Research Article

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On topological polynomials and indices for metal-organic and cuboctahedral bimetallic networks

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Abstract: A molecular graph consists of bonds and atoms, where atoms are present as vertices and bonds are present as edges. We can look at topological invariants and topological polynomials that furnish bioactivity and physio-chemical features for such molecular graphs. These topological invariants, which are usually known as graph invariants, are numerical quantities that relate to the topology of a molecular graph. Let $m_{pq}(X)$ be the number of edges in X such that $(\zeta^a, \zeta^b) = (p, q)$, where ζ^a (or ζ^b) present the degree of a (or b). The M-polynomial for X can be determined with the help of relation $M(X;x, y) = \sum_{p \le q} m_{pq}(X)x^p y^q$. In this study, we calculate the M-polynomial, forgotten polynomial, sigma polynomial and Sombor polynomial, and different topological invariants of critical importance, referred to as first, second, modified and augmented Zagreb, inverse and general Randić, harmonic, symmetric division; forgotten and inverse invariants of chemical structures namely metal-organic networks (transition metal-tetra cyano benzene organic network) and cuboctahedral bimetallic networks (MOPs) are retrieved using a generic topological polynomial approach. We also draw the two-dimensional graphical representation of outcomes that express the relationship between topological indices and polynomial structural parameters.

Keywords: M-polynomial, sigma polynomial, Sombor polynomial, metal-organic networks, cuboctahedral bimetallic, topological indices

1 Introduction

The topological invariants, which are usually known as graph invariants, are numerical quantities that relate to the topology of a molecular graph. Topological invariants are used in graph theory to investigate the structural possession of graphs. These compounds are used in a wide range of fields including chemistry, drug discovery, pharmaceutical, and discrete dynamical systems. Graph theory is an important part of mathematics that allows us to explore the features of any structure with ease. Chemical graph theory is crucial in the modeling and designing of any chemical structure. Mathematical chemistry appeals to scientists since it studies and works on a large number of topological invariants of a chemical compound in order to anticipate its physicochemical properties (Brückler et al., 2011). Molecular compounds have a wide range of applications in business, industrial, medicinal chemistry, commercial, everyday life, and research (Imran et al., 2018a,b).

Let X be a simple and finite graph with $V(X)$ be a vertex set and $E(X)$ be an edge set. A graph $X = (V(X), E(X))$ is connected if each pair of its vertices has a path connecting them. A network is simply defined as a connected graph with numerous edges and no loops. The degree of a given vertex a is the number of edges in X which are connecting directly to the vertex, and it is represented as ζ^a. When calculating topological invariants, one should have a solid understanding of the fundamentals of graph theory. The topological invariants are calculated by figuring out the single polynomial. Several graph polynomials

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have been established in the literature and have played a major role in mathematical chemistry, including matching (Farrell, 1979), Schultz (Hassani et al., 2013), and Tutte (Došlić, 2013) polynomials, with M-polynomials and Hosoya polynomials (Hosoya, 1988) being the most notable. The Hosoya polynomial, also known as the Wiener polynomial, is used to establish the distance-based topological invariants in chemistry. Similarly, in defining degree-based topological invariants of graphs, the M-polynomial (Ajmal et al., 2017a,b) is key. According to Deutsch and Klavžar (2015), the M-polynomial for X is defined as follows:

$$M(X;x,y) = \sum_{\delta \le p \le q \le \Delta} m_{pq}(X)x^p y^q \tag{1}$$

where $\delta = \min\{\zeta^a: \forall a \in V(X)\}$, $\Delta = \max\{\zeta^a: \forall a \in V(X)\}$, and $m_{pq}(X)$ be the number of edges $ab \in E(X)$ as $(\zeta^a, \zeta^b) = (p, q)$.

The forgotten polynomial for X is written as follows:

$$F(X;x) = \sum_{ab \in E(X)} x^{((\zeta^a)^2 + (\zeta^b)^2)} \tag{2}$$

The sigma polynomial for X is characterized as:

$$S(X;x) = \sum_{ab \in E(X)} x^{(\zeta^a - \zeta^b)^2} \tag{3}$$

The Sombor polynomial for X is defined as:

$$\mathrm{SO}(X;x) = \sum_{ab \in E(X)} x^{\sqrt{(\zeta^a)^2 + (\zeta^b)^2}} \tag{4}$$

In most cases, multiple equations can be used to compute topological invariants for certain classes. We can obtain several vertex-based invariants with the help of M-polynomial by using only the specific differential, integral, or both operators on corresponding polynomials. The authors were able to construct closed forms of degree-related invariants for triangular boron nanotubes (Munir et al., 2016) and the Jahangir graph (Munir et al., 2017) using M-polynomial. Experiments demonstrate that no one topological invariant is powerful enough to deliberate all of a compound's physiochemical possessions, although they can do so to some extent when used in combination. Randić (1975) introduced the first degree-based topological invariant, which is known as the Randić invariant, 1975, and in some literature, it was also written as molecular connectivity invariant (Amic et al., 1998). Bollobás and Erdos (1998) developed a general form of the Randić invariant, which is presented as follows:

$$R_\rho(X) = \sum_{ab \in E(X)} \frac{1}{(\zeta^a \zeta^b)^\rho} \tag{5}$$

where $\rho \in \mathbb{R}$. Chemists and mathematicians investigated this invariant extensively; after that, they concluded that the Randić invariant has a correlation in the Kovats constants of the molecules and the calculations of the boiling point. The inverse Randić $RR_\rho(X)$ invariant is stated as follows:

$$RR_\rho(X) = \sum_{ab \in E(X)} (\zeta^a \zeta^b)^\rho \tag{6}$$

where $\rho \in \mathbb{R}$. The Randić invariant's compatibility with alkane physicochemical properties is remarkable. Several remarkable applications of the Randić invariant (Randić, 1975) are discovered. The first M_1 and the second M_2 Zagreb invariants were presented by Gutman and Trinastić (1972):

$$M_1(X) = \sum_{a \in V(X)} (\zeta^a)^2 = \sum_{ab \in E(X)} (\zeta^a + \zeta^b) \tag{7}$$

$$M_2(X) = \sum_{ab \in E(X)} \zeta^a \zeta^b \tag{8}$$

For a simple graph X, the modified Zagreb invariant can be introduced in the study by Baig et al. (2017) as follows:

$$M_2^m(X) = \sum_{ab \in E(X)} \frac{1}{\zeta^a \zeta^b} \tag{9}$$

The symmetric division SDD(X) is a most effective and good predictor for the computation of the total surface area of polychlorobiphenyl and is investigated for simple and connected graphs as:

$$\mathrm{SDD}(X) = \sum_{ab \in E(X)} \left(\frac{\min(\zeta^a, \zeta^b)}{\max(\zeta^a, \zeta^b)} + \frac{\max(\zeta^a, \zeta^b)}{\min(\zeta^a, \zeta^b)} \right) \tag{10}$$

Another generalization of the Randić invariant is the harmonic invariant and that is introduced as follows:

$$H(X) = \sum_{ab \in E(X)} \frac{2}{\zeta^a + \zeta^b} \tag{11}$$

The inverse sum indeg (or ISI) invariant is a reliable and most important predictor for the computation of the surface area of octane isomer, and its extremal graphs can be found by using mathematical chemistry. The inverse sum indeg ISI(X) invariant is specified as follows:

$$\mathrm{ISI}(X) = \sum_{ab \in E(X)} \frac{\zeta^a \zeta^b}{\zeta^a + \zeta^b} \tag{12}$$

The augmented Zagreb invariant of X was established by Furtula et al. (2010), and it is defined as follows:

$$A(X) = \sum_{ab \in E(X)} \left(\frac{\zeta^a \zeta^b}{\zeta^a + \zeta^b - 2} \right)^3 \tag{13}$$

Furtula and Gutman (2015) proposed the forgotten invariant (also known as F-invariant) and is written as follows:

Table 1: Derivation of some degree-related topological invariants from polynomials

Topological invariant	Formulae based on polynomials
First Zagreb invariant $M_1(X)$	$(D_x+D_y)M(X; x, y)\|_{x=y=1}$
Second Zagreb invariant $M_2(X)$	$(D_xD_y)M(X; x, y)\|_{x=y=1}$
Modified second Zagreb invariant $M_2^m(X)$	$(S_xS_y)M(X; x, y)\|_{x=y=1}$
Randić invariant $R_\rho(X)$.	$(D_x^\rho D_y^\rho)M(X; x, y)\|_{x=y=1}$
Inverse Randić invariant $RR_\rho(X)$	$(S_x^\rho S_y^\rho)M(X; x, y)\|_{x=y=1}$
Harmonic invariant $H(X)$	$2S_xJM(X; x, y)\|_{x=1}$
Inverse sum indeg invariant ISI(X)	$S_xJD_xD_yM(X; x, y)\|_{x=1}$
Augmented Zagreb invariant $A(X)$	$(S_x^3Q_{-2}JD_x^3D_y^3)M(X; x, y)\|_{x=1}$
Forgotten invariant FI(X)	$D_xF(X; x)\|_{x=1}$
Sigma invariant $S(X)$	$D_xS(X; x)\|_{x=1}$
Sombor invariant SO(X)	$D_x\mathrm{SO}(X; x)\|_{x=1}$

$$\mathrm{FI}(X) = \sum_{ab\in E(X)} ((\zeta^a)^2 + (\zeta^b)^2) \tag{14}$$

The sigma invariant (Grigory and Alexander, 2021) is defined as follows:

$$S(X) = \sum_{ab\in E(X)} (\zeta^a - \zeta^b)^2 \tag{15}$$

Gutman (2021) recently developed the concept of Sombor invariant, which is defined as follows:

$$\mathrm{SO}(X) = \sum_{ab\in E(X)} \sqrt{(\zeta^a)^2 + (\zeta^b)^2} \tag{16}$$

We refer to the concerned readers some indices-related articles such as those of Ajmal et al. (2017a,b), Akhter and Imran (2016), Akhter et al. (2016, 2017, 2018, 2020, 2021), Ali et al. (2016, 2017), Gao et al. (2019, 2020), Imran et al. (2020a,b), Yang et al. (2019), and Yasmeen et al. (2021). In Table 1, we give the relation of polynomials and the degree-related topological invariants, where $D_x = x\frac{\partial f(x,y)}{\partial x}$, $D_y = y\frac{\partial f(x,y)}{\partial y}$, $S_x = \int_0^x \frac{f(t,y)}{t}\mathrm{d}t$, $S_y = \int_0^y \frac{f(x,t)}{t}\mathrm{d}t$, $J(f(x, y)) = f(x, x)$, and $Q_\rho(f(x, y)) = x^\rho f(x, y)$.

2 Main results

The novel planar metal-organic networks (transition metal-tetra cyano benzene organic network [TM-TCNB]) and cuboctahedral bimetallic networks (MOPs) are now discussed in terms of their degree-based topological features. Interestingly, the metal-organic networks (TM-TCNB) and cuboctahedral bimetallic (MOPs) systems are metallic in any case in one turn heading and show long-run ferromagnetic coupling on the off chance that for attractive structures, which speak to ideal candidates and an intriguing possibility of uncommon applications in spintronics.

In this article, we calculate the *M*-, *F*-, sigma, and Sombor polynomials for these metal-organic networks (TM-TCNB) and cuboctahedral bimetallic networks (MOPs), and then with the help of these polynomials, we compute first, second, modified, and augmented Zagreb invariants, general and inverse Randić, symmetric division, harmonic, inverse sum indeg, forgotten invariants, sigma, and Sombor invariants of TM-TCNB and MOPs. In the computation of above polynomials and invariants, we use some techniques from combinatorial and analytic computations, also vertex and edge partition, graph theoretical tools, counting of vertex degrees and sum of degrees of neighboring vertices, and also, we use the MATLAB for plotting our results.

3 Molecular structure of TM-TCNB

The attractive frameworks of TM-TCNB have a fragmentary absolute attractive second, so the entire arrangement of TM-TCNB is metallic or half-metallic (metallic a solitary way of turn and protecting in the other heading of the turn). The neighborhood attractive snapshots of the TM (TM = Ti, V, Cr, and Co) in TM-TCNB structures are diminished by turn electrons inverse to the neighborhood turn which are found on the natural ligands and which encompass the focal molecule of TM. The materials of Fe-TCNB, Co-TCNB, Ni-TCNB, and Zn-TCNB are completely metallic. Be that as it may, the metal–natural systems of Ti-TCNB, VTCNB, Cr-TCNB, and Mn-TCNB are half-metallic since they speak to a hole in a solitary turn bearing (Figure 1). Additionally, the TM-TCNB monolayers are attractive with TM = Ti, V, Cr, and Co.

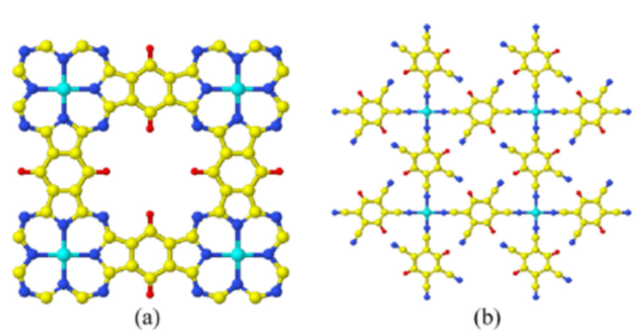

Figure 1: Structures of (a) 2DTM-Pc and the TM-TCNB, (b) metal-organic networks. The TM, N, C, and H atoms are highlighted in cyan, blue, yellow, and red, respectively.

Conversely, Ni-TCNB and Zn-TCNB are non-attractive. For the entire arrangement of TM-TCNB (with the exception of TM = Ni and Zn), there is a fragmented screening impact (lessening of the attractive second), and the nearby attractive snapshot of the molecule (Ti, V, Cr, and Co) is somewhat screened by turn captivated electrons on the natural ligands encompassing TM on account of TM-TCNB. The physical wonder of screening is thoroughly missing in TM-Pc.

Let TM-TCNB be the chemical graph with n unit cells in the plane (Figure 1).

The number of vertices and edges of TM-TCNB are $26n–16$ and $152n–24$, respectively. Since there are four types of vertices in TM-TCNB namely the vertices of degrees $1, 2, 3, 4$. The edge partition of TM-TCNB based on degrees of end vertices of each edge is depicted in Table 2.

3.1 Polynomials of TM-TCNB

Let X be a molecular graph of TM-TCNB. Then, by using Table 2 in Eqs. 1–4, the M-polynomial, F-polynomial, S-polynomial, and SO-polynomial for TM-TCNB are computed as follows:

Table 2: Edge partition based on degrees of end vertices of each edge

$(\zeta(a), \zeta(b))$	**(1,3)**	**(2,2)**	**(2,3)**	**(3,3)**	**(3,4)**
Frequency	$12n-4$	$8n+8$	$32n$	$84n-28$	$16n$
Set of edges	E_1	E_2	E_3	E_4	E_5

$$\begin{aligned} S((\text{TM-TCNB});x) &= \sum_{ab\in E(X)} x^{(\zeta^a-\zeta^b)^2} \\ &= \sum_{ab\in E_1} m_{13}(\text{TM-TCNB})x^4 \\ &\quad + \sum_{ab\in E_2} m_{22}(\text{TM-TCNB}) \\ &\quad + \sum_{ab\in E_3} m_{23}(\text{TM-TCNB})x \\ &\quad + \sum_{ab\in E_4} m_{33}(\text{TM-TCNB}) \\ &\quad + \sum_{ab\in E_5} m_{34}(\text{TM-TCNB})x \end{aligned}$$

$$\begin{aligned} &S((\text{TM-TCNB});x) \\ &= |E_1|x^4 + |E_2| + |E_3|x + |E_4| + |E_5|x \\ &= 4(3n-1)x^4 + 8(n+1) + 32nx + 28(3n-1) + 16nx \\ &= 4(3n-1)x^4 + 48nx + 4(23n-5) \end{aligned}$$

$$\begin{aligned} M((\text{TM-TCNB});x,y) &= \sum_{\delta\le p\le q\le\triangle} m_{pq}(\text{TM-TCNB})x^p y^q \\ &= \sum_{ab\in E_1} m_{13}(\text{TM-TCNB})xy^3 + \sum_{ab\in E_2} m_{22}(\text{TM-TCNB})x^2y^2 \\ &\quad + \sum_{ab\in E_3} m_{23}(\text{TM-TCNB})x^2y^3 + \sum_{ab\in E_4} m_{33}(\text{TM-TCNB})x^3y^3 \\ &\quad + \sum_{ab\in E_5} m_{34}(\text{TM-TCNB})x^3y^4 \\ &= |E_1|xy^3 + |E_2|x^2y^2 + |E_3|x^2y^3 + |E_4|x^3y^3 + |E_5|x^3y^4 \\ &= 4(3n-1)xy^3 + 8(n+1)x^2y^2 + 32nx^2y^3 + 28(3n-1)x^3y^3 + 16nx^3y^4 \end{aligned}$$

$$\begin{aligned} F((\text{TM-TCNB});x) &= \sum_{ab\in E(X)} x^{((\zeta^a)^2+(\zeta^b)^2)} \\ &= \sum_{ab\in E_1} m_{13}(\text{TM-TCNB})x^{10} + \sum_{ab\in E_2} m_{22}(\text{TM-TCNB})x^8 \\ &\quad + \sum_{ab\in E_3} m_{23}(\text{TM-TCNB})x^{13} + \sum_{ab\in E_4} m_{33}(\text{TM-TCNB})x^{18} \\ &\quad + \sum_{ab\in E_5} m_{34}(\text{TM-TCNB})x^{25} \\ &= |E_1|x^{10} + |E_2|x^8 + |E_3|x^{13} + |E_4|x^{18} + |E_5|x^{25} \\ &= 4(3n-1)x^{10} + 8(n+1)x^8 + 32nx^{13} + 28(3n-1)x^{18} + 16nx^{25} \end{aligned}$$

$$\begin{aligned}
\mathrm{SO}((\text{TM-TCNB});x) &= \sum_{ab\in E(X)} x^{\sqrt{(\zeta^a)^2+(\zeta^b)^2}} \\
&= \sum_{ab\in E_1} m_{13}(\text{TM-TCNB})x^{\sqrt{10}} + \sum_{ab\in E_2} m_{22}(\text{TM-TCNB})x^{\sqrt{8}} \\
&\quad + \sum_{ab\in E_3} m_{23}(\text{TM-TCNB})x^{\sqrt{13}} + \sum_{ab\in E_4} m_{33}(\text{TM-TCNB})x^{\sqrt{18}} \\
&\quad + \sum_{ab\in E_5} m_{34}((\text{TM-TCNB}))x^{\sqrt{25}} \\
&= |E_1|x^{\sqrt{10}} + |E_2|x^{2\sqrt{2}} + |E_3|x^{\sqrt{13}} + |E_4|x^{\sqrt{18}} + |E_5|x^{5} \\
&= 4(3n-1)x^{\sqrt{10}} + 8(n+1)x^{2\sqrt{2}} + 32nx^{\sqrt{13}} + 28(3n-1)x^{3\sqrt{2}} + 16nx^{5}
\end{aligned}$$

Figure 2 shows a graphical presentation of M-polynomial, F-polynomial, S-polynomial, and SO-polynomial of TM-TCNB, respectively.

3.2 Computation of topological invariants with the help of polynomials of TM-TCNB

Now, we calculate the topological invariants for TM-TCNB, including first, second, modified, and augmented Zagreb

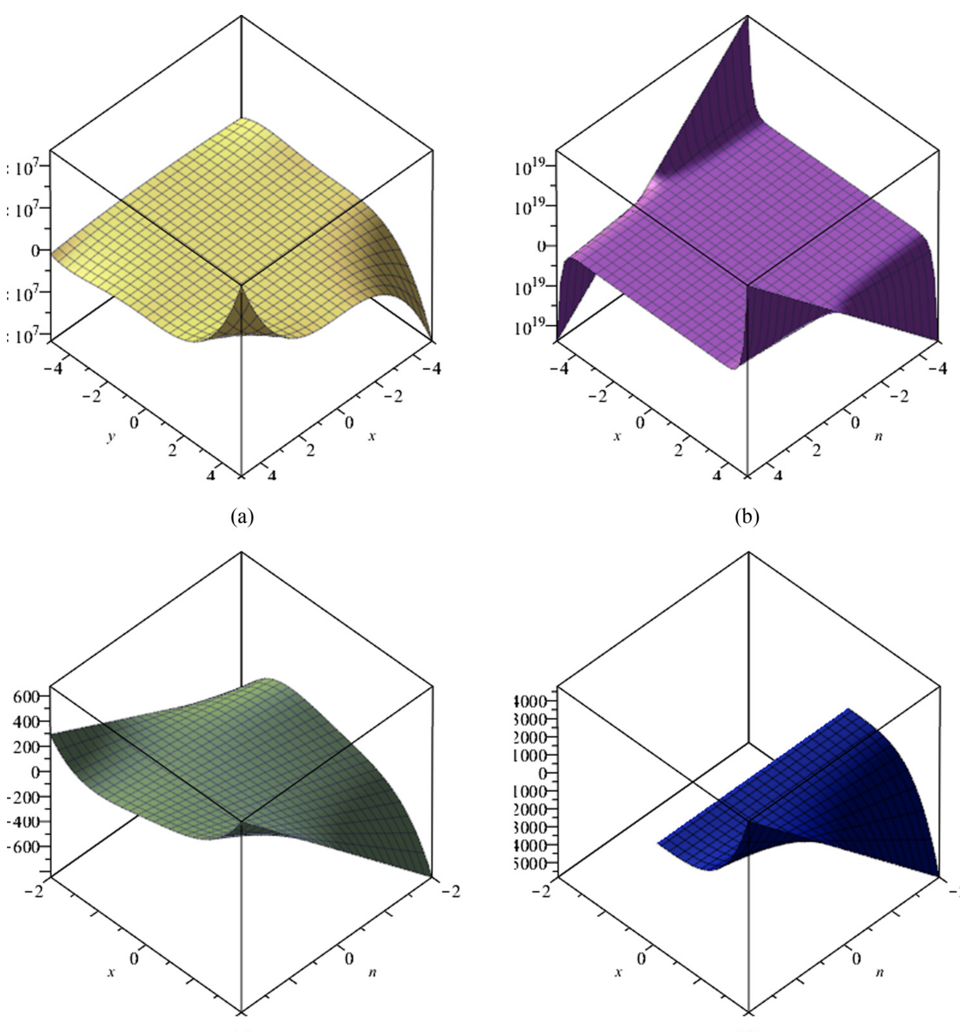

Figure 2: (a) M-polynomial, (b) F-polynomial, (c) S-polynomial, and (d) SO-polynomial of TM-TCNB.

invariants, Randić invariants, SSD invariant, harmonic invariant, ISI invariant, F invariant, S invariant, and SO invariant. From Table 1 and the result of M-polynomial, we acquire the following invariants:

$$\begin{aligned}D_x(f(x,y)) &= x\frac{\partial f(x,y)}{\partial x}\\ &= x((12n-4)y^3+2(8n+8)xy^2+2(32n)xy^3\\ &\quad +3(84n-28)x^2y^3+3(16n)x^2y^4)\\ &= 4(3n-1)xy^3+16(n+1)x^2y^2+64nx^2y^3\\ &\quad +84(3n-1)x^3y^3+48nx^3y^4\end{aligned}$$

$$\begin{aligned}D_y(f(x,y)) &= y\frac{\partial f(x,y)}{\partial y}\\ &= y(3(12n-4)xy^2+2(8n+8)x^2y\\ &\quad +3(32n)x^2y^2+3(84n-28)x^3y^2\\ &\quad +4(16n)x^3y^3)\\ &= 12(3n-1)xy^3+16(n+1)x^2y^2+96nx^2y^3\\ &\quad +84(3n-1)x^3y^3+64nx^3y^4\end{aligned}$$

$$\begin{aligned}D_xD_y(f(x,y)) &= x\frac{\partial}{\partial x}(D_y(f(x,y)))\\ &= x(12(3n-1)y^3+2\times 16(n+1)xy^2\\ &\quad +2(96n)xy^3+3(252n-84)x^2y^3\\ &\quad +3(64n)x^2y^4)\\ &= 12(3n-1)xy^3+32(n+1)x^2y^2+192nx^2y^3\\ &\quad +252(3n-1)x^3y^3+192nx^3y^4\end{aligned}$$

$$\begin{aligned}S_x(f(x,y)) &= \int_0^x \frac{f(t,y)}{t}\mathrm{d}t\\ &= (12n-4)xy^3+\frac{1}{2}(8n+8)x^2y^2+\frac{1}{2}(32n)x^2y^3\\ &\quad +\frac{1}{3}(84n-28)x^3y^3+\frac{1}{3}(16n)x^3y^4\\ &= 4(3n-1)xy^3+4(n+1)x^2y^2+16nx^2y^3\\ &\quad +\frac{28}{3}(3n-1)x^3y^3+\frac{16n}{3}x^3y^4\end{aligned}$$

$$\begin{aligned}S_y(f(x,y)) &= \int_0^y \frac{f(x,t)}{t}\mathrm{d}t\\ &= \frac{1}{3}(12n-4)xy^3+\frac{1}{2}(8n+8)x^2y^2\\ &\quad +\frac{1}{3}(32n)x^2y^3+\frac{1}{3}(84n-28)x^3y^3\\ &\quad +\frac{1}{4}(16n)x^3y^4\\ &= \frac{4}{3}(3n-1)xy^3+4(n+1)x^2y^2+\frac{32n}{3}x^2y^3\\ &\quad +\frac{28}{3}(3n-1)x^3y^3+4nx^3y^4\end{aligned}$$

$$\begin{aligned}S_xS_y(f(x,y)) &= \frac{4}{3}(3n-1)xy^3+\frac{1}{2}(4(n+1))x^2y^2\\ &\quad +\frac{1}{2}\frac{32n}{3}x^2y^3\\ &\quad +\frac{1}{3}\frac{28}{3}(3n-1)x^3y^3+\frac{1}{3}(4n)x^3y^4\\ &= \frac{4}{3}(3n-1)xy^3+2(n+1)x^2y^2+\frac{16n}{3}x^2y^3\\ &\quad +\frac{28}{9}(3n-1)x^3y^3+\frac{4n}{3}x^3y^4\end{aligned}$$

$$\begin{aligned}D_x^{\rho}D_y^{\rho}(f(x,y)) &= 4(3n-1)(3)^{\rho+1}xy^3+(n+1)(2)^{2\rho+5}x^2y^2\\ &\quad +32n(6)^{\rho+1}x^2y^3+28(3n-1)(9)^{\rho+1}x^3y^3\\ &\quad +16n(12)^{\rho+1}x^3y^4\end{aligned}$$

$$\begin{aligned}S_x^{\rho}S_y^{\rho}(f(x,y)) &= \frac{4}{3^{\rho+1}}(3n-1)xy^3+2^{1-2\rho}(n+1)x^2y^2\\ &\quad +\frac{2^{4-\rho}}{3^{\rho+1}}nx^2y^3+\frac{28}{9^{\rho+1}}(3n-1)x^3y^3\\ &\quad +\frac{4^{1-\rho}}{3^{\rho+1}}nx^3y^4\end{aligned}$$

$$\begin{aligned}S_yD_x(f(x,y)) &= \frac{1}{3}(12n-4)xy^3+\frac{1}{2}(16n+16)x^2y^2\\ &\quad +\frac{1}{3}(64n)x^2y^3\\ &\quad +\frac{1}{3}(252n-84)x^3y^3+\frac{1}{4}(48n)x^3y^4\\ &= \frac{4}{3}(3n-1)xy^3+8(n+1)x^2y^2+\frac{64n}{3}x^2y^3\\ &\quad +28(3n-1)x^3y^3+12nx^3y^4\end{aligned}$$

$$\begin{aligned}S_xD_y(f(x,y)) &= (36n-12)xy^3+\frac{1}{2}(16n+16)x^2y^2\\ &\quad +\frac{1}{2}(96n)x^2y^3+\frac{1}{3}(252n-84)x^3y^3\\ &\quad +\frac{1}{3}(64n)x^3y^4\\ &= 12(3n-1)xy^3+8(n+1)x^2y^2+48nx^2y^3\\ &\quad +28(3n-1)x^3y^3+\frac{64n}{3}x^3y^4\end{aligned}$$

$$\begin{aligned}J(f(x,y)) = f(x,x) &= 4(3n-1)x^4+8(n+1)x^4\\ &\quad +32nx^5+28(3n-1)x^6+16nx^7\\ &= 4(5n+1)x^4+32nx^5+28(3n-1)x^6+16nx^7\end{aligned}$$

$$\begin{aligned}S_xJ(f(x,y)) &= \tfrac{1}{4}\times 4(5n+1)x^4+\tfrac{1}{5}(32n)x^5+\tfrac{1}{6}\\ &\quad \times 28(3n-1)x^6+\tfrac{1}{7}(16n)x^7\\ &= (5n+1)x^4+\tfrac{32n}{5}x^5+\tfrac{14}{3}(3n-1)x^6\\ &\quad +\tfrac{16n}{7}x^7\end{aligned}$$

$$\begin{aligned}2S_xJ(f(x,y)) &= 2(5n+1)x^4+\tfrac{64n}{5}x^5+\tfrac{28}{3}(3n-1)x^6\\ &\quad +\tfrac{32n}{7}x^7\end{aligned}$$

$$\begin{aligned} JD_xD_y(f(x,y)) &= 12(3n-1)x^4+32(n+1)x^4+192nx^5+252(3n-1)x^6+192nx^7\\ &= 4(17n-5)x^4+192nx^5+252(3n-1)x^6+192nx^7\\ S_xJD_xD_y(f(x,y)) &= \frac{1}{4}\times 4(17n-5)x^4+\frac{1}{5}(192n)x^5+\frac{1}{6}\times 252(3n-1)x^6+\frac{1}{7}(192n)x^7\\ &= (17n-5)x^4+\frac{192n}{5}x^5+42(3n-1)x^6+\frac{192n}{7}x^7 \end{aligned}$$

$$D_y^2(f(x,y)) = 36(3n-1)xy^3+32(n+1)x^2y^2+288nx^2y^3+252(3n-1)x^3y^3+256nx^3y^4$$

$$D_y^3(f(x,y)) = 108(3n-1)xy^3+64(n+1)x^2y^2+864nx^2y^3+756(3n-1)x^3y^3+1024nx^3y^4$$

$$D_xD_y^3(f(x,y)) = 108(3n-1)xy^3+128(n+1)x^2y^2+1728nx^2y^3+2268(3n-1)x^3y^3+3072nx^3y^4$$

$$D_x^2D_y^3(f(x,y)) = 108(3n-1)xy^3+256(n+1)x^2y^2+3456nx^2y^3+6804(3n-1)x^3y^3+9216nx^3y^4$$

$$D_x^3D_y^3(f(x,y)) = 108(3n-1)xy^3+512(n+1)x^2y^2+6912nx^2y^3+20412(3n-1)x^3y^3+27648nx^3y^4$$

$$\begin{aligned} JD_x^3D_y^3(f(x,y)) &= 108(3n-1)x^4+512(n+1)x^4+6912nx^5+20412(3n-1)x^6+27648nx^7\\ &= 4(209n+101)x^4+6912nx^5+20412(3n-1)x^6+27648nx^7\\ Q_{-2}JD_x^3D_y^3(f(x,y)) &= 4(209n+101)x^2+6912nx^3+20412(3n-1)x^4+27648nx^5\\ S_xQ_{-2}JD_x^3D_y^3(f(x,y)) &= 2(209n+101)x^2+2304nx^3+5103(3n-1)x^4+\frac{27648n}{5}x^5\\ S_x^2Q_{-2}JD_x^3D_y^3(f(x,y)) &= (209n-101)x^2+768nx^3+\frac{5103}{4}(3n-1)x^4+\frac{27648n}{25}x^5\\ S_x^3Q_{-2}JD_x^3D_y^3(f(x,y)) &= \frac{1}{2}(209n-101)x^2+256nx^3+\frac{5103}{16}(3n-1)x^4+\frac{27648n}{125}x^5 \end{aligned}$$

Now, the second condition, i.e., $x=y=1$ on above-computed expressions is applied to get the exact formulae of topological indices.

$$\begin{aligned} M_1(\text{TM-TCNB}) &= (D_x+D_y)(\text{TM-TCNB};x,y)|_{x=y=1}\\ &= (16(3n-1)xy^3+32(n+1)x^2y^2+160nx^2y^3+168(3n-1)x^3y^3+112nx^3y^4)|_{x=y=1}\\ &= 16(3n-1)+32(n+1)+160n+168(3n-1)+112n) = 856n-152 \end{aligned}$$

$$\begin{aligned} M_2(\text{TM-TCNB}) &= (D_xD_y)(\text{TM-TCNB};x,y)|_{x=y=1}\\ &= (12(3n-1)xy^3+32(n+1)x^2y^2+192nx^2y^3+252(3n-1)x^3y^3+192nx^3y^4)|_{x=y=1}\\ &= 12(3n-1)+32(n+1)+192n+252(3n-1)+192n = 1208n-232 \end{aligned}$$

$$\begin{aligned} M_1^m(\text{TM-TCNB}) &= (S_xS_y)(\text{TM-TCNB});x,y)|_{x=y=1}\\ &= \left(\frac{4}{3}(3n-1)x^1y^3+2(n+1)x^2y^2+\frac{16n}{3}x^2y^3+\frac{28}{9}(3n-1)x^3y^3+\frac{4n}{3}x^3y^4\right)|_{x=y=1}\\ &= \frac{4}{3}(3n-1)+2(n+1)+\frac{16n}{3}+\frac{28}{9}(3n-1)+\frac{4n}{3} = 22n-\frac{22}{9} \end{aligned}$$

$$\begin{aligned} RR_\rho(\text{TM-TCNB})) &= (S_x^\rho S_y^\rho)(\text{TM-TCNB};x,y)|_{x=y=1}\\ &= \left(\frac{4}{3^{\rho+1}}(3n-1)xy^3+2^{1-2\rho}(n+1)x^2y^2+\frac{2^{4-\rho}}{3^{\rho+1}}nx^2y^3+\frac{28}{9^{\rho+1}}(3n-1)x^3y^3+\frac{4^{1-\rho}}{3^{\rho+1}}nx^3y^4\right)\Big|_{x=y=1}\\ &= \frac{4}{3^{\rho+1}}(3n-1)+2^{1-2\rho}(n+1)+\frac{2^{4-\rho}}{3^{\rho+1}}n+\frac{28}{9^{\rho+1}}(3n-1)+\frac{4^{1-\rho}}{3^{\rho+1}}n \end{aligned}$$

$$\begin{aligned}
\mathrm{SSD(TM\text{-}TCNB)} &= (D_xS_y + D_yS_x)(\mathrm{TM\text{-}TCNB};x,y)|_{x=y=1}\\
&= \left(\frac{4}{3}(3n-1)xy^3 + 8(n+1)x^2y^2 + \frac{64n}{3}x^2y^3 + 28(3n-1)x^3y^3 + (12n)x^3y^4\right.\\
&\quad \left. + 12(3n-1)xy^3 + 8(n+1)x^2y^2 + 64nx^2y^3 + 28(3n-1)x^3y^3 + \frac{64n}{3}x^3y^4\right)\Big|_{x=y=1}\\
&= \frac{40}{3}(3n-1) + 16(n+1) + \frac{208n}{3} + 56(3n-1) + \frac{100n}{3}\\
&= \frac{980}{3}n - \frac{160}{3}
\end{aligned}$$

$$\begin{aligned}
I(\mathrm{TM\text{-}TCNB}) &= (S_xJD_xD_y)(\mathrm{TM\text{-}TCNB};x,y)|_{x=1}\\
&= \left((17n-5)x^4 + \frac{192n}{5}x^5 + 42(3n-1)x^6 + \frac{192n}{7}x^7\right)|_{x=1}\\
&= (17n-5) + \frac{192n}{5} + 42(3n-1) + \frac{192n}{7}\\
&= \frac{7309}{35}n - 47
\end{aligned}$$

$$\begin{aligned}
H(\mathrm{TM\text{-}TCNB}) &= (2S_xJ)(\mathrm{TM\text{-}TCNB};x,y)|_{x=1}\\
&= \left(2(5n+1)x^4 + \frac{64n}{5}x^5 + \frac{28}{3}(3n-1)x^6 + \frac{32n}{7}x^7\right)|_{x=1}\\
&= 2(5n+1) + \frac{64n}{5} + \frac{28}{3}(3n-1) + \frac{32n}{7}\\
&= \frac{1938}{35}n - \frac{22}{3}
\end{aligned}$$

$$\begin{aligned}
A(\mathrm{TM\text{-}TCNB}) &= (S_x^3Q_{-2}JD_x^3D_y^3)(\mathrm{TM\text{-}TCNB};x,y)|_{x=1}\\
&= \left(2(209n+101)x^2 + 2304nx^3 + 5103(3n-1)x^4 + \frac{27648n}{5}x^5\right)|_{x=1}\\
&= 2(209n+101) + 2304n + 5103(3n-1) + \frac{27648n}{5}\\
&= \frac{117803}{5}n - 4901.
\end{aligned}$$

$$\begin{aligned}
\mathrm{FI(TM\text{-}TCNB)} &= D_x(\mathrm{TM\text{-}TCNB};x)|_{x=1}\\
&= (40(3n-1)x^{10} + 64(n+1)x^8 + 416nx^{13} + 504(3n-1)x^{18} + 400nx^{25})|_{x=1}\\
&= 40(3n-1) + 64(n+1) + 416nx + 504(3n-1) + 400n\\
&= 2512n - 24
\end{aligned}$$

$$\begin{aligned}
S(\mathrm{TM\text{-}TCNB}) &= D_x(\mathrm{TM\text{-}TCNB};x)|_{x=1} = (16(3n-1)x^4 + 48nx)|_{x=1}\\
&= 16(3n-1) + 48n + = 96n - 16\\
\mathrm{SO(TM\text{-}TCNB)} &= D_x(\mathrm{TM\text{-}TCNB};x)|_{x=1}\\
&= (4\sqrt{10}(3n-1)x^{\sqrt{10}} + 16\sqrt{2}(n+1)x^{2\sqrt{2}} + 32\sqrt{13}nx^{\sqrt{13}}\\
&\quad + 84\sqrt{2}(3n-1)x^{3\sqrt{2}} + 80nx^5)|_{x=1}\\
&= 4\sqrt{10}(3n-1) + 16\sqrt{2}(n+1) + 32\sqrt{13}n + 84\sqrt{2}(3n-1) + 80n
\end{aligned}$$

Table 3: Computation of topological invariants by the help of *M*-polynomial of TM-TCNB

[*n*]	M_1	M_2	M_1^m	RR_p	SSD	*A*	*I*	*H*
[1]	704	976	19.556	0.0000	273.333	1270.059	208.828	48.038
[2]	1,560	2,814	41.556	0.0001	600	2808.555	417.657	103.409
[3]	2,416	3,392	64	0.0002	926.667	4347.052	626.485	158.780
[4]	3,272	4,600	85.556	0.0003	1253.333	5885.548	835.314	214.152
[5]	4,128	5,808	107.556	0.0003	1580	7424.045	1044.142	269.5238
[6]	4,984	7,016	129.556	0.0004	1906.667	8962.541	1252.971	324.895
[7]	5,840	8,224	151.556	0.0005	2233.333	10501.038	1461.800	380.266
[8]	6,696	9,432	173.556	0.0005	2560	12039.534	1670.628	435.638
[9]	7,552	10,640	195.556	0.0006	2886.667	13578.031	1879.457	491.009
[10]	8,408	11,848	217.556	0.0007	3213.333	15116.527	2088.285	546.380

3.3 Comparison

In this section, we present a numerical (Tables 3 and 4) and graphical (Figure 3) comparison of topological indices of *M*-polynomials, *F*-polynomial, sigma polynomial, and Sombor polynomial for $n = 1, 2, 3, 4, \ldots, 10$ for TM-TCNB.

3.4 Cuboctahedral bimetallic structure (MOPs)

The number of vertices and edges of cuboctahedral bimetallic networks (MOPs) (Figure 4) are $196n$ and $240n$, respectively. In cuboctahedral bimetallic networks (MOPs), there are four types of vertices: degrees 1, 2, 3, and 4, respectively. Table 5 shows the edge partition of cuboctahedral bimetallic networks (MOPs) depending on the degrees of end vertices of each edge.

Table 4: Computation of topological invariants by the help of *F*-polynomial, *S*-polynomial, and SO-polynomial of TM-TCNB

[*n*]	*F*1	*S*	SO
[1]	2,488	80	1299.326
[2]	5,000	176	2922.429
[3]	7,512	272	4545.532
[4]	10,024	368	6168.635
[5]	12,536	464	7791.738
[6]	15,048	560	9414.841
[7]	17,560	656	11037.944
[8]	20,072	752	12661.047
[9]	22,584	848	14284.1500
[10]	25,096	944	15907.252

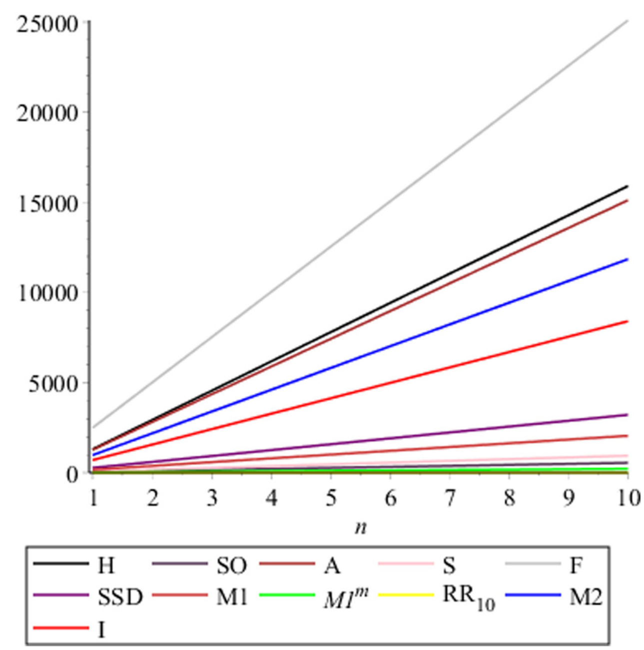

Figure 3: Comparison of topological invariants by applying polynomials for TM-TCNB at $x = 1$ and $y = 1$.

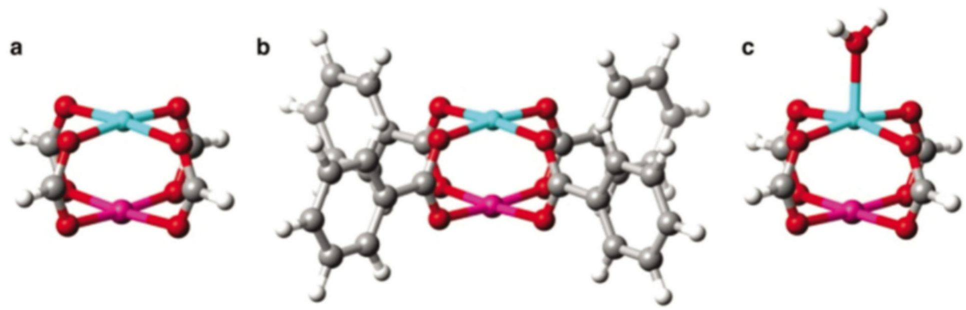

Figure 4: Clusters investigated a unit cell of cuboctahedral bimetallic networks using density functional theory methods: (a) formate, (b) benzoate, and (c) water solvated.

Table 5: Edge partition of MOPs based on degrees of end vertices of each edge

(ζ(a), ζ(b))	**(1,4)**	**(2,2)**	**(2,3)**	**(2,4)**	**(3,3)**	**(3,4)**
Frequency	36*n*	16*n*	120*n*	42*n*	24*n*	16*n*
Set of edges	E_1	E_2	E_3	E_4	E_5	E_6

3.5 Polynomials of cuboctahedral bimetallic networks (MOPs)

Let G be a molecular graph of MOPs. Then, using Table 5 in Eqs. 1–4, respectively, the M-, F-, S-, and SO-polynomials for MOPs are computed as follows:

$$\begin{aligned}
S((\mathrm{MOPs});x) &= \sum_{ab\in E(X)} x^{(\zeta^a-\zeta^b)^2}\\
&= \sum_{ab\in E_1} m_{14}((\mathrm{MOPs}))x^9 + \sum_{ab\in E_2} m_{22}((\mathrm{MOPs}))\\
&\quad + \sum_{ab\in E_3} m_{23}((\mathrm{MOPs}))x + \sum_{ab\in E_4} m_{24}((\mathrm{MOPs}))x^4\\
&\quad + \sum_{ab\in E_5} m_{33}((\mathrm{MOPs})) + \sum_{ab\in E_6} m_{34}((\mathrm{MOPs}))x\\
&= |E_1|x^9 + |E_2| + |E_3|x + |E_4|x^4 + |E_5| + |E_6|x\\
&= 36nx^9 + 16n + 120nx + 42nx^4 + 24n + 16nx\\
&= 36nx^9 + 42nx^4 + 136nx + 40n
\end{aligned}$$

$$\begin{aligned}
M((\mathrm{MOPs});x,y) &= \sum_{\delta\le p\le q\le\triangle} m_{pq}((\mathrm{MOPs}))x^p y^q\\
&= \sum_{ab\in E_1} m_{14}((\mathrm{MOPs}))x^1y^4 + \sum_{ab\in E_2} m_{22}((\mathrm{MOPs}))x^2y^2 + \sum_{ab\in E_3} m_{23}((\mathrm{MOPs}))x^2y^3 + \sum_{ab\in E_4} m_{24}((\mathrm{MOPs}))x^2y^4\\
&\quad + \sum_{ab\in E_5} m_{33}((\mathrm{MOPs}))x^3y^3 + \sum_{ab\in E_6} m_{34}((\mathrm{MOPs}))x^3y^4\\
&= |E_1|xy^4 + |E_2|x^2y^2 + |E_3|x^2y^3 + |E_4|x^2y^4 + |E_5|x^3y^3 + |E_6|x^3y^4\\
&= 36nxy^4 + 16nx^2y^2 + 120nx^2y^3 + 42nx^2y^4 + 24nx^3y^3 + 16nx^3y^4
\end{aligned}$$

$$\begin{aligned}
\mathrm{FI}((\mathrm{MOPs});x) &= \sum_{ab\in E(X)} x^{((\zeta^a)^2+(\zeta^b)^2)}\\
&= \sum_{ab\in E_1} m_{14}((\mathrm{MOPs}))x^{17} + \sum_{ab\in E_2} m_{22}((\mathrm{MOPs}))x^8\,\mathrm{x}+ \sum_{ab\in E_3} m_{23}((\mathrm{MOPs}))x^{13} + \sum_{ab\in E_4} m_{24}((\mathrm{MOPs}))x^{20}\\
&\quad + \sum_{ab\in E_5} m_{33}((\mathrm{MOPs}))x^{18} + \sum_{ab\in E_6} m_{34}((\mathrm{MOPs}))x^{25}\\
&= |E_1|x^{17} + |E_2|x^8 + |E_3|x^{13} + |E_4|x^{20} + |E_5|x^{18} + |E_6|x^{25}\\
&= 36nx^{17} + 16nx^8 + 120nx^{13} + 42nx^{20} + 24nx^{18} + 16nx^{25}
\end{aligned}$$

$$
\begin{aligned}
\mathrm{SO}((\mathrm{MOPs});x) &= \sum_{ab\in E(X)} x^{\sqrt{(\zeta^{a})^{2}+(\zeta^{b})^{2}}} \\
&= \sum_{ab\in E_1} m_{14}((\mathrm{MOPs}))x^{\sqrt{17}} + \sum_{ab\in E_2} m_{22}((\mathrm{MOPs}))x^{\sqrt{8}} \\
&\quad + \sum_{ab\in E_3} m_{23}((\mathrm{MOPs}))x^{\sqrt{13}} + \sum_{ab\in E_4} m_{24}((\mathrm{MOPs}))x^{\sqrt{20}} \\
&\quad + \sum_{ab\in E_5} m_{33}((\mathrm{MOPs}))x^{\sqrt{18}} + \sum_{ab\in E_6} m_{34}((\mathrm{MOPs}))x^{\sqrt{25}}
\end{aligned}
$$

$$
\begin{aligned}
\mathrm{SO}((\mathrm{MOPs});x) &= |E_1|x^{\sqrt{17}} + |E_2|x^{2\sqrt{2}} + |E_3|x^{\sqrt{13}} + |E_4|x^{2\sqrt{5}} \\
&\quad + |E_5|x^{3\sqrt{2}} + |E_6|x^{5} \\
&= 36nx^{\sqrt{17}} + 16nx^{2\sqrt{2}} + 120nx^{\sqrt{13}} + 42nx^{2\sqrt{5}} \\
&\quad + 24nx^{3\sqrt{2}} + 16nx^{5}
\end{aligned}
$$

Figure 5 shows the graphical presentation of M-polynomial, F-polynomial, S-polynomial, and SO-polynomial of transition cuboctahedral bimetallic systems (MOPs).

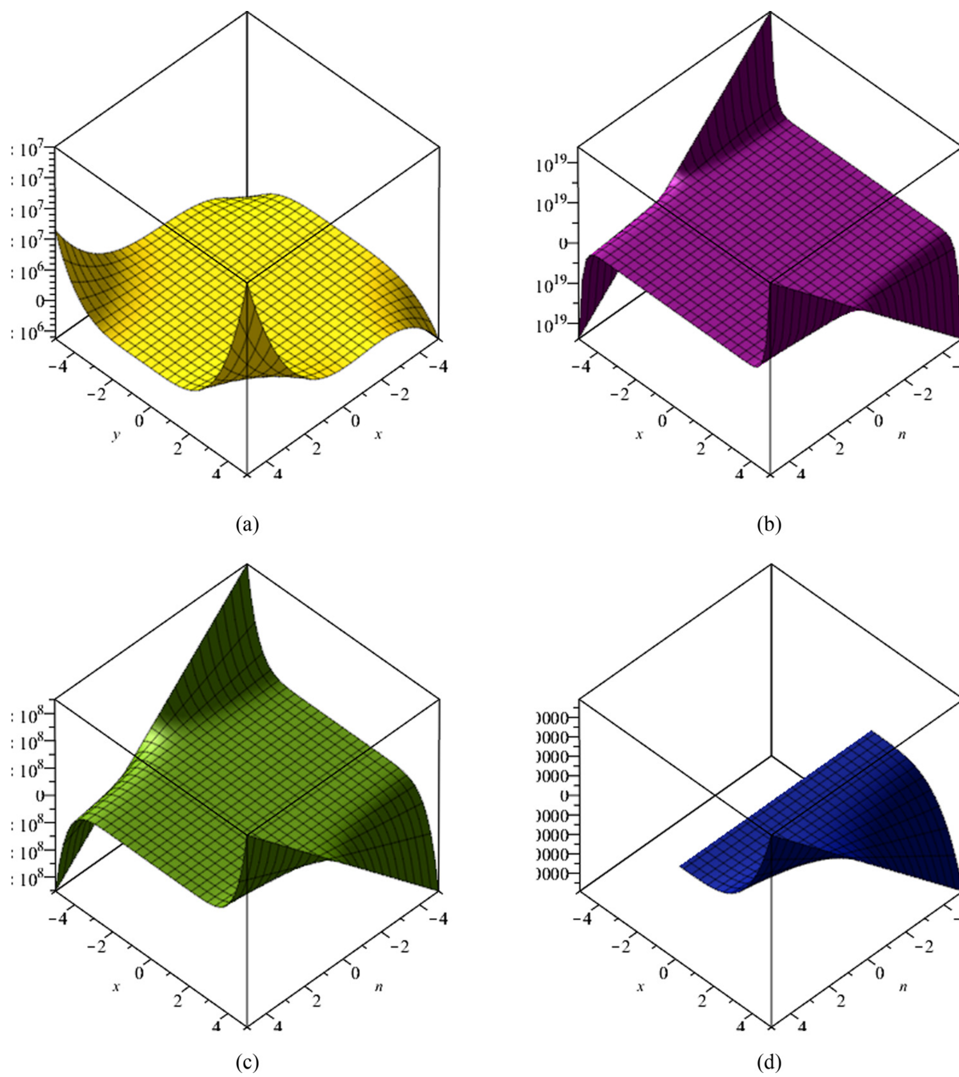

Figure 5: (a) M-polynomial, (b) F-polynomial, (c) S-polynomial, and (d) SO-polynomial of transition cuboctahedral bimetallic networks (MOPs).

3.6 Computation of topological invariants by applying polynomials for cuboctahedral bimetallic networks (MOPs)

Now, we calculate the topological invariants for cuboctahedral bimetallic networks (MOPs), known first, second, modified, and augmented Zagreb invariants, Randić invariants, SSD invariant, harmonic invariant, ISI invariant, F invariant, S invariant, and SO invariant. From Table 1, we acquire the results of M-polynomial as follows:

$$\begin{aligned}D_x(f(x,y)) &= x\frac{\partial f(x,y)}{\partial x}\\ &= x((36n)y^4 + 2(16n)x^1y^2 + 2(120n)x^1y^3 + 2(42n)x^1y^4 + 3(24n)x^2y^3 + 3(16n)x^2y^4)\\ &= 36nxy^4 + 32nx^2y^2 + 240nx^2y^3 + 84nx^2y^4 + 72nx^3y^3 + 48nx^3y^4\end{aligned}$$

$$\begin{aligned}D_y(f(x,y)) &= y\frac{\partial f(x,y)}{\partial y}\\ &= y(4(36n)xy^3 + 2(16n)x^1y^2 + 3(120n)x^2y^2 + 4(42n)x^2y^3 + 3(24n)x^3y^2 + 4(16n)x^3y^3)\\ &= 144nxy^4 + 32nx^2y^2 + 360nx^2y^3 + 168nx^2y^4 + 72nx^3y^3 + 64nx^3y^4\end{aligned}$$

$$\begin{aligned}D_xD_y(f(x,y)) &= x\frac{\partial}{\partial x}D_y(f(x,y))\\ &= x((144n)xy^4 + 2(32n)x^1y^2 + 2(360n)x^1y^3 + 2(168n)x^1y^4 + 3(72)x^2y^3 + 3(64n)x^2y^4)\\ &= 144nxy^4 + 64nx^2y^2 + 720nx^2y^3 + 336nx^2y^4 + 216nx^3y^3 + 192nx^3y^4\end{aligned}$$

$$\begin{aligned}S_x(f(x,y)) &= \int_0^x \frac{f(t,y)}{t}\mathrm{d}t\\ &= (36n)xy^4 + \frac{1}{2}(32n)x^2y^2 + \frac{1}{2}(240n)x^2y^3 + \frac{1}{2}(84n)x^2y^4 + \frac{1}{3}(72)x^3y^3 + \frac{1}{3}(48n)x^3y^4\\ &= 36nxy^4 + 16nx^2y^2 + 120nx^2y^3 + 42nx^2y^4 + 24nx^3y^3 + 16nx^3y^4\end{aligned}$$

$$\begin{aligned}S_y(f(x,y)) &= \int_0^y \frac{f(x,t)}{t}\mathrm{d}t\\ &= \frac{1}{4}(144n)xy^4 + \frac{1}{2}(32n)x^2y^2 + \frac{1}{3}(360n)x^2y^3 + \frac{1}{4}(168n)x^2y^4 + \frac{1}{3}(72n)x^3y^3 + \frac{1}{4}(64n)x^3y^4\\ &= 36nxy^4 + 16nx^2y^2 + 120nx^2y^3 + 42nx^2y^4 + 24nx^3y^3 + 16nx^3y^4\end{aligned}$$

$$\begin{aligned}S_xS_y(f(x,y)) &= (36n)xy^4 + \frac{1}{2}(16n)x^2y^2 + \frac{1}{2}(120n)x^2y^3 + \frac{1}{2}(42n)x^2y^4 + \frac{1}{3}(24n)x^3y^3 + \frac{1}{3}(16n)x^3y^4\\ &= 36nxy^4 + 8nx^2y^2 + 60nx^2y^3 + 21nx^2y^4 + 8nx^3y^3 + \frac{16n}{3}x^3y^4\end{aligned}$$

$$\begin{aligned}D_x^{\rho}D_y^{\rho}(f(x,y)) &= 144(4)^{\rho}nxy^4 + 64(4)^{\rho}nx^2y^2 + 720(6)^{\rho}nx^2y^3 + 336(8)^{\rho}nx^2y^4 + 216(9)^{\rho}nx^3y^3 + 192(12)^{\rho}nx^3y^4\end{aligned}$$

$$\begin{aligned}S_x^{\rho}S_y^{\rho}(f(x,y) &= 9(4)^{1-\rho}nxy^4 + (4)^{2-\rho}nx^2y^2 + 20(6)^{1-\rho}nx^2y^3 + 42(8)^{-\rho}nx^2y^4 + 8(3)^{1-2\rho}nx^3y^3 + 16(12)^{-\rho}nx^3y^4\end{aligned}$$

$$\begin{aligned}S_yD_x(f(x,y)) &= \frac{1}{4}(36n)xy^4 + \frac{1}{2}(32n)x^2y^2 + \frac{1}{3}(240n)x^2y^3 + \frac{1}{4}(84n)x^2y^4 + \frac{1}{3}(72n)x^3y^3 + \frac{1}{4}(48n)x^3y^4\\ &= 9nxy^4 + 16nx^2y^2 + 80nx^2y^3 + 21nx^2y^4 + 24nx^3y^3 + 12nx^3y^4,\end{aligned}$$

$$\begin{aligned}S_xD_y(f(x,y)) &= (144n)xy^4 + \frac{1}{2}(32n)x^2y^2 + \frac{1}{2}(360n)x^2y^3 + \frac{1}{2}(168n)x^2y^4 + \frac{1}{3}(72n)x^3y^3 + \frac{1}{3}(64n)x^3y^4\\ &= 144nxy^4 + 16nx^2y^2 + 180nx^2y^3 + 84nx^2y^4 + 24nx^3y^3 + \frac{64n}{3}x^3y^4\end{aligned}$$

$$J(f(x,y)) = f(x,x) = 16nx^4 + 156nx^5 + 66nx^6 + 16nx^7$$

$$S_xJ(f(x,y)) = \frac{1}{4}(16n)x^4 + \frac{1}{5}(156n)x^5 + \frac{1}{6}(66n)x^6 + \frac{1}{7}(16n)x^7$$
$$= 4nx^4 + \frac{156n}{5}x^5 + 11nx^6 + \frac{16}{7}nx^7$$

$$2S_xJ(f(x,y)) = 8nx^4 + \frac{312n}{5}x^5 + 22nx^6 + \frac{32}{7}nx^7$$
$$JD_xD_y(f(x,y)) = 64nx^4 + 864nx^5 + 552nx^6 + 192nx^7$$

$$S_xJD_xD_y(f(x,y)) = \frac{1}{4}(64n)x^4 + \frac{1}{5}(864n)x^5 + \frac{1}{6}(552n)x^6 + \frac{1}{7}(192n)x^7$$
$$= 16nx^4 + \frac{864}{5}nx^5 + 92nx^6 + \frac{192}{7}nx^7,$$

$$D_y^3f(x,y) = 4^2(144n)x^1y^4 + 2^2(32n)x^2y^2 + 3^2(360n)x^2y^3 + 4^2(168n)x^2y^4 + 3^2(72n)x^3y^3 + 4^2(64n)x^3y^4$$
$$= 2304nx^1y^4 + 128nx^2y^2 + 3240nx^2y^3 + 2688nx^2y^4 + 648nx^3y^3 + 1024nx^3y^4$$

$$D_x^3D_y^3(f(x,y)) = 2304nxy^4 + 2^3(128n)x^2y^2 + 2^3(3240n)x^2y^3 + 2^3(2688n)x^2y^4 + 3^3(648n)x^3y^3 + 3^3(1024n)x^3y^4$$
$$= 2304nxy^4 + 1024nx^2y^2 + 25920nx^2y^3 + 21504nx^2y^4 + 17496nx^3y^3 + 27648nx^3y^4$$

$$JD_x^3D_y^3(f(x,y)) = 1024nx^4 + 28224nx^5 + 39000nx^6 + 27648nx^7$$
$$Q_{-2}JD_x^3D_y^3(f(x,y)) = 1024nx^2 + 28224nx^3 + 39000nx^4 + 27648nx^5$$
$$S_x^3Q_{-2}JD_x^3D_y^3(f(x,y)) = \left(\frac{1}{2}\right)^3(1024n)x^2 + \left(\frac{1}{3}\right)^3(28224n)x^3 + \left(\frac{1}{4}\right)^3(39000n)x^4 + \left(\frac{1}{5}\right)^3(27648n)x^5$$
$$= 128nx^2 + \frac{3136}{3}nx^3 + \frac{4875}{8}nx^4 + \frac{27648}{125}nx^5$$

Now, the second condition, i.e., $x = y = 1$ on above-calculated expressions is applied to get the exact formulas of all topological indices.

$$M_1(\text{MOPs}) = (D_x + D_y)(\text{MOPs};x,y)|_{x=y=1}$$
$$= (180nxy^4 + 64nx^2y^2 + 600nx^2y^3 + 252nx^2y^4 + 144nx^3y^3 + 112nx^3y^4)|_{x=y=1}$$
$$= 1352n$$

$$M_2(\text{MOPs}) = (D_xD_y)(\text{MOPs};x,y)|_{x=y=1}$$
$$= (144nxy^4 + 64nx^2y^2 + 720nx^2y^3 + 336nx^2y^4 + 216nx^3y^3 + 192nx^3y^4)|_{x=y=1}$$
$$= 1672n$$

$$M_1^m(\text{MOPs}) = (S_xS_y)(\text{MOPs};x,y)|_{x=y=1}$$
$$= \left(36nxy^4 + 8nx^2y^2 + 60nx^2y^3 + 21nx^2y^4 + 8nx^3y^3 + \frac{16}{3}nx^3y^4\right)|_{x=y=1}$$
$$= \frac{415n}{3}$$

$$RR_\rho(\text{MOPs}) = (S_x^\rho S_y^\rho)(\text{MOPs};x,y)|_{x=y=1}$$
$$= (9(4)^{1-\rho}nxy^4 + (4)^{2-\rho}nx^2y^2 + 20(6)^{1-\rho}nx^2y^3 + 42(8)^{-\rho}nx^2y^4 + 8(3)^{1-2\rho}nx^3y^3 + 16(12)^{-\rho}nx^3y^4)|_{x=y=1}$$
$$= 9(4)^{1-\rho}n + (4)^{2-\rho}n + 20(6)^{1-\rho}n + 42(8)^{-\rho}n + 8(3)^{1-2\rho}n + 16(12)^{-\rho}n$$

$$\text{SSD}(\text{MOPs}) = (S_xD_y + S_yD_x)(\text{MOPs};x,y)|_{x=y=1}$$
$$= \left(153nxy^4 + 32nx^2y^2 + 260nx^2y^3 + 105nx^2y^4 + 48nx^3y^3 + \frac{100}{3}nx^3y^4\right)|_{x=y=1}$$
$$= \frac{1894n}{3}$$

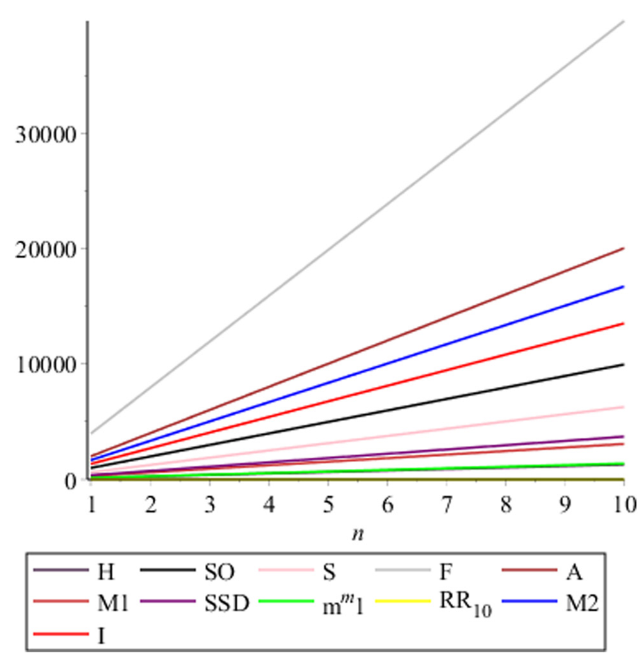

Figure 6: Comparision of topological invariants by applying polynomials for cuboctahedral bimetallic networks (MOPs) at $x = 1$ and $y = 1$.

Table 6: Comparison of topological invariants by applying M-polynomial for cuboctahedral bimetallic networks (MOPs) at $x = 1$ and $y = 1$

[*n*]	M_1	M_2	M_1^m	RR_p	SSD	*A*	*I*	*H*
[1]	1,352	1,672	138.333	0.0000	371.333	2003.892	308.228	128.971
[2]	2,704	3,344	276.667	0.0001	742.666	4007.784	616.4571	257.942
[3]	4,056	5,016	415	0.0002	1114	6011.677	924.685	386.914
[4]	5,408	6,688	553.333	0.0002	1485.333	8015.569	1232.914	515.885
[5]	6,760	8,360	691.666	0.0003	1856.666	10019.461	1541.142	644.8571
[6]	8,112	10,032	830	0.0003	2228	12023.354	1849.371	773.828
[7]	9,464	11,704	968.333	0.0004	2599.333	14027.246	2157.60	902.8
[8]	10,816	13,376	1106.667	0.0004	2970.666	16031.138	2465.828	1031.771
[9]	12,168	15,048	1245	0.0005	3342	18035.031	2774.0571	1160.742
[10]	13,520	16,720	1383.333	0.0005	3713.333	20038.923	3082.285	1289.714

Table 7: Comparison of topological invariants by applying *F*-, *S*-, and SO-polynomials for cuboctahedral bimetallic networks (MOPs) at $x = 1$

[*n*]	FI	*S*	SO
[1]	3,972	628	996.005
[2]	7,944	1256	1992.011
[3]	11,916	1884	2988.017
[4]	15,888	2512	3984.023
[5]	19,860	3140	4980.029
[6]	23,832	3768	5976.035
[7]	27,804	4396	6972.041
[8]	31,776	5024	7968.047
[9]	35,748	5652	8964.052
[10]	39,720	6280	9960.058

$$\begin{aligned} I(\text{MOPs}) &= (S_xJD_xD_y)(\text{MOPs};x,y)|_{x=1} \\ &= \left(16nx^4 + \frac{864}{5}nx^5 + 92nx^6 + \frac{192}{7}nx^7\right)\Big|_{x=y=1} \\ &= \frac{10788}{35}n \end{aligned}$$

$$\begin{aligned} H(\text{MOPs}) &= (2S_xJ)(\text{MOPs};x,y)|_{x=1} \\ &= \left(8nx^4 + \frac{312n}{5}x^5 + 22nx^6 + \frac{32}{7}nx^7\right)\Big|_{x=1} \\ &= \frac{3394}{35}n \end{aligned}$$

$$\begin{aligned} A(\text{MOPs}) &= (S_x^3Q_{-2}JD_x^3D_y^3)(\text{MOPs};x,y)|_{x=1} \\ &= \left(128nx^2 + \frac{3136}{3}nx^3 + \frac{4875}{8}nx^4 \right. \\ &\quad \left. + \frac{27648}{125}nx^5\right)\Big|_{x=1} \\ &= \frac{6011677}{3000}n \end{aligned}$$

$$\begin{aligned} FI(\text{MOPs}) &= (D_x)(\text{MOPs};x,y)|_{x=1} \\ &= (612nx^{17} + 128nx^8 + 1560nx^{13} + 840nx^{20} + 432nx^{18} \\ &\quad + 400nx^{25})|_{x=1} \\ &= 3972n \end{aligned}$$

$$\begin{aligned} S(\text{MOPs}) &= (D_x)(\text{MOPs};x,y)|_{x=1} = (D_x)(\text{MOPs};x,y)|_{x=1} \\ &= (324nx^9 + 120nx + 168nx^4 + 16nx)|_{x=1} \\ &= 628n \end{aligned}$$

$$\begin{aligned} SO(\text{MOPs}) &= (D_x)(\text{MOPs};x,y)|_{x=1} \\ &= (36\sqrt{17}nx^{\sqrt{17}} + 32\sqrt{2}nx^{2\sqrt{2}} + 120\sqrt{13}nx^{\sqrt{13}} \\ &\quad + 84\sqrt{5}nx^{2\sqrt{5}} + 72\sqrt{2}nx^{3\sqrt{2}} + 80nx^5)|_{x=1} \\ &= 36\sqrt{17}n + 32\sqrt{2}n + 120\sqrt{13}n + 84\sqrt{5}n + 72\sqrt{2}n \\ &\quad + 80n \end{aligned}$$

In Figure 6 and Tables 6 and 7, a comparison of topological invariants by applying polynomials for cuboctahedral bimetallic networks (MOPs) at $x = 1$ and $y = 1$ is presented. We can analyze that all topological invariants are increasing as the values of n increases.

4 Conclusion

In this article, we give *M*-, *F*-, *S*-, and SO-polynomials of the two most appealing networks metal-organic networks (TM-TCNB) and cuboctahedral bimetallic networks (MOPs). We also calculated the formulae for various degree-dependent topological invariants of critical importance, such as the first, second, modified, and augmented Zagreb invariants, general and inverse Randić invariants, SSD, harmonic invariants, ISI, F invariant, sigma invariant, and Sombor invariant of metal-organic networks (TM-TCNB) and cuboctahedral bimetallic (MOPs) by using topological polynomials derived in the previous topic. The Zagreb invariants of metal-organic networks (TM-TCNB) and cuboctahedral bimetallic networks (MOPs) furnish total π-electron energy in increasing form for higher quantities of n. One can analyze that the strain energy of metal-organic networks (TM-TCNB) and cuboctahedral bimetallic networks (MOPs) is high as the values of n increase. The physical properties, chemical reactivity, and biological activities of these structures can all be better understood using topological invariants.

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