathbb{G} a^2 b^4) \\ &\quad + \sum_{3 \leq 3} (m_{3,3} \mathbb{G} a^3 b^3) + \sum_{3 \leq 4} (m_{3,4} \mathbb{G} a^3 b^4) \\ &\quad + \sum_{4 \leq 4} (m_{4,4} \mathbb{G} a^4 b^4) \\ &= |E_1| a^2 b^3 + |E_2| a^2 b^4 + |E_3| a^3 b^3 \\ &\quad + |E_4| a^3 b^4 + |E_5| a^4 b^4 \\ &= 12(n+2)a^2b^3 + 12(n+1)a^2b^4 \\ &\quad + 24(n-1)a^3b^3 + 12(n-1)a^3b^4 \\ &\quad + 12(n-1)a^4b^4 \end{aligned}$$

Theorem 4.2

Let $\mathbb{G} \cong \text{MON}_2(n)$ be the second metal-organic network, where $n \geq 2$. The M-polynomial of $\mathbb{G}$ is:

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

Then, the first Zagreb index ($M_1(\mathbb{G})$), the second Zagreb index ($M_2(\mathbb{G})$), the second modified Zagreb index ($MM_2(\mathbb{G})$), general Randić index ($R_\alpha(\mathbb{G})$), and reciprocal

General Randić index ($RR_\alpha(\mathbb{G})$), where $\alpha \in \mathbb{N}$ 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) $MM_2(\mathbb{G}) = \binom{95}{12}n + \frac{13}{12}$,
- (iv) $R_\alpha(\mathbb{G}) = (6)^\alpha 12(n+2) + (8)^\alpha 12(n+1) \\ + (9)^\alpha 24(n-1) + (12)^\alpha 12(n-1) + (16)^\alpha 12(n-1)$
- (v) $RR_\alpha(\mathbb{G}) = \frac{12}{(6)^\alpha} (n+2) + \frac{12}{(8)^\alpha} (n+1) + \frac{24}{(9)^\alpha} (n-1) \\ + \frac{12}{(12)^\alpha} (n-1) + \frac{12}{(16)^\alpha} (n-1)$,
- (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:

$$\begin{aligned} f(a, b) &= 12(n+2)a^2b^3 + 12(n+1)a^2b^4 \\ &\quad + 24(n-1)a^3b^3 + 12(n-1)a^3b^4 \\ &\quad + 12(n-1)a^4b^4 \end{aligned}$$

The needed partial derivatives and integrals are computed as:

$$\begin{aligned} D_a(f(a, b)) &= 24(n+2)ab^3 + 24(n+1)ab^4 \\ &\quad + 72(n-1)a^2b^3 + 36(n-1)a^2b^4 \\ &\quad + 48(n-1)a^3b^4, \\ D_b(f(a, b)) &= 36(n+2)a^2b^2 + 48(n+1)a^2b^3 \\ &\quad + 72(n-1)a^3b^2 + 48(n-1)a^3b^3 \\ &\quad + 48(n-1)a^4b^3, \\ D_a(D_b(f(a, b))) &= 72(n+2)ab^2 + 96(n+1)ab^3 \\ &\quad + 216(n-1)a^2b^2 + 144(n-1)a^2b^3 \\ &\quad + 192(n-1)a^3b^3, \\ S_a(f(a, b)) &= 6(n+2)a^2b^3 + 6(n+1)a^2b^4 \\ &\quad + 8(n-1)a^3b^3 + 4(n-1)a^3b^4 \\ &\quad + 3(n-1)a^4b^4, \\ S_b(f(a, b)) &= 4(n+2)a^2b^3 + 3(n+1)a^2b^4 \\ &\quad + 8(n-1)a^3b^3 + 3(n-1)a^3b^4 \\ &\quad + 3(n-1)a^4b^4, \\ S_a(S_b(f(a, b))) &= 2(n+2)a^2b^3 + \frac{3}{2}(n+1)a^2b^4 \\ &\quad + \frac{8}{3}(n-1)a^3b^3 + (n-1)a^3b^4 \\ &\quad + \frac{3}{4}(n-1)a^4b^4, \\ D_bS_a(f(a, b)) &= 18(n+2)a^2b^2 + 24(n+1)ab^4 \\ &\quad + 24(n-1)a^3b^2 + 16(n-1)a^3b^3 \\ &\quad + 12(n-1)a^4b^3, \end{aligned}$$

$$\begin{aligned}
D_a S_b(f(a, b)) &= 8(n+2)a^2 b^3 + 6(n+1)ab^4 \\
&\quad + 24(n-1)a^2 b^3 + 9(n-1)a^2 b^4 \\
&\quad + 12(n-1)a^3 b^4, \\
(D^{\alpha_a} D^{\alpha_b})(f(a, b)) &= (6)^{\alpha} 12(n+2)ab^2 \\
&\quad + (8)^{\alpha} 12(n+1)ab^3 \\
&\quad + (9)^{\alpha} 24(n-1)a^2 b^2 \\
&\quad + (12)^{\alpha} 12(n-1)a^2 b^3 \\
&\quad + (16)^{\alpha} 12(n-1)a^3 b^3, \\
(S^{\alpha_a} S^{\alpha_b})(f(a, b)) &= \frac{12}{(6)^{\alpha}}(n+2)a^2 b^3 + \frac{12}{(8)^{\alpha}}(n+1)a^2 b^4 \\
&\quad + \frac{24}{(9)^{\alpha}}(n-1)a^3 b^3 + \frac{12}{(12)^{\alpha}}(n-1)a^3 b^4 \\
&\quad + \frac{12}{(16)^{\alpha}}(n-1)a^4 b^4,
\end{aligned}$$

Now, we obtained:

$$\begin{aligned}
D_a(f(a, b))|_{a=|b} &= 24(n+2) + 24(n+1) \\
&\quad + 72(n-1) + 36(n-1) + 48(n-1), \\
D_b(f(a, b))|_{a=|b} &= 36(n+2) + 48(n+1) \\
&\quad + 72(n-1) + 48(n-1) + 48(n-1), \\
D_a(D_b(f(a, b)))|_{a=|b} &= 72(n+2) + 96(n+1) \\
&\quad + 216(n-1) + 144(n-1) \\
&\quad + 192(n-1), \\
S_a(f(a, b))|_{a=|b} &= 6(n+2) + 6(n+1) \\
&\quad + 8(n-1) + 4(n-1) + 3(n-1), \\
S_b(f(a, b))|_{a=|b} &= 4(n+2) + 3(n+1) \\
&\quad + 8(n-1) + 3(n-1) + 3(n-1), \\
S_a(S_b(f(a, b)))|_{a=|b} &= 2(n+2) + \frac{3}{2}(n+1) \\
&\quad + \frac{8}{3}(n-1) + (n-1) \\
&\quad + \frac{3}{4}(n-1), \\
D_b S_a(f(a, b))|_{a=|b} &= 18(n+2) + 24(n+1) \\
&\quad + 24(n-1) + 16(n-1) \\
&\quad + 12(n-1), \\
D_a S_b(f(a, b))|_{a=|b} &= 8(n+2) + 6(n+1) \\
&\quad + 24(n-1) + 9(n-1) \\
&\quad + 12(n-1), \\
(D^{\alpha_a} D^{\alpha_b})(f(a, b))|_{a=|b} &= (6)^{\alpha} 12(n+2) \\
&\quad + (8)^{\alpha} 12(n+1) \\
&\quad + (9)^{\alpha} 24(n-1) \\
&\quad + (12)^{\alpha} 12(n-1) \\
&\quad + (16)^{\alpha} 12(n-1), \\
(S^{\alpha_a} S^{\alpha_b})(f(a, b))|_{a=|b} &= \frac{12}{(6)^{\alpha}}(n+2) + \frac{12}{(8)^{\alpha}}(n+1) \\
&\quad + \frac{24}{(9)^{\alpha}}(n-1) + \frac{12}{(12)^{\alpha}}(n-1) \\
&\quad + \frac{12}{(16)^{\alpha}}(n-1),
\end{aligned}$$

Consequently:

$$\begin{aligned}
\text{(i)} \quad M_1(\mathbb{G}) &= (D_a + D_b)(f(a, b))|_{a=|b} \\
&= D_a(f(\mathbb{G}, a, b))|_{a=|b} + D_b(f(\mathbb{G}, a, b))|_{a=|b} = 456n - 132 \\
\text{(ii)} \quad M_2(\mathbb{G}) &= (D_a D_b)(f(a, b))|_{a=|b} \\
&= (D_a(D_b(f(\mathbb{G}, a, b))))|_{a=|b} = 720n - 312 \\
\text{(iii)} \quad MM_2(\mathbb{G}) &= (S_a S_b)(f(a, b))|_{a=|b} \\
&= S_a(S_b(f(\mathbb{G}, a, b)))|_{a=|b} = 2(n+2) \\
&\quad + \frac{3}{2}(n+1) + \frac{8}{3}(n-1) + (n-1) + \frac{3}{4}(n-1) = \left(\frac{95}{12}\right)n + \frac{13}{12}, \\
\text{(iv)} \quad R_{\alpha}(\mathbb{G}) &= (D^{\alpha_a} D^{\alpha_b})(f(a, b))|_{a=|b} \\
&= (6)^{\alpha} 12(n+2) + (8)^{\alpha} 12(n+1) \\
&\quad + (9)^{\alpha} 24(n-1) + (12)^{\alpha} 12(n-1) \\
&\quad + (16)^{\alpha} 12(n-1), \\
\text{(v)} \quad RR_{\alpha}(\mathbb{G}) &= (S^{\alpha_a} S^{\alpha_b})(f(a, b))|_{a=|b} \\
&= \frac{12}{(6)^{\alpha}}(n+2) + \frac{12}{(8)^{\alpha}}(n+1) + \frac{24}{(9)^{\alpha}}(n-1) \\
&\quad + \frac{12}{(12)^{\alpha}}(n-1) + \frac{12}{(16)^{\alpha}}(n-1), \\
\text{(vi)} \quad SDD(\mathbb{G}) &= (D_a S_b + D_b S_a)(f(a, b))|_{a=|b} \\
&= (D_a S_b)(f(a, b))|_{a=|b} + (D_b S_a)(f(a, b))|_{a=|b} \\
&= (D_a(S_b(f(a, b))))|_{a=|b} + (D_b(S_a(f(a, b))))|_{a=|b} \\
&= 153n - 15 \triangleright
\end{aligned}$$

Theorem 4.3

Let $\mathbb{G} \cong \text{MON}_2(n)$ be the second metal-organic network, where $n \geq 2$. The M-polynomial of $\mathbb{G}$ is:

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

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

$$\begin{aligned}
\text{(i)} \quad H(\mathbb{G}) &= 2S_a(J(f(a, b)))|_{a=|b} = \left(\frac{813}{35}\right)n - \frac{29}{35}, \\
\text{(ii)} \quad IS(\mathbb{G}) &= S_a Q_2(J(D_a(D_b(f(a, b)))))|_{a=|b} \\
&= \left(\frac{3884}{35}\right)n - \left(\frac{1252}{35}\right), \\
\text{(iii)} \quad AZI(\mathbb{G}) &= S_a^3 J D^3_a D^3_b(f(a, b))|_{a=|b} \\
&= 12(8)(n+2) + 12(8)(n+1) \\
&\quad + 24\left(\frac{729}{64}\right)(n-1) + 12\left(\frac{1728}{125}\right)(n-1) + 12\left(\frac{512}{27}\right)(n-1) \\
&= \left(\frac{7729367}{9000}\right)n - \left(\frac{3409367}{9000}\right).
\end{aligned}$$

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

$$\begin{aligned} f(a, b) = & 12(n+2)a^2b^3 + 12(n+1)a^2b^4 \\ & + 24(n-1)a^3b^3 + 12(n-1)a^3b^4 \\ & + 12(n-1)a^4b^4. \end{aligned}$$

The needed partial derivatives and integrals are computed as:

$$\begin{aligned} J(f(a, b)) = & 12(n+2)a^5 + 12(n+1)a^6 \\ & + 24(n-1)a^6 + 12(n-1)a^7 \\ & + 12(n-1)a^8, \end{aligned}$$

$$\begin{aligned} S_a(J(f(a, b))) = & \frac{12}{5}(n+2)a^5 + 2(n+1)a^6 \\ & + 4(n-1)a^6 + \frac{12}{7}(n-1)a^7 \\ & + \frac{3}{2}(n-1)a^8, \end{aligned}$$

$$\begin{aligned} J(D_a(D_b(f(a, b)))) = & 72(n+2)a^3 + 96(n+1)a^4 \\ & + 216(n-1)a^4 \\ & + 144(n-1)a^5 \\ & + 192(n-1)a^6, \end{aligned}$$

$$\begin{aligned} Q_2(J(D_a(D_b(f(a, b)))))) = & 72(n+2)a^5 + 96(n+1)a^6 \\ & + 216(n-1)a^6 \\ & + 144(n-1)a^7 \\ & + 192(n-1)a^8, \end{aligned}$$

$$\begin{aligned} S_a Q_2(J(D_a(D_b(f(a, b)))))) = & \frac{72}{5}(n+2)a^5 + 16(n-1)a^6 \\ & + 36(n-1)a^6 + \frac{144}{7}(n-1)a^7 \\ & + 24(n-1)a^8, \end{aligned}$$

$$\begin{aligned} D^3_a(D^3_b(f(a, b))) = & 6^3(12)(n+2)ab^2 \\ & + 8^3(12)(n+1)ab^3 \\ & + 9^3(24)(n-1)a^2b^2 \\ & + 12^3(12)(n-1)a^2b^3 \\ & + 16^3(12)(n-1)a^3b^3, \end{aligned}$$

$$\begin{aligned} J D^3_a(D^3_b(f(a, b))) = & 6^3(12)(n+2)a^3 \\ & + 8^3(12)(n+1)a^4 \\ & + 9^3(24)(n-1)a^4 \\ & + 12^3(12)(n-1)a^5 \\ & + 16^3(12)(n-1)a^6, \end{aligned}$$

$$\begin{aligned} S_a^3 J D^3_a(D^3_b(f(a, b))) = & \left(\frac{6}{3}\right)^3(12)(n+2)a^3 \\ & + \left(\frac{8}{4}\right)^3 12(n+1)a^4 \\ & + \left(\frac{9}{4}\right)^3 24(n-1)a^4 \\ & + \left(\frac{12}{5}\right)^3 12(n-1)a^5 \\ & + \left(\frac{16}{6}\right)^3 12(n-1)a^6. \end{aligned}$$

Now we obtained:

$$\begin{aligned} S_a(J(f(a, b)))|_{a=1=b} = & \frac{12}{5}(n+2) + 2(n+1) \\ & + 4(n-1) + \left(\frac{12}{7}\right)(n-1) \\ & + \left(\frac{3}{2}\right)(n-1), \end{aligned}$$

$$\begin{aligned} S_a Q_2(J(D_a(D_b(f(a, b)))))|_{a=1=b} = & \frac{72}{5}(n+2) + 16(n-1) \\ & + 36(n-1) + \frac{144}{7}(n-1) \\ & + 24(n-1), \end{aligned}$$

$$\begin{aligned} S_a^3 J(D^3_a D^3_b(f(a, b)))|_{a=1=b} = & 2^3(12)(n+2) \\ & + (2)^3 12(n+1) \\ & + \left(\frac{9}{4}\right)^3 24(n-1) \\ & + \left(\frac{12}{5}\right)^3 12(n-1) \\ & + \left(\frac{8}{3}\right)^3 12(n-1). \end{aligned}$$

Consequently:

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

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

$$(iii) \quad AZI(\mathbb{G}) = \left(\frac{7729367}{9000}\right)n - \left(\frac{3409367}{9000}\right).$$

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

Figure 3: Graphical comparison of $M_1(\mathbb{G})$, $M_2(\mathbb{G})$, and $MM_2(\mathbb{G})$ are labeled in blue, cyan, and gold graphs, respectively, for $MON_1(n)$.

Figure 4: Graphical comparison of $R_o(G)$, $RR_o(G)$, and $SSD(G)$ are labeled in blue, cyan, and gold graphs, respectively, for $MON_1(n)$.

Figure 5: Graphical comparison of $H(G)$, $IS(G)$, and $AZI(G)$ are labeled in blue, cyan, and gold graphs, respectively, for $MON_1(n)$.

$MON_1(n)$ 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

Figure 6: Graphical comparison of $M_1(G)$, $M_2(G)$, and $MM_2(G)$ are labeled in blue, cyan, and gold graphs, respectively, for $MON_2(n)$.

Figure 7: Graphical comparison of $R_o(G)$, $RR_o(G)$, and $SSD(G)$ are labeled in blue, cyan, and gold graphs, respectively, for $MON_2(n)$.

Figure 8: Graphical comparison of $H(G)$, $IS(G)$, and $AZI(G)$ are labeled in blue, cyan, and gold graphs, respectively, for $MON_2(n)$.

Table 5: Comparison among $M_1(G)$, $M_2(G)$, and $MM_2(G)$ of $MON_1(n)$

n	$M_1(G)$	$M_2(G)$	$MM_2(G)$
2	852	1272	16
3	1380	2136	23
4	1908	3000	30
5	2436	3864	37
6	2964	4728	44
7	3492	5592	51
8	4020	6456	58
9	4548	7320	65
10	5076	8184	72

Table 6: Comparison among $R_\alpha(G)$, $RR_\alpha(G)$, and $SSD(G)$ of $MON_1(n)$, where $\alpha = 1$

n	$R_\alpha(G)$	$RR_\alpha(G)$	$SSD(G)$
2	1272	16	334
3	2136	23	530
4	3000	30	726
5	3864	37	922
6	4728	44	1118
7	5592	51	1314
8	6456	58	1510
9	7320	65	1706
10	8184	72	1902

Table 7: Comparison among $H(G)$, $IS(G)$, and $AZI(G)$ of $MON_1(n)$

n	$H(G)$	$IS(G)$	$AZI(G)$
2	42.80	188	1284
3	63.20	300.8	2088
4	83.60	413.6	2892
5	104	526.4	3696
6	124.40	639.2	4500
7	144.80	752	5304
8	165.20	864.8	6108
9	185.60	977.6	6912
10	206	1090.4	7716

Table 8: Comparison among $M_1(G)$, $M_2(G)$, and $MM_2(G)$ of $MON_2(n)$

n	$M_1(G)$	$M_2(G)$	$MM_2(G)$
2	780	1128	16.9166
3	1236	1848	24.8333
4	1692	2568	32.7500
5	2148	3288	40.6666
6	2604	4008	48.5833
7	3060	4728	56.5000
8	3516	5448	64.4166
9	3972	6168	72.3333
10	4428	6888	80.2500

Table 9: Comparison among $R_\alpha(G)$, $RR_\alpha(G)$, and $SSD(G)$ of $MON_2(n)$, where $\alpha = 1$

n	$R_\alpha(G)$	$RR_\alpha(G)$	$SSD(G)$
2	1128	17	291
3	1848	25	444
4	2568	33	597
5	3288	41	750
6	4008	49	903
7	4728	57	1056
8	5448	64	1209
9	6168	72	1326
10	6888	80	1515

Table 10: Comparison among $H(G)$, $IS(G)$, and $AZI(G)$ of $MON_2(n)$

N	$H(G)$	$IS(G)$	$AZI(G)$
2	45.6285	186.1714	1338.8186
3	68.8571	297.1428	2197.6371
4	92.0857	408.1142	3056.45567
5	115.3142	519.0857	3915.2742
6	138.5428	630.0571	4774.09278
7	161.7714	741.0285	5632.91133
8	185	852	6491.7299
9	208.2285	962.9714	7350.5484
10	231.4571	1073.9428	8209.367

these two networks. Figures 4-6 present that $M_2(G)$, $R_\alpha(G)$, and $AZI(G)$ are better for both networks discussed in this paper. These M-polynomials and calculated TIs 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.

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