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Topological Aspects of Certain Transition Metals via Neighbourhood $M-$Polynomial

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Abstract

Graph theory is extensively used in chemistry for modeling molecular structures, resulting in the formation of molecular graphs. These molecular graphs serve as a crucial link between mathematics and the natural sciences. By associating chemical networks with molecular characteristics, they facilitate the design of biologically active substances through quantitative structure-activity relationship studies. One of the fundamental tools for investigating such relationships is the use of topological indices. These indices can be derived through mathematical operations involving polynomials. Among the existing techniques for structural characterization of molecular graphs, the approach based on neighborhood $M-$polynomials proves to be particularly effective. The neighborhood $M-$polynomials offer significant advantages in identifying structural patterns, analyzing molecular configurations, encoding structural information, evaluating structural variance under graph isomorphisms and acting as mathematical descriptors in quantitative structure-activity relationship investigations. They are essential in predicting biological activities and, more importantly, in designing new molecules with specific desired properties. Transition metals such as zinc (II), manganese (II), cobalt (II) and copper (II) are well-known for their extraordinary properties, which have attracted significant attention in medicine, food industries and production industries. This article aims to mathematically depict the above-mentioned transition metals through the use of neighborhood $M-$polynomials.

Keywords: zinc (II); Mn(II); neighborhood $M-$polynomials; cobalt (II) and copper (II).

1 Introduction

Chemical compounds are characterized by a wide range of physical, chemical and biological properties. Many of these compounds exhibit significant biological activities, making them candidates for therapeutic applications. The ongoing quest to discover novel antibacterial agents and other medically relevant substances drives pharmaceutical companies to synthesize and evaluate thousands of new compounds annually. However, despite their potential, the extensive cost and time associated with experimental biological testing pose substantial challenges. In response, numerous theoretical frameworks have been established to predict biological activity or physicochemical properties based on molecular structure [4, 12].

Among these frameworks, a widely adopted approach is the use of topological indices numerical parameters derived from the graph-theoretical representation of molecules. These indices provide a bridge between discrete molecular structures and continuous biological data, facilitating quantitative studies of structure activity and structure-property relationships. The concept of topological indices dates back to Wieners pioneering work in 1947 [14] and was further formalized by Hosoya through the introduction of the Z-index in 1949 [15, 9].

One of the most universal mathematical tools for generating numerous degree-based topological indices is the $M-$polynomial. This polynomial encapsulates degree-based information about molecular graphs and enables systematic computation of a wide variety of descriptors [5]. A notable extension of this approach is the neighborhood $M-$polynomial, which offers enhanced capabilities for characterizing structural patterns, encoding molecular information and assessing invariance under graph isomorphisms. These polynomials have proven effective as descriptors in both structure-activity and structure-property modeling.

Transition metal complexes represent an important class of compounds due to their diverse coordination chemistry and functional versatility. In particular, transition metals such as zinc in the $+2$ oxidation state, manganese in the $+2$ oxidation state, copper in the $+2$ oxidation state and cobalt in the $+2$ oxidation state are of growing interest for their roles in chemical, biological and industrial applications. This study focuses on the mathematical modeling of molecular structures involving these transition metals using the neighborhood $M-$polynomial framework. Below, we briefly introduce the significance of each metal.

1.1 Zinc (II)

Zinc has been known since ancient times, first identified in India in the 14th century and later recognized in Europe in the 16th century [10]. It is widely distributed in nature and plays a vital role in numerous biological functions. Zinc is the only metal found in all enzyme classes and is essential for immune function, enzymatic catalysis and structural biology [10]. Zinc compounds also find applications in antimicrobial treatments, nanotechnology and advanced materials for industrial use [6, 11].

1.2 Manganese (II)

Manganese was first isolated by Johan Gottlieb Gahn in 1774 [17]. Compounds of the Manganese (II) oxidation state exhibit diverse applications, ranging from magnetic resonance imaging

(MRI) contrast agents and antioxidants to components in sensors and water purification systems [2, 13]. They also play an essential role in steel manufacturing [3] and have emerging potential in energy storage and hydrogen production technologies [1].

1.3 Copper (II)

Copper has been used by civilizations for millennia and derives its name from the island of Cyprus [8]. Copper in the $+2$ oxidation state forms compounds that are widely used in industrial and environmental applications. These compounds serve as precursors to other copper salts and are employed in wood preservatives, ceramics, animal nutrition and electronics [5]. Environmentally, they are also used in water purification systems and in energy storage technologies such as supercapacitors and batteries [7, 10]. In addition, copper-based materials have attracted attention for their role in advanced electrochemical and catalytic processes [6, 13].

1.4 Cobalt (II)

Cobalt was discovered by Georg Brandt in 1735 and its compounds were historically used in pigments and enamels. Modern applications of cobalt include high-performance materials for aerospace and industrial processes, catalysis for petroleum refining and the synthesis of alternative fuels [11, 17]. Biologically, cobalt is an essential element in vitamin B_{12}, a cofactor necessary for DNA synthesis and red blood cell formation [2]. Cobalt-based enzymes are also involved in critical metabolic pathways [1, 13] and play important roles in several biochemical processes [8, 16].

This paper aims to mathematically characterize the molecular frameworks of these transition metal-based compounds through neighborhood $M-$polynomials, providing insights into their structural properties and potential applications in materials science and pharmacology.

2 Literature Review

Graph theory has been widely applied in chemistry to model molecular structures through molecular graphs. These graphs serve as a bridge between mathematical analysis and the natural sciences, enabling quantitative structure activity relationship (QSAR) studies that assist in the design of biologically active molecules [10]. Among various mathematical approaches, topological indices play a crucial role in (QSAR) analysis [14, 9]. One of the most effective techniques in this domain is the neighborhood M-polynomial approach. Neighborhood M-polynomials are valuable for identifying structural patterns, analyzing molecular configurations and encoding structural information for both (QSAR) and quantitative structure property relationship (QSPR) studies [15, 5]. They facilitate the prediction of biological activity and the design of molecules with desired properties, making them highly useful in pharmaceutical and materials sciences [7].

2.1 Role of transition metals in chemical and biological systems

Transition metals, including zinc (II), manganese (II), cobalt (II) and copper (II), exhibit unique electronic configurations in their d-orbitals, making them useful in diverse applications [7]. These metals are essential in various industrial, biological and chemical processes due to their versatile coordination chemistry and reactivity [10].

2.1.1 Zinc (II)

Zinc (II) plays a vital role in enzymatic reactions, catalysis and structural biology. It is widely used in medical research and nanotechnology applications [6, 11].

2.1.2 Manganese (II)

Manganese (II) is important for magnetic resonance imaging (MRI) contrast agents, sensors, water treatment technologies and steel production. It is also being explored for next-generation solar cells and hydrogen storage systems [2, 17].

2.1.3 Copper (II)

Copper (II) is utilized in environmental chemistry, remediation of contaminated water and energy storage technologies such as supercapacitors [3, 13].

2.1.4 Cobalt (II)

Cobalt (II) is crucial for the development of lithium-ion batteries, hydrogen production through water splitting and petroleum refining. Biologically, it plays an important role as a component of vitamin B_{12} [1, 8].

2.2 Preliminaries and methods

Let $\mathbb{W} = \mathbb{W}(P, L)$ be a graph, where $P(w)$ and $L(w)$ denote the set of points (vertices) and links (edges), respectively, of the graph $\mathbb{W}$, such that $|P(w)| = n$ and $|L(w)| = k$. The degree of a vertex is a fundamental parameter in graph analysis. The degree of a point (vertex) z in a graph W, denoted by $\deg(z)$, is defined as the total number of links connected to z.

The neighborhood of a vertex z in a graph $\mathbb{W}$ is denoted by $N_w(z)$ and refers to the set of all vertices adjacent to z. For more on basic graph theory definitions, see [14].

The $M-$polynomial of a graph W is defined as,

$$M(w; x, y) = \sum_{p \leq q} \Delta_{pq} x^p y^q,$$

where Δ_{pq} denotes the number of edges $uz \in L(w)$ such that $\{\deg(u), \deg(z)\} = \{p, q\}$.

The neighborhood $M-$polynomial associated with the graph W is given by,

$$M(w; x, y) = \sum_{p \leq q} \delta_{pq} x^p y^q,$$

where δ_{pq} denotes the number of edges $uz \in L(w)$ such that $\{N_w(u), N_w(z)\} = \{p, q\}$. Henceforth, we denote the neighborhood $M-$polynomial by $N_w(x, y)$ for simplicity.

This article explores the topological aspects of the aforementioned metal-based molecular graphs by computing their neighborhood $M-$polynomials as Table 1,

Table 1: Derivation of selected topological indices from the neighborhood $M-$polynomial.

No.	**Topological index**	**Symbol**	**Function** $f(x,y)$	**Derived from** $NM(G^{\cdot})$
1	First Zagreb index	M_1^*	$x+y$	$(d_x + d_y) \cdot NM(G^{\cdot})\big\|_{x=y=1}$
2	Second Zagreb index	M_2^*	xy	$(d_x d_y) \cdot NM(G^{\cdot})\big\|_{x=y=1}$
3	Forgotten index	M_T^*	x^2+y^2	$(d_x^2 + d_y^2) \cdot NM(G^{\cdot})\big\|_{x=y=1}$
4	Modified second Zagreb index	M_2^{**}	$\frac{1}{xy}$	$(S_x S_y) \cdot NM(G^{\cdot})\big\|_{x=y=1}$
5	Third Randić index	ND_3	$xy(x+y)$	$d_x d_y (d_x + d_y) \cdot NM(G^{\cdot})\big\|_{x=y=1}$
6	Fifth Randić index	ND_5	$\frac{x^2+y^2}{xy}$	$(d_x S_x + d_y S_y) \cdot NM(G)\big\|_{x=y=1}$
7	Harmonic index	NH	$\frac{2}{x+y}$	$2S_x J \cdot NM(G^{\cdot})\big\|_{x=y=1}$
8	Inverse sum index	NI	$\frac{xy}{x+y}$	$S_x J d_x d_y \cdot NM(G^{\cdot})\big\|_{x=y=1}$

where the operators are defined as follows;

$$d_x\left(f(x,y)\right) = x\frac{\partial f(x,y)}{\partial x}, \qquad d_y(f(x,y)) = y\frac{\partial f(x,y)}{\partial y},$$
$$S_x(f(x,y)) = \int_0^x \frac{f(t,y)}{t}dt, \qquad S_y(f(x,y)) = \int_0^y \frac{f(x,t)}{t}dt,$$
$$\int\left(f(x,y)\right) = f(x,y).$$

Theorem 2.1. *The neighborhood polynomial of the molecular structure of the metal complex of zinc (II) with chalcone of pyridine-2-carbaldehyde is given by (Figure 1),*

$$NM(Zn) = 2x^3y^6 + 5x^4y^4 + 7x^4y^5 + x^4y^6 + 2x^5y^5 + 7x^5y^6 + 4x^5y^7 + 2x^6y^9 + 4x^7y^7 + 4x^7y^8 + 4x^7y^9.$$

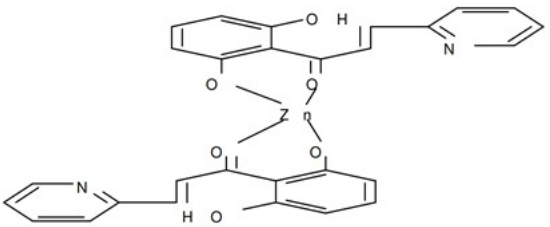

Figure 1: Topological analysis of Zinc(II) complex with chalcone of pyridine-2-carbaldehyde.

Proof. There are thirty seven vertices and forty two edges of this molecular structure. The neighbourhood edge partition of this chemical structure is as follows (Table 2 and Figure 2).

Table 2: Neighborhood edge partition with corresponding degree pairs and frequencies.

Nbgh.Degree	$(3,6)$	$(4,4)$	$(4,5)$	$(4,6)$	$(5,5)$	$(5,6)$	$(5,7)$	$(6,9)$	$(7,7)$	$(7,8)$	$(7,9)$
Frequency	2	5	7	1	2	7	4	2	4	4	4

Therefore, $NM-$polynomial is given as,

$$NM(Zn) = 2x^3y^6 + 5x^4y^4 + 7x^4y^5 + x^4y^6 + 2x^5y^5 + 7x^5y^6 + 4x^5y^7 + 2x^6y^9 + 4x^7y^7 + 4x^7y^8 + 4x^7y^9.$$

□

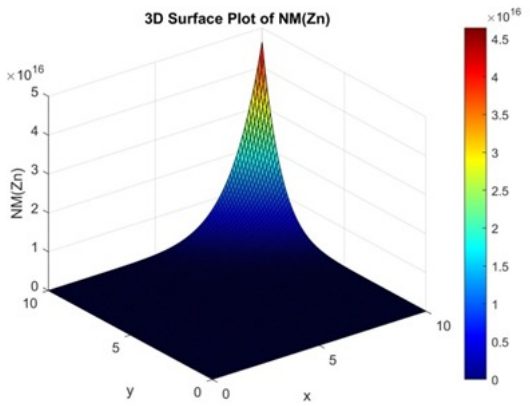

Figure 2: 3D surface plot of $NM(\text{Zn})$.

Theorem 2.2. *The $NM-$polynomial of Zinc (II) with chalcone of pyridine-2-carbaldehyde, then is in Theorem 2.1, then;*

1. *1st Zagreb index* $= M_1^* = 453$.
2. *2nd Zagreb index* $= M_2^* = 63729$.
3. *Forgotten topological index* $= F_N^* = 132642$.
4. *2nd modified Zagreb index* $= M_2^{nm} = 4.193650794$.

5. *3rd Randić topological index* $= ND_3 = 28869237.$
6. *5th Randić topological index* $= ND_5 = 2.08134444.$
7. *Harmonic topological index* $= NH = 0.003683.$
8. *Inverse sum topological index* $= NI = 140.6821192.$

Proof. Here,

$$NM(Zn) = 2x^3y^6 + 5x^4y^4 + 7x^4y^5 + x^4y^6 + 2x^5y^5 + 7x^5y^6 + 4x^5y^7 + 2x^6y^9 + 4x^7y^7 + 4x^7y^8 + 4x^7y^9,$$

now, compute the values by using formulas given in Table 1.

1. $M_1^* = (d_x + d_y)(NM(G))|x = y = 1.$

$$M_1^* = \left(6x^2y^6 + 20x^3y^4 + 28x^3y^5 + 4x^3y^6 + 10x^4y^5 + 35x^4y^6 + 20x^4y^7 + 12x^5y^9 + 28x^6y^7 + 28x^6y^9\right) + \left(36x^3y^5 + 20x^4y^3 + 35x^4y^4 + 6x^4y^5 + 10x^5y^4 + 42x^5y^5 + 28x^5y^6 + 18x^6y^8 + 28x^7y^6 + 32x^7y^7 + 36x^7y^8\right).$$

Combining like terms,

$$M_1^* = \left(42x^3y^5 + 20x^3y^4 + 63x^4y^4 + 34x^4y^5 + 10x^4y^6 + 10x^5y^4 + 52x^5y^5 + 48x^5y^6 + 20x^5y^7 + 12x^5y^9 + 18x^6y^8 + 28x^6y^9 + 32x^7y^7 + 36x^7y^8\right).$$

Now, substituting $x = 1$ and $y = 1$,

$$M_1^* = \left(42(1)^3(1)^5 + 20(1)^3(1)^4 + 63(1)^4(1)^4 + 34(1)^4(1)^5 + 10(1)^4(1)^6 + 10(1)^5(1)^4 + 52(1)^5(1)^5 + 48x^5y^6 + 20x^5y^7 + 12(1)^5(1)^9 + 18(1)^6(1)^8 + 28(1)^6(1)^9 + 32(1)^7(1)^7 + 36(1)^7(1)^8\right),$$

$$M_1^* = 42 + 20 + 63 + 34 + 10 + 10 + 52 + 48 + 20 + 12 + 18 + 28 + 28 + 32 + 36.$$

First Zagreb index: $M_1^* = 453.$

2. Second Zagreb index: $M_2^* = (d_x + d_y) \cdot NM(G)\big|_{x=y=1}$

$$M_2^* = \left(6x^2y^6 + 20x^3y^4 + 28x^3y^5 + 4x^3y^6 + 10x^4y^5 + 35x^4y^6 + 20x^4y^7 + 12x^5y^9 + 28x^6y^7 + 28x^6y^9\right) + \left(36x^3y^5 + 20x^4y^3 + 35x^4y^4 + 6x^4y^5 + 10x^5y^4 + 42x^5y^5 + 28x^5y^6 + 18x^6y^8 + 28x^7y^6 + 32x^7y^7 + 36x^7y^8\right).$$

Multiplying and combining like terms,

$$M_2^* = \left(216x^5y^{11} + 720x^6y^9 + 1008x^6y^{10} + 140x^6y^{11} + 360x^7y^8 + 700x^8y^9 + 980x^7y^{10} + 160x^7y^{11} + 300x^8y^7 + 630x^8y^8 + 840x^8y^9 + 180x^8y^{10} + 252x^9y^6 + 504x^9y^7 + 756x^9y^8 + 1008x^9y^9 + 252x^{10}y^5 + 504x^{10}y^6 + 756x^{10}y^7 + 1008x^{10}y^8 + 1008x^{11}y^7 + 1344x^{11}y^8 + 2016x^{11}y^9 + 2016x^{12}y^8 + 2018x^{12}y^9 + 2018x^{13}y^9\right).$$

Now, substituting $x = 1$ and $y = 1$,

$$M_2^* = \left(216(1)^5(1)^{11} + 720(1)^6(1)^9 + 1008(1)^6(1)^{10} + \cdots + 2018(1)^{13}(1)^9\right).$$

2nd Zagreb index $= M_2^* = 63729.$

3. $F_N^* = (d_x^2 + d_y^2)(NM(G))|x = y = 1.$
Forgotten topological index: $F_N^* = (d_x^2 + d_y^2) \cdot NM(G)\big|_{x=y=1}.$

$$F_N^* = \left(6x^2y^6 + 20x^3y^4 + 28x^3y^5 + 4x^3y^6 + 10x^4y^5 + 35x^4y^6 + 20x^4y^7 + 12x^5y^9 + 28x^6y^7 + 28x^6y^9\right)^2 + \left(36x^3y^5 + 20x^4y^3 + 35x^4y^4 + 6x^4y^5 + 10x^5y^4 + 42x^5y^5 + 28x^5y^6 + 18x^6y^8 + 28x^7y^6 + 32x^7y^7 + 36x^7y^8\right)^2.$$

After expanding and simplifying and substituting $x = 1$ and $y = 1$, we get,

$$F_N^* = 84681 + 47961.$$

Forgotten topological index $= F_N^* = 132642,$

$$M_2^{nm} = (S_xS_y)(NM(G))|x = y = 1,$$

$$S_x(f(x,y)) = \left(\frac{1}{2}\right)x^4y^6 + x^5y^4 + \left(\frac{7}{5}\right)x^5y^5 + \left(\frac{1}{5}\right)x^5y^6 + \left(\frac{1}{3}\right)x^6y^5 + \left(\frac{7}{6}\right)x^6y^6 + \left(\frac{2}{3}\right)x^6y^7 + \left(\frac{2}{7}\right)x^7y^9 + \left(\frac{1}{2}\right)x^8y^7 + \left(\frac{1}{2}\right)x^8y^8\left(\frac{1}{2}\right)x^8y^9$$

$$S_y(f(x,y)) = \left(\frac{2}{7}\right)x^3y^7 + x^4y^5 + \left(\frac{7}{6}\right)x^4y^6 + \left(\frac{1}{7}\right)x^4y^7 + \left(\frac{1}{3}\right)x^5y^6 + x^5y^7 + \left(\frac{1}{2}\right)x^5y^8 + \left(\frac{1}{5}\right)x^6y^{10} + \left(\frac{1}{2}\right)x^7y^8 + \left(\frac{4}{9}\right)x^7y^9\left(\frac{2}{5}\right)x^7y^{10}.$$

Therefore, by using formula we get;

$$M_2^{mn} = \left(\frac{1}{7}\right)x^7y^{13} + \left(\frac{1}{7}\right)x^7y^{14} + \left(\frac{1}{3}\right)x^8y^{13} + \left(\frac{1}{3}\right)x^8y^{14} + \left(\frac{7}{15}\right)x^8y^{15} + \left(\frac{1}{5}\right)x^8y^{16} + \left(\frac{1}{9}\right)x^9y^{13} + \left(\frac{7}{18}\right)x^9y^{14} + \left(\frac{7}{9}\right)x^9y^{15} + \left(\frac{7}{18}\right)x^9y^{16} + \left(\frac{2}{9}\right)x^9y^{17} + \left(\frac{2}{7}\right)x^{10}y^{16} + \left(\frac{1}{5}\right)x^{10}y^{17} + \left(\frac{1}{5}\right)x^{10}y^{18} + \left(\frac{2}{35}\right)x^{11}y^{17} + \left(\frac{4}{35}\right)x^{11}y^{18} + \left(\frac{4}{35}\right)x^{11}y^{19} + \left(\frac{2}{105}\right)(2/105)x^{12}y^{19} + \left(\frac{4}{105}\right)x^{12}y^{19} + \left(\frac{4}{105}\right)x^{12}y^{20} + \left(\frac{4}{945}\right)x^{13}y^{19} + \left(\frac{4}{945}\right)x^{13}y^{20} + \left(\frac{4}{945}\right)x^{13}y^{21} + \left(\frac{4}{4725}\right)x^{14}y^{20} + \left(\frac{4}{4725}\right)x^{14}y^{21} + \left(\frac{4}{4725}\right)x^{14}y^{22} + \left(\frac{4}{225}\right)x^{14}y^{19} + \left(\frac{4}{175}\right)x^{14}y^{20}.$$

Putting $x = y = 1$, we have;

$$M_2^{mn} = \left(\frac{1}{7}\right)(1)^7(1)^{13} + \left(\frac{1}{7}\right)(1)^7(1)^{14} + \cdots + \left(\frac{4}{175}\right)(1)^{14}(1)^{20}.$$

4. 2nd modified Zagreb index $= M_2^{nm} = 4.193650794.$
So, the final simplified result is approximately $4.193650794.$
Similarly by using Table 2 we can easily calculate the other values.

5. 3rd Randić topological index: $ND_3 = d_xd_y(d_x + d_y) \cdot NM(G)\big|_{x=y=1}.$
3rd Randić topological index $= ND_3 = (xy)(x + y).$

3rd Randić topological index $= ND_3 = M_1^* \star M_2^*$.
3rd Randić topological index $= ND_3 = 453 \star 63729$.
3rd Randić topological index $= ND_3 = 28869237$.

6. Fifth Randić topological index: $ND_5 = (d_x S_x + d_y S_y) \cdot NM(G)\big|_{x=y=1}$.
   Fifth Randić topological index: $ND_5 = \dfrac{x^2+y^2}{xy}$.
   Fifth Randić topological index $= ND_5 = 132642/63729$
   Fifth Randić topological index $= ND_5 = 2.08134444$.

7. Harmonic topological index: $NH = 2S_x J \cdot NM(G)\big|_{x=y=1}$.
   Harmonic topological index $= NH = \dfrac{2}{x+y}$.
   Harmonic topological index $= NH = \dfrac{2}{453}$.
   Harmonic topological index $= NH = 0.003683$.

8. Inverse sum topological index: $NI = S_x d_x d_y \cdot NM(G)\big|_{x=y=1}$.
   Inverse sum topological index: $NI = \dfrac{xy}{x+y}$.
   Inverse sum topological index $= NI = \dfrac{63729}{453}$.
   Inverse sum topological index $= NI = 140.6821192$.

Topological Indices for $NM(\text{Zn})$ can be refer to Figure 3.

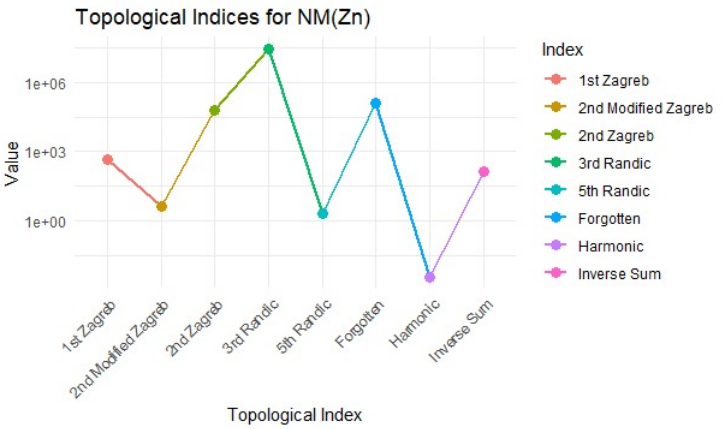

Figure 3: Topological Indices for $NM(\text{Zn})$.

□

Theorem 2.3. *The neighbourhood polynomial of the molecular structure of metal complex of Manganese (II) with (E)-3-(furan-2-yl)-1-(2, 6-dihydroxyphenyl) prop-2-en-1-one R = H, M = Mn(II) (in Figure*

4) is

$$NM(Zn) = 2x^3y^5 + 2x^3y^6 + 4x^4y^5 + 8x^5y^5 + 8x^5y^6 + 4x^5y^7 + x^5y^9 + x^6y^6 + 2x^6y^9 + 4x^7y^8 + 3x^7y^9.$$

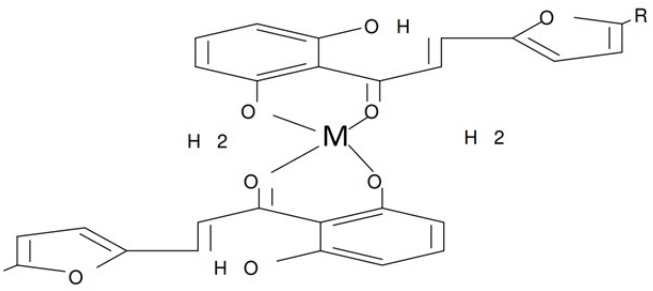

Figure 4: Topological analysis of Manganese(II) complex with (E)-3-(furan-2-yl)-1-(2,6-dihydroxyphenyl)prop-2-en-1-one.

Proof. There are thirty seven vertices and forty two edges of this molecular structure. The neighbourhood edge partition of this chemical structure is as follows (Table 3 and Figure 5),

Table 3: Neighborhood edge partition with corresponding degree pairs and frequencies.

Nbgh.Dgr	(3,5)	(3,6)	(4,5)	(5,5)	(5,6)	(5,7)	(5,9)	(6,6)	(6,9)	(7,7)	(7,8)	(7,9)
Frequency	2	2	4	8	8	4	1	1	2	3	4	3

Therefore, $NM-$polynomial is given as,

$$NM(Mn) = 2x^3y^5 + 2x^3y^6 + 4x^4y^5 + 8x^5y^5 + 8x^5y^6 + 4x^5y^7 + x^5y^9 + x^6y^6 + 2x^6y^9 + 4x^7y^8 + 3x^7y^9.$$

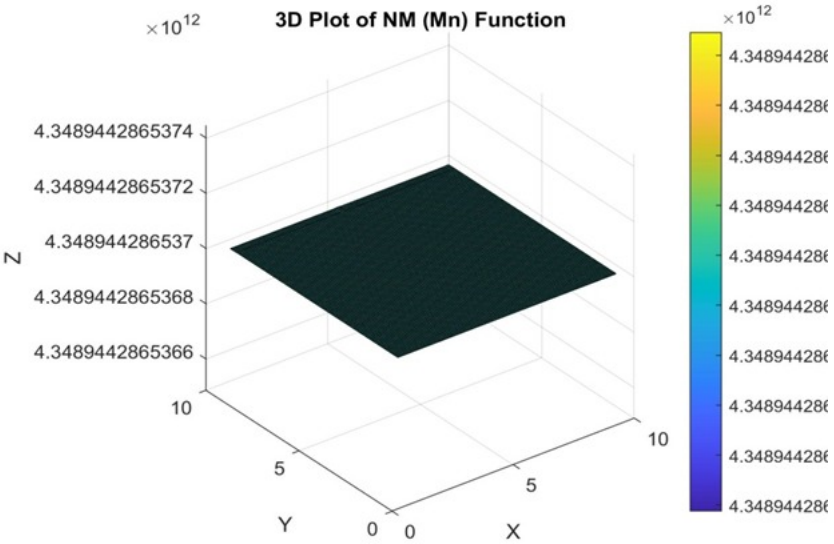

Figure 5: 3D plot of NM9(Mn) function.

□

Theorem 2.4.

$$NM(Mn) = 2x^3y^5 + 2x^3y^6 + 4x^4y^5 + 8x^5y^5 + 8x^5y^6 + 4x^5y^7 + x^5y^9 + x^6y^6 + 2x^6y^9 + 4x^7y^8 + 3x^7y^9.$$

The $NM-$polynomial of Mn(II) with chalcone of pyridine-2-carbaldehyde is the given above, then we have;

1. *1st Zagreb index* $= M_1^* = 450.$
2. *2nd Zagreb index* $= M_2^* = 5000.$
3. *Forgotten topological index* $= F_N^* = 102500.$
4. *2nd modified Zagreb index* $= M_2^{nm} = 3.96904762.$
5. *3rd Randić topological index* $= ND_3 = 22500000.$
6. *5th Randić topological index* $= ND_5 = 2.05.$
7. *Harmonic topological index* $= NH = 0.004444.$
8. *Inverse sum topological index* $= NI = 111.1111.$

Proof. Here,

$$NM(Mn) = 2x^3y^5 + 2x^3y^6 + 4x^4y^5 + 8x^5y^5 + 8x^5y^6 + 4x^5y^7 + x^5y^9 + x^6y^6 + 2x^6y^9 + 4x^7y^8 + 3x^7y^9.$$

Now, we calculate its topological indices in Table 1.

1. First Zagreb index: $M_1^* = (d_x + d_y)(NM(G))|x = y = 1.$
   where

$$d_x(f(x,y)) = x\frac{\delta(f(x,y))}{\delta x}, \qquad d_y(f(x,y)) = y\frac{\delta(f(x,y))}{\delta y},$$

$$M_1^* = \big(6x^2y^5 + 6x^2y^6 + 16x^3y^5 + 40x^4y^5 + 40x^4y^6 + 20x^4y^7 + 5x^4y^9 + 6x^5y^6 + 12x^5y^9 + 21x^6y^9\big) + \big(10x^3y^4 + 12x^3y^5 + 20x^4y^4 + 40x^5y^4 + 48x^5y^5 + 9x^5y^8 + 6x^6y^5 + 18x^6y^8 + 32x^7y^7 + 27x^7y^8\big).$$

   Combining like terms,

$$M_1^* = \big(16x^2y^5 + 26x^3y^4 + 28x^3y^5 + 36x^4y^4 + 56x^4y^5 + 40x^4y^6 + 20x^4y^7 + 5x^4y^9 + 54x^5y^4 + 88x^5y^5 + 28x^5y^6 + 9x^6y^8 + 6x^5y^6 + 12x^5y^9 + 34x^6y^5 + 46x^6y^8 + 21x^6y^9 + 32x^7y^7 + 27x^7y^8\big)$$

   Now, substituting $x = 1$ and $y = 1$,

$$M_1^* = \big(16(1)^2(1)^5 + 26(1)^3(1)^4 + 28(1)^3(1)^5 + \cdots + 27(1)^7(1)^8\big).$$

   1st Zagreb index $= M_1^* = 450.$

2. Second Zagreb index: $M_2^* = (d_x + d_y) \cdot NM(G)\big|_{x=y=1}$.

$$M_2^* = \big(6x^2y^5 + 6x^2y^6 + 16x^3y^5 + 40x^4y^5 + 40x^4y^6 + 20x^4y^7 + 5x^4y^9 + 6x^5y^6 + 12x^5y^9 + 21x^6y^9\big)^2 \times \big(10x^3y^4 + 12x^3y^5 + 20x^4y^4 + 40x^5y^4 + 48x^5y^5 + 9x^5y^8 + 6x^6y^5 + 18x^6y^8 + 32x^7y^7 + 27x^7y^8\big)^2.$$

Multiplying and combining like terms,

$$M_2^* = \big(60x^5y^9 + 72x^5y^{10} + 160x^6y^9 + 400x^7y^7 + \cdots + 1728x^{15}y^{12} + 1296x^{15}y^{13}\big).$$

Now, substituting $x = 1$ and $y = 1$,

$$M_2^* = 60 + 72 + 160 + 400 + 200 + \cdots + 1036 + 1728 + 1296.$$

2nd Zagreb index $= M_2^* = 5000$.

3. Forgotten topological index: $F_N^* = (d_x^2 + d_y^2) \cdot NM(G)\big|_{x=y=1}$.

$$F_N^* = \big(6x^2y^5 + 6x^2y^6 + 16x^3y^5 + 40x^4y^5 + 40x^4y^6 + 20x^4y^7 + 5x^4y^9 + 6x^5y^6 + 12x^5y^9 + 21x^6y^9\big)^2 \times \big(10x^3y^4 + 12x^3y^5 + 20x^4y^4 + 40x^5y^4 + 48x^5y^5 + 9x^5y^8 + 6x^6y^5 + 18x^6y^8 + 32x^7y^7 + 27x^7y^8\big)^2.$$

After expanding and simplifying and substituting $x = 1$ and $y = 1$, we get;

$$\text{Forgotten topological index} = F_N^* = 5000,$$
$$M_2^{nm} = (S_xS_y)(NM(G))|x = y = 1.$$

First, we find S_x and S_xS_y from the above formula that is,

$$S_x(f(x,y)) = \int_0^x \frac{f(t,y)}{t}dt, \qquad S_y(f(x,y)) = \int_0^y \frac{f(x,t)}{t}dt,$$
$$\int(f(x,y)) = f(x,y)$$

$$S_x(f(x,y)) = \left(\frac{1}{2}\right)x^4y^5 + \left(\frac{1}{2}\right)x^4y^6 + \left(\frac{4}{5}\right)x^5y^5 + \left(\frac{4}{3}\right)x^6y^6 + \left(\frac{2}{3}\right)x^6y^7 + \left(\frac{1}{6}\right)x^6y^9 + \left(\frac{1}{7}\right)x^7y^6 + \left(\frac{2}{7}\right)x^7y^9 + \left(\frac{1}{2}\right)x^8y^8 + \left(\frac{3}{8}\right)x^8y^9,$$

$$S_y(f(x,y)) = \left(\frac{2}{3}\right)y^6 + \left(\frac{2x^3}{7}\right)y^7 + \left(\frac{2x^4}{3}\right)y^6 + \left(\frac{4x^5}{3}\right)y^6 + \left(\frac{8x^5}{7}\right)y^7 + \left(\frac{x^5}{2}\right)y^8 + \left(\frac{x^5}{10}\right)y^{10} + \left(\frac{x^6}{7}\right)y^7 + \left(\frac{x^6}{5}\right)y^{10} + \left(\frac{4x^7}{8}\right)y^9 + \left(\frac{3x^7}{10}\right)y^{10},$$

$$M_2^{mn} = \left(\frac{1}{6}\right)x^7y^{11} + \left(\frac{1}{7}\right)x^7y^{12} + \left(\frac{2}{9}\right)x^8y^{12} + \cdots + \left(\frac{3}{280}\right)x^{15}y^{20}.$$

Putting $x = y = 1$, we have

$$M_2^{mn} = \left(\frac{1}{6}\right) + \left(\frac{1}{7}\right) + \left(\frac{2}{9}\right) + \left(\frac{1}{3}\right) + \left(\frac{4}{15}\right) + \cdots + \left(\frac{3}{2880}\right)(1^8)(1^8),$$
$$M_2^{mn} = \left(\frac{1}{7}\right)(1)^7(1)^{13} + \left(\frac{1}{7}\right)(1)^7(1)^{14} + \cdots + \left(\frac{4}{175}\right)(1)^{14}(1)^{20}.$$

4. 2nd modified Zagreb index: $M_2^{nm} = 3.96904762$.
   So, the final simplified result is approximately 3.96904762.
   Similarly by using table we can easily calculate the other values.

5. 3rd Randić topological index: $ND_3 = (xy)(x+y)$.
   3rd Randić topological index: $ND_3 = M_1^* \star M_2^*$.
   3rd Randić topological index $= ND_3 = 50000 \star 450$.
   3rd Randić topological index $= ND_3 = 22500000$.

6. Fifth Randić topological index: $ND_5 = (d_x S_x + d_y S_y) \cdot NM(G)\big|_{x=y=1}$.
   5th Randić topological index: $ND_5 = \dfrac{x^2+y^2}{xy}$.
   5th Randić topological index $= ND_5 = \dfrac{102500}{50000}$.
   5th Randić topological index $= ND_5 = 2.05$.

7. Harmonic topological index: $NH = 2S_x J \cdot NM(G)\big|_{x=y=1}$.
   Harmonic topological index: $NH = \dfrac{2}{x+y}$.
   Harmonic topological index $= NH = \dfrac{2}{450}$.
   Harmonic topological index $= NH = 0.004444$.

8. Inverse sum topological index: $NI = S_x d_x d_y \cdot NM(G)\big|_{x=y=1}$.
   Inverse sum topological index: $NI = \dfrac{xy}{x+y}$.
   Inverse sum topological index $= NI = \dfrac{50000}{450}$.
   Inverse sum topological index $= NI = 111.1111$.

Topological indices for $NM(\mathrm{Mn})$ can be refer to Figure 6. □

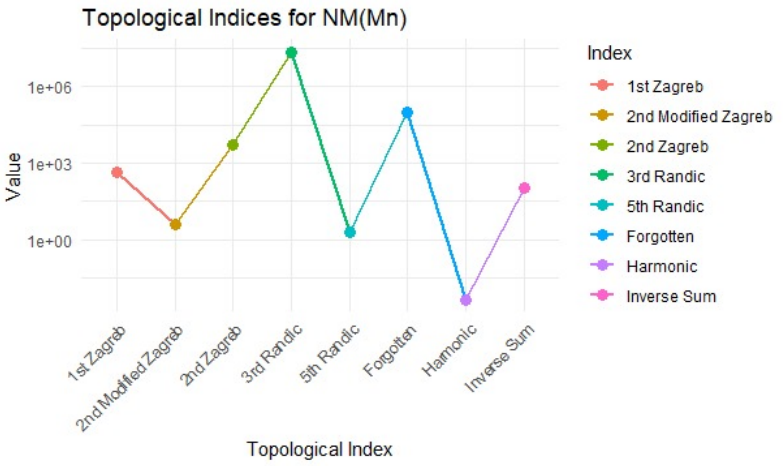

Figure 6: Topological indices for $NM(\mathrm{Mn})$.

Theorem 2.5. *The neighbourhood polynomial of the molecular structure of Metal complexes of cobalt (II)*

and copper (II) with chalcone of 5-methyl furaldehyde (Figure 7) is

$$NM(G) = 2x^3y^5 + 2x^3y^6 + 4x^4y^5 + 6x^5y^5 + 10x^5y^6 + 2x^5y^7 + 2x^6y^6 + 2x^6y^7 + 4x^6y^9 + 2x^7y^7 + 4x^7y^8 + 2x^7y^9$$

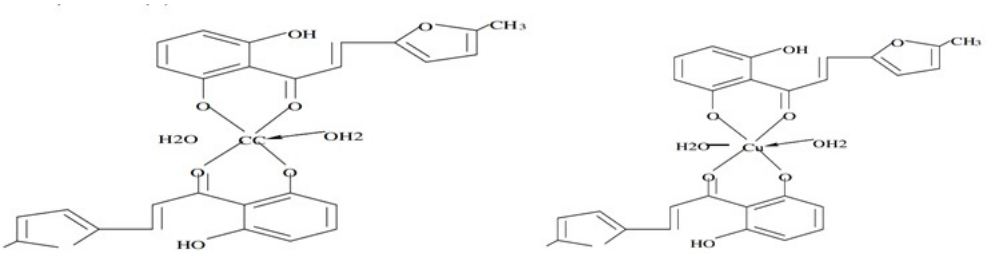

Figure 7: Topological analysis of cobalt (II) and copper (II) with chalcone of 5-methyl furaldehyde.

Proof. There are thirty seven vertices and forty two edges of this molecular structure. The neighbourhood edge partition of this chemical structure is as follows (Table 4 and Figure 8):

Table 4: Neighborhood edge partition with corresponding degree pairs and frequencies.

Nbh.dgr	(3,5)	(3,6)	(4,5)	(5,5)	(5,6)	(5,7)	(6,6)	(6,7)	(6,9)	(7,7)	(7,8)	(7,9)
Frqncy	2	2	4	6	10	2	2	2	4	2	4	2

Therefore, $NM-$polynomial is given as,

$$NM(CO) = 2x^3y^5 + 2x^3y^6 + 4x^4y^5 + 6x^5y^5 + 10x^5y^6 + 2x^5y^7 + 2x^6y^6 + 2x^6y^7 + 4x^6y^9 + 2x^7y^7 + 4x^7y^8 + 2x^7y^9.$$

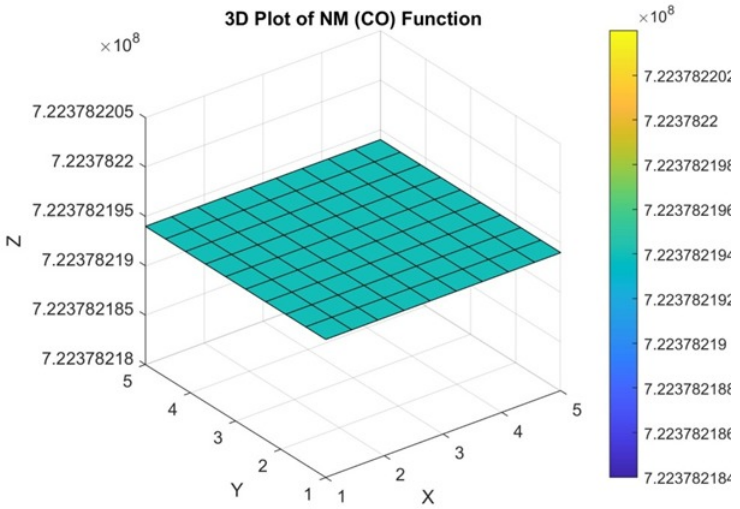

Figure 8: 3D plot of NM(CO) function.

□

Theorem 2.6. *If*

$$NM(CO) = 2x^3y^5 + 2x^3y^6 + 4x^4y^5 + 6x^5y^5 + 10x^5y^6 + 2x^5y^7 + 2x^6y^6 + 2x^6y^7 + 4x^6y^9 + 2x^7y^7 + 4x^7y^8 + 2x^7y^9,$$

is $NM-$polynomial of Metal complexes of cobalt (II) and copper (II) with chalcone of 5-methyl furaldehyde, then;

1. *1st Zagreb index* $= M_1^* = 624$.
2. *2nd Zagreb index* $= M_2^* = 73440$.
3. *Forgotten topological index* $= F_N^* = 123268$.
4. *2nd modified Zagreb index* $= M_2^{nm} = 4.554048072$.
5. *3rd Randić topological index* $= ND_3 = 45826560$.
6. *5th Randić topological index* $= ND_5 = 1.7684858$.
7. *Harmonic topological index* $= NH = 0.00320513$.
8. *Inverse sum topological index* $= NI = 117.69231$.

Proof. In this case, we have

$$NM(G) = 2x^3y^5 + 2x^3y^6 + 4x^4y^5 + 6x^5y^5 + 10x^5y^6 + 2x^5y^7 + 2x^6y^6 + 2x^6y^7 + 4x^6y^9 + 2x^7y^7 + 4x^7y^8 + 2x^7y^9.$$

1. $M_1^* = (d_x + d_y)(NM(G))|x = y = 1$,
   where

$$d_x(f(x,y)) = x\frac{\delta(f(x,y))}{\delta x}, \qquad d_y(f(x,y)) = y\frac{\delta(f(x,y))}{\delta y},$$

$$M_1^* = \big(2x^3y^5 + 2x^3y^6 + 4x^4y^5 + 6x^5y^5 + 10x^5y^6 + 2x^5y^7 + 2x^6y^6 + 2x^6y^7 + 4x^6y^9 + 2x^7y^7 + 4x^7y^8 + 2x^7y^9\big) + \big(2x^3y^5 + 2x^3y^6 + 4x^4y^5 + 6x^5y^5 + 10x^5y^6 + 2x^5y^7 + 2x^6y^6 + 2x^6y^7 + 4x^6y^9 + 2x^7y^7 + 4x^7y^8 + 2x^7y^9\big).$$

   Combining like terms,

$$M_1^* = \big(16x^2y^5 + 16x^2y^6 + 28x^3y^5 + 36x^4y^4 + 46x^4y^5 + 50x^4y^6 + 10x^4y^7 + 30x^5y^4 + 90x^5y^5 + 75x^5y^6 + 12x^5y^7 + 24x^5y^9 + 12x^6y^5 + 26x^6y^6 + 36x^6y^8 + 14x^6y^6 + 14x^7y^6 + 32x^7y^7 + 32x^7y^8\big).$$

   Now, substituting $x = 1$ and $y = 1$,

$$M_1^* = (16(1)^2(1)^5 + 16(1)^2(1)^6 + 26(1)^3(1)^5 + \cdots + 32(1)^7(1)^8)$$
$$M_1^* = 16 + 16 + 26 + 28 + 36 + 46 + 50 + 10 + 30 + 90 + 74 + 12 + 24 + 12 + 26 + 36 + 14 + 14 + 32 + 32.$$

   1st Zagreb index $= M_1^* = 624$.

2. Second Zagreb index: $M_2^* = (d_x + d_y) \cdot NM(G)\big|_{x=y=1}$.

$$M_2^* = \big(2x^3y^5 + 2x^3y^6 + 4x^4y^5 + 6x^5y^5 + 10x^5y^6 + 2x^5y^7 + 2x^6y^6 + 2x^6y^7 + 4x^6y^9 + 2x^7y^7 + 4x^7y^8 + 2x^7y^9\big)^2 \times \big(2x^3y^5 + 2x^3y^6 + 4x^4y^5 + 6x^5y^5 + 10x^5y^6 + 2x^5y^7 + 2x^6y^6 + 2x^6y^7 + 4x^6y^9 + 2x^7y^7 + 4x^7y^8 + 2x^7y^9\big)^2.$$

Multiplying and combining like terms,

$$M_2^* = \big(600x^5y^9 + 720x^5y^{10} + 1600x^6y^9 + 3000x^7y^9 + \cdots + 288x^6y^{13} + 144x^6y^{14}\big).$$

Now, substituting $x = 1$ and $y = 1$,

$$M_2^* = 600 + 720 + 1600 + 3000 + 5000 + \cdots + 576 + 288 + 144.$$

2nd Zagreb index $= M_2^* = 73440$.

3. Forgotten topological index: $F_N^* = (d_x^2 + d_y^2) \cdot NM(G)\big|_{x=y=1}$.

$$F_N^* = \big(2x^3y^5 + 2x^3y^6 + 4x^4y^5 + 6x^5y^5 + 10x^5y^6 + 2x^5y^7 + 2x^6y^6 + 2x^6y^7 + 4x^6y^9 + 2x^7y^7 + 4x^7y^8 + 2x^7y^9\big)^2 + \big(2x^3y^5 + 2x^3y^6 + 4x^4y^5 + 6x^5y^5 + 10x^5y^6 + 2x^5y^7 + 2x^6y^6 + 2x^6y^7 + 4x^6y^9 + 2x^7y^7 + 4x^7y^8 + 2x^7y^9\big)^2.$$

After expanding and simplifying and substituting $x = 1$ and $y = 1$ we get

$$\text{Forgotten topological index} = F_N^* = 123268.$$

4. $M_2^{nm} = (S_xS_y)(NM(G))|x = y = 1$.
First, we find S_x and S_xS_y from the above formula that is

$$S_x(f(x,y)) = \int_0^x \frac{f(t,y)}{t}dt, \qquad S_y(f(x,y)) = \int_0^y \frac{f(x,t)}{t}dt, \qquad \int(f(x,y)) = f(x,y),$$

$$S_x(f(x,y)) = \left(\frac{1}{2}\right)x^4y^5 + \left(\frac{1}{2}\right)x^4y^6 + \left(\frac{4}{5}\right)x^5y^5 + x^6y^5 + \left(\frac{5}{3}\right)x^6y^6 + \left(\frac{1}{3}\right)x^6y^7 + \left(\frac{2}{7}\right)x^7y^6 + \left(\frac{2}{7}\right)x^7y^7 + \left(\frac{4}{7}\right)x^7y^9 + \left(\frac{1}{4}\right)x^8y^7 + \left(\frac{1}{2}\right)x^8y^8 + \left(\frac{1}{4}\right)x^8y^9,$$

$$S_y(f(x,y)) = \left(\frac{1}{3}\right)x^3y^6 + \left(\frac{2}{7}\right)x^3y^7 + \left(\frac{2}{3}\right)x^4y^6 + x^5y^6 + \left(\frac{10}{7}\right)x^5y^7 + \left(\frac{1}{4}\right)x^5y^8 + \left(\frac{2}{7}\right)x^6y^7 + \left(\frac{1}{4}\right)x^6y^8 + \left(\frac{2}{5}\right)x^6y^{10} + \left(\frac{1}{4}\right)x^7y^8 + \left(\frac{4}{9}\right)x^7y^9 + \left(\frac{1}{5}\right)x^7y^{10},$$

$$M_2^{mn} = \left(\frac{1}{6}\right)x^7y^{11} + \left(\frac{1}{7}\right)x^7y^{12} + \left(\frac{2}{9}\right)x^8y^{12} + \cdots + \left(\frac{1}{24956885536}\right)x^{19}y^{23}.$$

Now, putting $x = y = 1$, we have

$$M_2^{mn} = \left(\frac{1}{6}\right)(1)^7(1)^{11} + \left(\frac{1}{7}\right)(1)^7(1)^{12} + \left(\frac{2}{9}\right)(1)^8(1)^{12} + \cdots + \left(\frac{1}{24956885536}\right)(1)^{19}(1)^{23}.$$

2nd modified Zagreb index $= M_2^{nm} = 4.554048072$.
So, the final simplified result is approximately 4.554048072.
Similarly by using table we can easily calculate the other values.

5. 3rd Randić topological index: $ND_3 = d_x d_y (d_x + d_y) \cdot NM(G)\big|_{x=y=1}$.
   3rd Randić topological index $= ND_3 = (xy)(x+y)$.
   3rd Randić topological index $= ND_3 = M_1^* \star M_2^*$.
   3rd Randić topological index $= ND_3 = 624 \star 73440$.
   3rd Randić topological index $= ND_3 = 45826560$.

6. Fifth Randić topological index: $ND_5 = (d_x S_x + d_y S_y) \cdot NM(G)\big|_{x=y=1}$.
   Fifth Randić topological index: $ND_5 = \dfrac{x^2+y^2}{xy}$.
   5th Randić topological index $= ND_5 = \dfrac{123268}{73440}$.
   5th Randić topological index $= ND_5 = 2.05$.

7. Harmonic topological index: $NH = 2S_x J \cdot NM(G)\big|_{x=y=1}$.
   Hamonic topological index: $NH = \dfrac{2}{x+y}$.
   Harmonic topological index $= NH = \dfrac{2}{624}$.
   Harmonic topological index $= NH = 0.00320513$.

8. Inverse sum topological index: $NI = S_x d_x d_y \cdot NM(G)\big|_{x=y=1}$.
   Invers sum topological index: $NI = \dfrac{xy}{x+y}$.
   Inverse sum topological index $= NI = \dfrac{73440}{624}$.
   Inverse sum topological index $= NI = 117.67231$.

Topological indices for $NM(\mathrm{CO})$ can be refer to Figure 9 and Table 5.

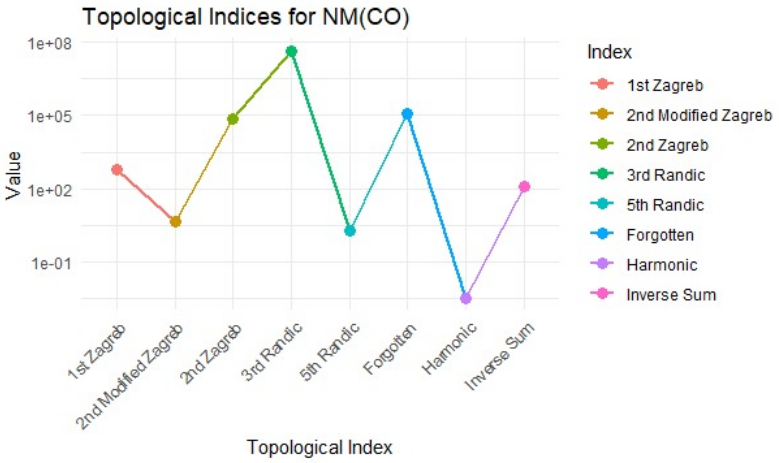

Figure 9: Topological indices for $NM(\mathrm{CO})$.

Table 5: Computed degree-based topological indices for Zn(II), Mn(II), and Co(II)/Cu metal complexes.

Metal	M_1^*	M_2^*	F_N^*	M_2^{nm}	ND_3^*	ND_5^*	NH	NI
Zn(II)	453	63729	132642	4.19	28869237	2.08	0.0037	140.68
Mn(II)	450	50000	102500	3.96	22500000	2.05	0.0044	111.11
Co(II) and Cu	624	73440	123268	4.55	45836560	1.68	0.0032	117.69

□

Comparison of the graphs (Tables 10 and 11)

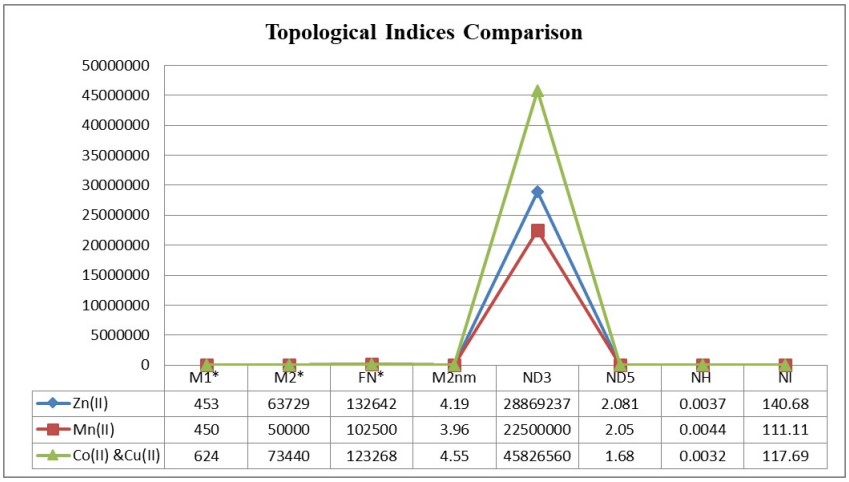

Figure 10: Degree-based topological indices comparison.

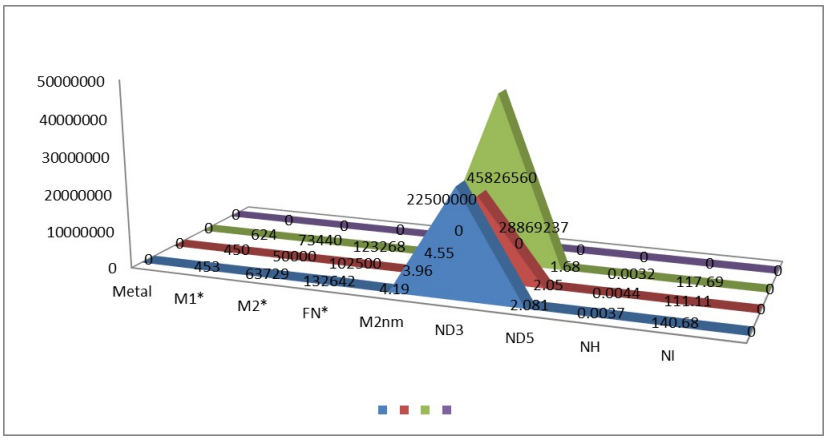

Figure 11: Comparison of Degree-based topological indices.

1. **Graph type and representation**
   - The first graph is a 2D line chart comparing the topological indices of Zn(II), Mn(II) and Co(II) and Cu(II).

- The second graph is a 3D bar chart, presenting the same data with an added depth effect for a visual comparison.

2. **Observations on data trends**

   - ND_3 index shows a sharp peak for all three metals, with Co(II) and Cu(II) having the highest value $(45, 826, 560)$, followed by Zn(II) $(28, 869, 237)$ and Mn(II) $(22, 500, 000)$.
   - $M_1, M_2, F_N^\star$ and NI values remain relatively low across all metals.
   - M_2^{nm} index has small values (between 3.96 and 4.55), indicating less variation.
   - NH and ND_5 indices show significantly lower values compared to others.

3. **Key differences in representation**

   - The 2D graph provides a clear comparison of trends but lacks depth perception.
   - The 3D graph enhances visual impact but might be harder to read due to overlapping data.

Inferene / Deduction

- The ND_3 index dominates the trend for all metals.
- Co(II) and Cu(II) have the highest values in almost all indices except for ND_5 and NH.
- Zn(II) and Mn(II) show similar patterns, with Zn(II) slightly higher in most cases.
- The 2D graph is better for precise comparisons, while the 3D graph adds visual appeal but may be harder to interpret.

3 Conclusion

This study presents a novel methodology for deriving neighborhood $M-$polynomials and various topological indices such as the zagreb, forgotten, inverse sum and harmonic indices are computed for transition metal complexes. The results reveal a strong correlation between these indices and the underlying physical and chemical properties of the metal complexes, underscoring their effectiveness as predictive tools. By integrating neighborhood $M-$polynomials with topological descriptors, the proposed approach establishes a robust framework for analyzing the structural and functional characteristics of metal-containing compounds from both mathematical and chemical perspectives. This methodology not only advances the field of chemical graph theory but also opens new avenues for practical applications. Future research will aim to extend this framework to a wider range of metal complexes and to explore its potential applications in advanced materials science, nanotechnology and pharmaceutical chemistry.

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Conflicts of Interest The authors declare no conflict of interest.

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