

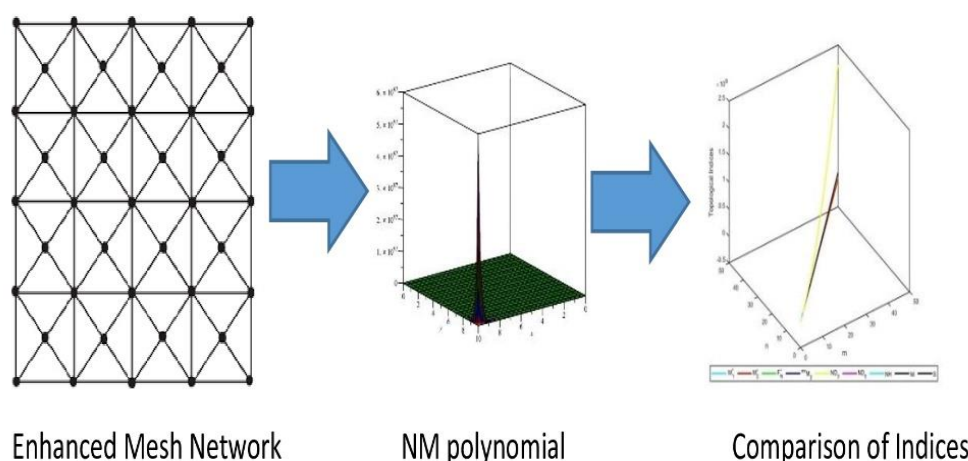
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NM-polynomial and neighborhood degree-based indices of Some Complex Networks

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Abstract: A topological index is a numerical value derived from the molecular graph structure, widely used to characterize molecular topology and predict chemical, physical, or biological properties. This study presents an in-depth exploration of neighborhood degree-based topological indices within the realm of chemical graph theory, focusing on four diverse molecular structures: the Enhanced Mesh Network, Triangular Mesh Network, Star of Silicate Network, and Rhenium Trioxide Lattice. Employing advanced mathematical techniques, including the NM Polynomial and calculus operators, in tandem with computational tools like Maple 2020 and MATLAB, we meticulously analyze the structural intricacies and connectivity patterns inherent in each molecular architecture. The calculated topological indices provide a quantitative framework for characterizing the unique graph-theoretical features of these complex molecular systems. Visualization through MATLAB facilitates a nuanced understanding of the molecular topology. This research not only advances the field of chemical graph theory

but also opens avenues for tailoring molecular designs with implications for materials science, catalysis, and network analysis.

Keywords: Topological index, degree, Enhanced Mesh, Triangular Mesh, Star of Silicate Network, Rhenium Trioxide Lattice

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Introduction

Every graph in this work is a simple graph Γ without any loops or multiple edges. Let the set of vertices and edges of a graph, respectively, be $V(\Gamma)$ and $E(\Gamma)$. The degree of the vertex $v \in V(\Gamma)$, indicated by du , is the sum of the degrees of u 's neighbours in Γ , where δu is the number of edges incident on v . The vertices that are adjacent to a vertex are referred as its neighbours. Chemical graph theory focuses on the relationship between a compound's molecular graph and its various characteristics and activities.

Topological indices are numerical descriptors that characterize the topology of a molecular graph, where atoms are represented as vertices and chemical bonds as edges. These indices quantify the structural information of a molecule by encoding connectivity patterns, distances, and bonding relationships within the graph. Topological indices are invariant under graph isomorphisms and serve as essential tools in chemoinformatics for predicting various molecular properties, such as boiling points, stability, and biological activity. In the process of creating new drugs, it has become more and more common to predict the physicochemical properties and biological activity of molecules. Quantitative structure-property/activity-relationships (QSPR/QSAR) mathematical models link the chemical composition of substances to their physical and biological properties. Without using a wet lab, it uses topological index to characterise molecular properties. The first widely recognized topological index is the Wiener Index [1], introduced for alkanes, which calculates the sum of distances between all pairs of vertices in a graph. This index has proven effective in correlating molecular structure with boiling points and other physical properties of compounds. Since then, numerous topological indices have been proposed to capture various structural aspects of molecules.

Degree-based indices such as the Randic Index [2], which focuses on the branching of molecular structures, and the Balaban Index [3], which considers distance-based measures of atom pairs, have been extensively used in Quantitative Structure-Property Relationships (QSPR) and Quantitative Structure-Activity Relationships (QSAR) studies. These indices are particularly useful in predicting biological activity, toxicity, and molecular stability.

Topological indexes are used in QSPR/QSAR analysis to convert graph into a real number that characterise the topology of the graph. For graphs that are isomorphic, it doesn't change. When attempting to create several indices of a certain category, it is difficult to compute topological indices using their traditional definitions. [4–6] developed a number of algebraic polynomials whose differentiation or integration or combination of the two obtained at a certain point generates topological indices. The M-polynomial is the most generic polynomial that could offer a significant number of degree-based topological indices [7]. To generate more indices, efforts are carried out on a daily basis.

Several academics have lately been interested in the neighbourhood degree sum based indexes [8–12]. The computation of these kinds of indices was made easier by the creation of the neighbourhood M-polynomial (NM) by contemporary authors [9, 13]. Similar to the M-polynomial for degree-based indices, it has a similar function for neighbourhood degree sum based indices. [14] computed degree-based topological indices and M-polynomials for Vphenylenic nanotubes and nanotori.

M-polynomials were employed by [15] to produce topological indices for the praline network of a chosen number of beautiful structures. The use of M-polynomial-based topological descriptors of chemical crystal structures was discussed in [16]. M-polynomials and topological indices for the linear chains of benzene, naphthalene, and anthracene were described in [17]). [18] computed the topological indices of the silicate network using an M-polynomial. M-polynomials and degree-based topological indices for copper (I) oxide were established in [19].

[20] developed topological indices for nanotubes using an M-polynomial. Closed formula for the M-polynomial and topological descriptors of boron triangular nanotubes were calculated in [21]. The development of several M-polynomials for nanostructures and the zigzag edge coronoid of starphene were discovered in [22,23]. The topological features of titanium difluoride TiF_2 crystal structures were discovered in [24]. The M- and NM-polynomials of certain anti- COVID-19 medicines were evaluated in [25].

The introduction of algebraic polynomials has simplified the computation of topological indices. The M-polynomial has proven to be an effective tool in deriving a wide range of degree-based topological indices. Building on this, the neighborhood M-polynomial (NM-polynomial) was introduced to facilitate the computation of neighborhood degree sum-based indices. This approach has been successfully applied to various nanostructures and molecular networks. This study hypothesizes that neighborhood degree sum-based topological indices derived through the NM-polynomial framework can effectively characterize the structural properties of complex molecular networks, providing deeper

insights into their connectivity patterns and potential applications in materials science and cheminformatics. Additionally, we propose that these indices exhibit distinct trends across different network structures, offering valuable quantitative descriptors for molecular topology. Unlike previous studies that primarily focused on well-established molecular graphs, this research extends the application of NM-polynomials to analyze complex network structures, including the Enhanced Mesh Network, Triangular Mesh Network, Star of Silicate Network, and Rhenium Trioxide Lattice. By employing advanced computational techniques, we provide a comparative analysis of various neighborhood degree sum-based indices, highlighting their significance in capturing molecular structural nuances. By using a neighbourhood M-polynomial technique, we hope to derive certain neighbourhood degree sum-based indices of Some Complex Networks.

The remainder of this paper is structured as follows: Section 2 provides preliminary definitions and theoretical background. Section 3 outlines the methodology for deriving NM-polynomials and neighborhood degree sum-based indices. Section 4 presents detailed computations for the four molecular networks under study. Section 5 discusses graphical representations and comparative analyses of the computed indices. Finally, Section 6 concludes the study, summarizing key findings and potential future directions.

Definitions

The neighborhood M-polynomial of a graph Γ is defined as

$$NM(\Gamma; x, y) = \sum_{i \leq j} \Gamma_{i,j} x^i y^j, \quad (1)$$

where $\Gamma_{i,j} x^i y^j$ is the total count of edges $uv \in E(\Gamma)$ such that $\delta u, \delta v = i, j$. Table 1 displays the creation of neighborhood degree-based indices and how they relate to the NM-polynomial.

Here, $NM(\Gamma)$ is a function of x, y and

$$D_x = \frac{\partial(f(x,y))}{\partial x}, D_y = \frac{\partial(f(x,y))}{\partial y}, L_x = f(x^2, y), L_y = f(x, y^2), L_y = f(x, y^2), \\ S_x = \int_0^x \frac{f(t,y)}{t} dt, S_y = \int_0^y \frac{f(x,t)}{t} dt, J = f(x, x)$$

Table 1. Formulation of Topological Indices using NM-Polynomial for a Graph Γ .

S.No	Topological Index	$f(x, y)$	Derivation from $NM(\Gamma)$
1.	Third Version of Zagreb Index $M'_1(\Gamma)$ [11]	$x + y$	$(D_x + D_y)(M(\Gamma; x, y)) _{x=y=1}$
2.	Neighborhood second Zagreb index $M_2^*(\Gamma)$ ([12])	xy	$(D_x \cdot D_y)(M(\Gamma; x, y)) _{x=y=1}$
3.	Neighborhood forgotten topological index $F_N^*(\Gamma)$ ([12])	$x^2 + y^2$	$(D_x^2 + D_y^2)(M(\Gamma; x, y)) _{x=y=1}$
4.	Neighborhood second modified zagreb index $^{nm}M_2(\Gamma)$ ([11])	$\frac{1}{xy}$	$(S_x S_y)(M(\Gamma; x, y)) _{x=y=1}$
5.	Neighborhood general Randic index $NR\alpha(\Gamma)$ ([11])	$(xy)^\alpha$	$(D_x^\alpha + D_y^\alpha)(M(\Gamma; x, y)) _{x=y=1}$
6.	Third NDe Index $ND_3(\Gamma)$ ([12])	$xy(x + y)$	$D_x D_y (D_x + D_y)(M(\Gamma; x, y)) _{x=y=1}$
7.	Fifth NDe Index $ND_5(\Gamma)$ ([12])	$\frac{x^2 + y^2}{xy}$	$(D_x S_y + D_y S_x)(M(\Gamma; x, y)) _{x=y=1}$
8.	Neighborhood Harmonic index $NH(\Gamma)$ ([12])	$\frac{2}{x + y}$	$2(S_x)J(M(\Gamma; x, y)) _{x=1}$
9.	Neighborhood Inverse sum index $NI(\Gamma)$ ([11])	$\frac{xy}{x + y}$	$S_x J(D_x + D_y)(M(\Gamma; x, y)) _{x=y=1}$
10.	Sanskriti index $S(\Gamma)$ ([11])	$\frac{xy}{(x + y - 2)^3}$	$(S_x^3 Q_{-2} J D_x^3 D_y^3)(M(\Gamma; x, y)) _{x=1}$

Methodology

With in current study, certain neighbourhood degree sum-based indices of the Enhanced Mesh, Triangular Mesh, Star of Silicate Network, Rhenium Trioxide Lattice are discussed. The above- mentioned networks' NM-polynomials are first calculated, and then various neighbourhood degree sum-based indices are obtained using certain calculus operations. To get the results, we use edge partitioning, graph theoretical approaches, and combinatorial computation. Utilizing Maple 2020, the findings are displayed graphically. Using Matlab 2017, 3d line graphing is used to compare the results.

Enhanced mesh $M(m, n)$ network

The graph whose vertices correspond to the points in the plane with integer coordinates, x - coordinates in the range $1, 2, \dots, n$ and y -coordinates in the range $1, 2, \dots, m$, and two vertices are connected by an edge whenever the corresponding points are at

distance 1, is a common form of lattice graph [26]. In other words, for the point set mentioned, it is a unit distance graph. The term n -mesh has also been given to various other types of graphs with a certain structure in the literature, such as the Cartesian product of a number of path graphs. The Cartesian product of paths of order $a_1, a_2, \dots, a_n$ is an n -mesh $M(a_1, a_2, \dots, a_n)$, which is defined as:

For an n -mesh, $M(a_1, a_2, \dots, a_n)$, the Cartesian product is given by

$$M(a_1, a_2, \dots, a_n) = Pa_1 \times Pa_2 \times \dots \times Pa_n.$$

The order of $M(a_1, a_2, \dots, a_n)$ is

$$|V(M(a_1, a_2, \dots, a_n))| = a_1, a_2, \dots, a_n$$

the size is given by

$$|E(M(a_1, a_2, \dots, a_n))| = a_1, a_2, \dots, a_n \left(n - \frac{1}{a_1} - \frac{1}{a_2} - \dots - \frac{1}{a_n} \right).$$

Here, we discuss the enhanced 2-mesh network. A 2-mesh $M(Pa_1 \times Pa_2)$ has the vertex set

$$V = \{(i, j) : 1 \leq i \leq m, 1 \leq j \leq n\}.$$

The edge set E for the enhanced 2-mesh network is given by

$$E = \{((i, j), (i, j + 1)) : 1 \leq i \leq m, 1 \leq j \leq n - 1\} \cup \{((i, j), (i + 1, j)) : 1 \leq i \leq m - 1, 1 \leq j \leq n\}.$$

An edge set is defined for an enhanced mesh. An enhanced mesh $EM(Pa_1 \times Pa_2)$ is obtained by replacing each 4-cycle of $M(Pa_1 \times Pa_2)$ with a wheel W_4 on 4 vertices. Thus, a wheel W_4 is a graph obtained by connecting the central vertex to each vertex of cycle C_4 . The hub (central vertex) of W_4 is a new vertex. Assume that

$h_{ij}, 1 \leq i \leq m - 1, 1 \leq j \leq n - 1$, is the collection of all hub (central) vertices. We define the creation of a Enhanced mesh $M(5, 5)$ network in Figure1.

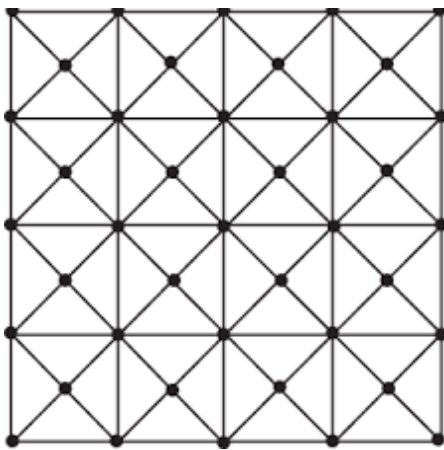


Fig. 1: Enhanced mesh $M(5, 5)$ network.

Table 2. Edge partition of Enhanced mesh $M(m, n)$ network.

(δ_u, δ_v)	frequency
(14, 21)	4
(14, 24)	8
(21, 24)	8
(21, 42)	4
(24, 26)	16
(24, 42)	$2(3m + 3n - 26)$
(26, 42)	8
(26, 45)	$6(m + n - 8)$
(32, 42)	4
(32, 45)	$4(m + n - 8)$
(32, 48)	$4(mn - 4m - 4n + 16)$
(42, 45)	8
(45, 45)	$2(m + n - 10)$
(45, 48)	$2(m + n - 8)$
(48, 48)	$(2mn - 9m - 9n + 40)$

NM-Polynomial Enhanced mesh $M(m, n)$ network

In this section we will find the NM-Polynomial of the enhanced mesh network.

Theorem 3.1. Let Γ be the graph of Enhanced mesh $M(m, n)$ network, then

$$NM(\Gamma; x, y) = 4x^{14}y^{21} + 8x^{14}y^{24} + 8x^{21}y^{24} + 4x^{21}y^{42} + 16x^{24}y^{26} + 8x^{24}y^{42} + 8x^{26}y^{42} + 2(3m + 3n - 26)x^{26}y^{26} + 6(m + n - 8)x^{26}y^{45} + 4(m + n - 8)x^{32}y^{45} + 4x^{32}y^{24} + 4(mn - 4m - 4n + 16)x^{32}y^{48} + 8x^{42}y^{45} + 2(m + n - 10)x^{45}y^{45} + 2(m + n - 8)x^{45}y^{48} + (2mn - 9m - 9n + 40)x^{48}y^{48}$$

Proof: Using Table 2 and definition of NM-polynomial, we have following computation

$$\begin{aligned} NM(\Gamma; x, y) &= \sum_{i \leq j} r_{i,j} x^i y^j \\ &= m(14, 21)x^{14}y^{21} + m(14, 24)x^{14}y^{24} + m(21, 24)x^{21}y^{24} + m(21, 42)x^{21}y^{42} + \\ &\quad m(24, 26)x^{24}y^{26} + m(24, 42)x^{24}y^{42} + m(26, 42)x^{26}y^{42} + m(26, 45)x^{26}y^{45} \\ &\quad + m(32, 42)x^{32}y^{42} + m(32, 45)x^{32}y^{45} + m(32, 48)x^{32}y^{48} + m(42, 45)x^{42}y^{45} \\ &\quad + m(45, 45)x^{45}y^{45} + m(45, 48)x^{45}y^{48} + m(48, 48)x^{48}y^{48} \\ &= 4x^{14}y^{21} + 8x^{14}y^{24} + 8x^{21}y^{24} + 4x^{21}y^{42} + 16x^{24}y^{26} + 8x^{24}y^{42} \\ &\quad + 8x^{26}y^{42} + 2(3m + 3n - 26)x^{26}y^{26} + 6(m + n - 8)x^{26}y^{45} + 4x^{32}y^{24} \\ &\quad + 8x^{42}y^{45} + 4(m + n - 8)x^{32}y^{45} + 4(mn - 4m - 4n + 16)x^{32}y^{48} \\ &\quad + 2(m + n - 10)x^{45}y^{45} + 2(m + n - 8)x^{45}y^{48} + (2mn - 9m - 9n + 40)x^{48}y^{48} \end{aligned}$$

4.1.2. Neighborhood degree based topological indices of Enhanced mesh $M(m, n)$ Network

In this section we will find the neighborhood degree based topological indices using Using Table 1 and Theorem 3.1 for the enhanced mesh $M(m,n)$.

Theorem 3.2. Let Γ be the graph of Enhanced mesh $M(m, n)$ network, then

$$M'_1(\Gamma, x, y) = 944 - 732n - 732m + 512m n$$

$$M_2^*(\Gamma, x, y) = 34412 - 20106n - 20106m + 10752m n$$

$$F_N^*(\Gamma, x, y) = 944 - 732n - 732m + 512m n$$

$$^{nm}M_2(\Gamma, x, y) = 0.01 + 0.004n + 0.004m + 0.003m n$$

$$NR_\alpha(\Gamma, x, y) = 4^\alpha + (3 + m + 2n) \cdot 5^\alpha + (-4 + 4m + 4n) \cdot 7^\alpha + (-9 + 6n + 3m) \cdot 8^\alpha + (15mn - 10m - 15n + 10) \cdot 9^\alpha$$

$$ND_3(\Gamma, x, y) = 4149128 - 2037624n - 2037624m + 933888m n$$

$$ND_5(\Gamma, x, y) = 10.146 - 10.338n - 10.338m + 12.667m n$$

$$NH(\Gamma, x, y) = 0.038 + 0.142m n + 0.004m + 0.004n$$

$$NI(\Gamma, x, y) = 4 + 6m n - 5m - 5n$$

$$S(\Gamma, x, y) = 59996.263m n - 131201.835m - 131201.835n + 267451.215$$

Proof: Using Table 1 and Theorem 3.1, we have following computation

$$\begin{aligned} M'_1(\Gamma, x, y) &= (D_x + D_y)(NM(\Gamma; x, y))|_{x=y=1} \\ &= (-2704 x^{26}y^{26} + 3840 x^{48}y^{48} - 1488 x^{45}y^{48} + 5120 x^{32}y^{48} - 1800 x^{45}y^{45} \\ &\quad - 3408 x^{26}y^{45} - 2464 x^{32}y^{45} + 180 x^{45}y^{45}n + 312 x^{26}y^{26}n + 308 x^{32}y^{45}n \\ &\quad + 426 x^{26}y^{45}m - 1280 x^{32}y^{48}n + 186 x^{45}y^{48}m - 1280 x^{32}y^{48}m + 426 x^{26}y^{45}n + 312 \\ &\quad x^{26}y^{26}m + 308 x^{32}y^{45}m + 320 x^{32}y^{48}m n + 186 x^{45}y^{48}n + 192 x^{48}y^{48}m n - 864 \\ &\quad x^{48}y^{48}m - 864 x^{48}y^{48}n + 180 x^{45}y^{45}m + 696 x^{42}y^{45} + 224 x^{32}y^{24} \\ &\quad + 800 x^{24}y^{26} + 528 x^{24}y^{42} + 544 x^{26}y^{42} + 140 x^{14}y^{21} + 304 x^{14}y^{24} + 360 x^{21}y^{24} \\ &\quad + 252 x^{21}y^{42})|_{x=y=1} = 944 - 732n - 732m + 512m n \end{aligned}$$

$$\begin{aligned} M_2^*(\Gamma, x, y) &= (D_x \cdot D_y)(NM(\Gamma; x, y))|_{x=y=1} \\ &= (-35152 x^{26}y^{26} + 92160 x^{48}y^{48} - 34560 x^{45}y^{48} + 98304 x^{32}y^{48} - 40500 x^{45}y^{45} \\ &\quad - 56160 x^{26}y^{45} - 46080 x^{32}y^{45} + 4050 x^{45}y^{45}n + 4056 x^{26}y^{26}n + 5760 x^{32}y^{45}n \\ &\quad + 7020 x^{26}y^{45}m - 24576 x^{32}y^{48}n + 4320 x^{45}y^{48}m - 24576 x^{32}y^{48}m + 7020 x^{26}y^{45}n \\ &\quad + 4056 x^{26}y^{26}m + 5760 x^{32}y^{45}m + 6144 x^{32}y^{48}m n + 4320 x^{45}y^{48}n + 4608 \\ &\quad x^{48}y^{48}mn - 20736 x^{48}y^{48}m - 20736 x^{48}y^{48}n + 4050 x^{45}y^{45}m + 15120 x^{42}y^{45} + \\ &\quad 3072 x^{32}y^{24} + 9984 x^{24}y^{26} + 8064 x^{24}y^{42} + 8736 x^{26}y^{42} + 1176 x^{14}y^{21} + 2688 \\ &\quad x^{14}y^{24} + 4032 x^{21}y^{24} + 3528 x^{21}y^{42})|_{x=y=1} = 34412 - 20106n - 20106m + 10752m n \end{aligned}$$

$$\begin{aligned}
 F_N^*(\Gamma, x, y) &= (D_x^2 + D_y^2)(NM(\Gamma; x, y))|_{x=y=1} \\
 &= (-2704 x^{26}y^{26} + 3840 x^{48}y^{48} - 1488 x^{45}y^{48} + 5120 x^{32}y^{48} - 1800 x^{45}y^{45} \\
 &\quad - 3408 x^{26}y^{45} - 2464 x^{32}y^{45} + 180 x^{45}y^{45}n + 312 x^{26}y^{26}n + 308 x^{32}y^{45}n \\
 &\quad + 426 x^{26}y^{45}m - 1280 x^{32}y^{48}n + 186 x^{45}y^{48}m - 1280 x^{32}y^{48}m + 426 x^{26}y^{45}n \\
 &\quad + 312 x^{26}y^{26}m + 308 x^{32}y^{45}m + 320 x^{32}y^{48}m \cdot n + 186 x^{45}y^{48}n + 192 x^{48}y^{48}m \\
 &\quad n \\
 &\quad - 864 x^{48}y^{48}m - 864 x^{48}y^{48}n + 180 x^{45}y^{45}m + 696 x^{42}y^{45} + 224 x^{32}y^{24} \\
 &\quad + 800 x^{24}y^{26} + 528 x^{24}y^{42} + 544 x^{26}y^{42} + 140 x^{14}y^{21} + 304 x^{14}y^{24} \\
 &\quad + 360 x^{21}y^{24} + 252 x^{21}y^{42})|_{x=y=1} = 944 - 732n - 732m + 512mn
 \end{aligned}$$

$$\begin{aligned}
 {}^{nm}M_2(\Gamma, x, y) &= (S_x S_y)(NM(\Gamma; x, y))|_{x=y=1} \\
 &= \left(-\frac{x^{26}y^{26}}{13} + \frac{5x^{48}y^{48}}{288} - \frac{x^{45}y^{48}}{24} + \frac{x^{32}y^{48}}{24} - \frac{4x^{45}y^{45}}{405} - \frac{8x^{26}y^{45}}{195} - \frac{x^{32}y^{45}}{45} + \frac{2x^{45}y^{45}n}{2025} + \frac{3x^{26}y^{26}n}{338} + \frac{x^{32}y^{45}n}{360} + \right. \\
 &\quad \left. \frac{x^{26}y^{45}m}{195} - \frac{x^{32}y^{48}n}{96} + \frac{x^{45}y^{48}m}{1080} - \frac{x^{32}y^{48}m}{96} + \frac{x^{26}y^{45}n}{195} + \frac{3x^{26}y^{26}m}{338} + \frac{x^{32}y^{45}m}{360} + \frac{x^{32}y^{48}mn}{384} + \frac{x^{45}y^{48}n}{1080} + \right. \\
 &\quad \left. \frac{x^{48}y^{48}mn}{1152} - \frac{x^{45}y^{48}m}{256} - \frac{x^{45}y^{48}n}{256} + \frac{2x^{45}y^{45}m}{2025} + \frac{4x^{42}y^{45}m}{945} + \frac{x^{32}y^{24}}{192} + \frac{x^{24}y^{26}}{39} + \frac{x^{24}y^{42}}{126} + \frac{2x^{14}y^{21}}{147} + \frac{x^{14}y^{24}}{42} + \right. \\
 &\quad \left. \frac{x^{21}y^{24}}{63} + \frac{2x^{21}y^{42}}{441} \right) |_{x=y=1} \\
 &= \frac{160829}{16511040} + \frac{383063n}{87609600} + \frac{383063m}{87609600} + \frac{m \cdot n}{288}.
 \end{aligned}$$

$$\begin{aligned}
 NR_\alpha(\Gamma, x, y) &= (D_x^\alpha + D_y^\alpha)(NM(\Gamma; x, y))|_{x=y=1} \\
 &= (4^\alpha x^4 y^2 + 5^\alpha x^5 y^3 + (m + 2n)5^\alpha x^5 y^5 + 5^\alpha x^5 y^5 + 7^\alpha x^7 y^4 + (2 + 2n)7^\alpha x^7 y^5 + \\
 &\quad 5^\alpha x^5 y^6 + (-7 + 4m + 2n)7^\alpha x^7 y^6 + (-2 + 2n)8^\alpha x^8 y^6 + (-5 + 2m + \\
 &\quad 2n)8^\alpha x^8 y^5 + 8^\alpha x^8 y^7 + (-4 + 2n + m)8^\alpha x^8 y^8 + (-3 + 2n + 2m)9^\alpha x^9 y^7 + \\
 &\quad (-7 + 4n + 2m)9^\alpha x^9 y^8 + (15mn - 14m - 21n + 20)9^\alpha x^9 y^9)|_{x=y=1} \\
 &= 4^\alpha + (3 + m + 2n) \cdot 5^\alpha + (-4 + 4m + 4n) \cdot 7^\alpha + (-9 + 6n + 3m) \cdot \\
 &\quad 8^\alpha + (15mn - 10m - 15n + 10) \cdot 9^\alpha
 \end{aligned}$$

$$\begin{aligned}
 ND_3(\Gamma, x, y) &= D_x D_y (D_x + D_y)(M(\Gamma; x, y))|_{x=y=1} \\
 &= (-1827904 x^{26}y^{26} + 8847360 x^{48}y^{48} - 3214080 x^{45}y^{48} + 7864320 \\
 &\quad x^{32}y^{48} - 3645000 x^{45}y^{45} - 3987360 x^{26}y^{45} - 3548160 x^{32}y^{45} + 364500 x^{45}y^{45}n \\
 &\quad + 210912 x^{26}y^{26}n + 443520 x^{32}y^{45}n + 498420 x^{26}y^{45}m - 1966080 x^{32}y^{48}n \\
 &\quad + 401760 x^{45}y^{48}m - 1966080 x^{32}y^{48}m + 498420 x^{26}y^{45}n + 210912 x^{26}y^{26}m \\
 &\quad + 443520 x^{32}y^{45}m + 491520 x^{32}y^{48}m \cdot n + 401760 x^{45}y^{48}n + 442368 x^{48}y^{48}m n \\
 &\quad - 1990656 x^{48}y^{48}m - 1990656 x^{48}y^{48}n + 364500 x^{45}y^{45}m + 1315440 x^{42}y^{45} \\
 &\quad + 172032 x^{32}y^{24} \\
 &\quad + 499200 x^{24}y^{26} + 532224 x^{24}y^{42} + 594048 x^{26}y^{42} + 41160 x^{14}y^{21} + 102144 \\
 &\quad x^{14}y^{24} + 181440 x^{21}y^{24} + 222264 x^{21}y^{42})|_{x=y=1} \\
 &= 4149128 - 2037624n - 2037624m + 933888mn
 \end{aligned}$$

$$ND_5(\Gamma, x, y) = (D_x S_y + D_y S_x)(NM(\Gamma; x, y))|_{x=y=1}$$

$$\begin{aligned}
 &= (-104 x^{26} y^{26} + 80 x^{48} y^{48} - 32.067 x^{45} y^{48} + 138.667 x^{32} y^{48} - 40 x^{45} y^{45} \\
 &- 110.81 x^{26} y^{45} - 67.756 x^{32} y^{45} + 4 x^{45} y^{45} n + 12 x^{26} y^{26} n + 8.469 x^{32} y^{45} n \\
 &+ 13.851 x^{26} y^{45} m - 34.667 x^{32} y^{48} n + 4.008 x^{45} y^{48} m - 34.667 x^{32} y^{48} m \\
 &+ 13.851 x^{26} y^{45} n + 12 x^{26} y^{26} m + 8.469 x^{32} y^{45} m + 8.667 x^{32} y^{48} m n \\
 &+ 4.008 x^{45} y^{48} n + 4 x^{48} y^{48} m \cdot n - 18 x^{48} y^{48} m - 18 x^{48} y^{48} n + 4 x^{45} y^{45} m \\
 &+ 16.038 x^{42} y^{45} + 8.333 x^{32} y^{24} + 32.103 x^{24} y^{26} + 18.571 x^{24} y^{42} + 17.875 x^{26} y^{42} \\
 &+ 8.667 x^{14} y^{21} + 18.381 x^{14} y^{24} + 16.143 x^{21} y^{24} + 10 x^{21} y^{42})|_{x=y=1} \\
 &= 10.146 - 10.338 n - 10.338 m + 12.667 m n
 \end{aligned}$$

$$\begin{aligned}
 NH(\Gamma, x, y) &= 2(S_x)J(NM(\Gamma; x, y))|_{x=1} \\
 &= (0.229 x^{35} + 0.421 x^{38} + 0.127 x^{63} + 0.64 x^{50} + 0.242 x^{66} + 0.235 x^{68} + \\
 &0.143 x^{56} + 0.184 x^{87} + 0.042 x^{96} m \cdot n + 0.1 x^{80} m \cdot n - 0.188 x^{96} m - 0.188 x^{96} n \\
 &+ 0.043 x^{93} m + 0.043 x^{93} n + 0.044 x^{90} m + 0.044 x^{90} n - 0.4 x^{80} m - 0.4 x^{80} n + \\
 &0.104 x^{77} m + 0.104 x^{77} n + 0.169 x^{71} m + 0.169 x^{71} n + 0.231 x^{52} m + 0.231 x^{52} n \\
 &+ 0.356 x^{45} - 2 x^{52} - 1.352 x^{71} - 0.831 x^{77} + 1.6 x^{80} - 0.444 x^{90} - 0.344 x^{93} + \\
 &0.833 x^{96})|_{x=1} \\
 &= 0.038 + 0.142 m \cdot n + 0.004 m + 0.004 n
 \end{aligned}$$

$$\begin{aligned}
 NI(\Gamma, x, y) &= S_x J(D_x + D_y)(NM(\Gamma; x, y))|_{x=y=1} \\
 &= (4 x^{35} + 8 x^{38} + 4 x^{63} + 16 x^{50} + 8 x^{66} + 8 x^{68} + 4 x^{56} + 8 x^{87} \\
 &+ 2 x^{96} m n + 4 x^{80} m \cdot n - 9 x^{96} m - 9 x^{96} n + 2 x^{93} m + 2 x^{93} n + 2 x^{90} m + 2 \\
 &x^{90} n - 16 x^{80} m - 16 x^{80} n + 4 x^{77} m + 4 x^{77} n + 6 x^{71} m + 6 x^{71} n + 6 x^{52} m + \\
 &6 x^{52} n + 8 x^{45} - 52 x^{52} - 48 x^{71} - 32 x^{77} + 64 x^{80} - 20 x^{90} - 16 x^{93} + 40 x^{96})|_{x=1} \\
 &= 4 + 6 m n - 5 m - 5 n
 \end{aligned}$$

$$\begin{aligned}
 S(\Gamma, x, y) &= (S_x^3 Q_{-2} J D_x^3 D_y^3)(NM(\Gamma; x, y))|_{x=1} \\
 &= (29450.58 x^{94} m \cdot n + 30545.682 x^{78} m \cdot n - 132527.612 x^{94} m - \\
 &132527.612 x^{94} n + 26746.507 x^{91} m + 26746.507 x^{91} n + 24370.086 x^{88} m + \\
 &24370.086 x^{88} n - 122182.729 x^{78} m - 122182.729 x^{78} n + 28311.552 x^{75} m + \\
 &28311.552 x^{75} n + 29252.404 x^{69} m + 29252.404 x^{69} n + 14827.957 x^{50} m + \\
 &14827.957 x^{50} n - 128508.963 x^{50} + 36234.819 x^{66} + 35152 x^{48} + 2828.526 x^{33} \\
 &+ 6504.296 x^{36} + 12091.39 x^{61} + 31255.875 x^{64} + 11507.007 x^{54} + 87946.513 \\
 &x^{85} + 12881.79 x^{43} - 234019.232 x^{69} - 226492.416 x^{75} + 488730.917 x^{78} - \\
 &243700.86 x^{88} - 213972.056 x^{91} + 589011.609 x^{94})|_{x=1} \\
 &= 59996.263 m n - 131201.835 m - 131201.835 n + 267451.215
 \end{aligned}$$

Triangular Mesh T_n network

In this section, we are going to study the degree-based topological descriptors for the triangular mesh network [26]. We denote the radix n triangular mesh network by T_n having node set

$$V_{T_n} = \{(x, y) | 0 \leq x \leq n \text{ and } 0 \leq x + y \leq n\} \quad (2)$$

and there exists a mesh arc between nodes

$$(x_1, y_1) \text{ and } (x_2, y_2) \text{ if } |x_1 - x_2| + |y_1 - y_2| \leq 1 \text{ and } x_1 + y_1 \leq x_2 + y_2.$$

The number of vertices (nodes) in a T_n is $n(n+1)/2$. The degree of a node in the aforementioned network may be 2, 4, or 6. There exist three vertices of degree 2, which we call corner vertices. Throughout this section, we represent G by the graph of the triangular mesh network T_n . The graph of triangular mesh T_5 is shown in Figure

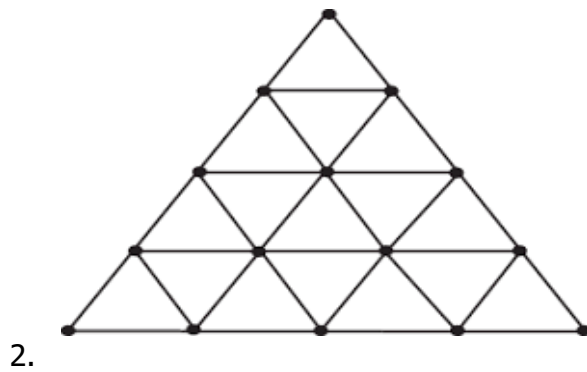


Figure 2. Triangular mesh T_n network.

Table 3. Edge partition of Triangular mesh T_n network.

(δ_u, δ_v)	frequency
(8, 16)	6
(16, 16)	3
(16, 20)	6
(16, 28)	6
(20, 20)	$3(n - 5)$
(20, 28)	6
(20, 32)	$6(n - 5)$
(28, 32)	6
(32, 32)	$3(n - 5)$
(32, 36)	$6(n - 6)$
(36, 36)	$\frac{3(n^2 - 13n + 42)}{2}$

NM-Polynomial of Triangular mesh T_n network

In this section we will find the NM –Polynomial of triangular mesh T_n .

Theorem 3.3. Let Γ be the graph of Triangular mesh T_n network, then

$$NM(\Gamma, x, y) = 6x^8y^{16} + 3x^{16}y^{16} + 6x^{16}y^{20} + 6x^{16}y^{28} + 3(n-5)x^{20}y^{20} + 6x^{20}y^{28} \\ + 6(n-5)x^{20}y^{32} + 6x^{28}y^{32} + 3(n-5)x^{32}y^{32} + 6(n-6)x^{32}y^{36} + \frac{3n^2-39n+126}{2}x^{36}y^{36}$$

Proof. Using Table 3 and definition of NM-polynomial, we have following computation

$$NM(\Gamma; x, y) = \sum_{i \leq j} \Gamma_{i,j} x^i y^j \\ = m(8,16)x^8y^{16} + m(16,16)x^{16}y^{16} + m(16,20)x^{16}y^{20} + m(16,28)x^{16}y^{28} \\ + m(20,20)x^{20}y^{20} + m(20,28)x^{20}y^{28} + m(20,32)x^{20}y^{32} + m(28,32)x^{28}y^{32} \\ + m(32,32)x^{32}y^{32} + m(32,36)x^{32}y^{36} + m(36,36)x^{36}y^{36} \\ = 6x^8y^{16} + 3x^{16}y^{16} + 6x^{16}y^{20} + 6x^{16}y^{28} + 3(n-5)x^{20}y^{20} + 6x^{20}y^{28} + 6(n-5)x^{20}y^{32} \\ + 6x^{28}y^{32} + 3(n-5)x^{32}y^{32} + 6(n-6)x^{32}y^{36} + \frac{3n^2-39n+126}{2}x^{36}y^{36} \quad \square$$

4.2.2. Neighborhood degree based topological indices of Triangular mesh T_n network

In this section we will find the neighborhood degree based topological indices using Table 1 and Theorem 3.3 for the triangular mesh T_n network.

Theorem 3.4. Let Γ be the graph of Triangular mesh T_n network, then

$$M'_1(\Gamma, x, y) = 108n^2 - 372n + 336 \\ M_2^*(\Gamma, x, y) = 1944n^2 - 10248n + 14496 \\ F_N^*(\Gamma, x, y) = 108n^2 - 372n + 336 \\ {}^{nm}M_2(\Gamma, x, y) = 0.001n^2 + 0.01n + 0.026 \\ NR_\alpha(\Gamma, x, y) = 3n^2 - 21n + 36 \cdot 32^\alpha + (12n - 48)20^\alpha + (-24 + 6n)36^\alpha \\ + 6 \cdot 8^\alpha + 24 \cdot 16^\alpha + 8 \cdot 24^\alpha + 18 \cdot 28^\alpha \\ ND_3(\Gamma, x, y) = 139968n^2 - 905280n + 1551360 \\ ND_5(\Gamma, x, y) = 3n^2 - 1.567n - 1.229 \\ NH(\Gamma, x, y) = 0.042n^2 + 0.109n + 0.062 \\ NI(\Gamma, x, y) = 1.5n^2 - 1.5n \\ S(\Gamma, x, y) = 9519.456n^2 - 62248.701n + 108665.21$$

Proof: Using Table 1 and Theorem 4.1, we have following computation

$$M'_1(\Gamma, x, y) = (D_x + D_y)(NM(\Gamma; x, y))|_{x=y=1} \\ = (108n^2x^{36}y^{36} - 1404nx^{36}y^{36} + 4536x^{36}y^{36} + 408nx^{32}y^{36} - 2448x^{32}y^{36} \\ + 192nx^{32}y^{32} - 960x^{32}y^{32} + 360x^{28}y^{32} + 312nx^{20}y^{32} - 1560x^{20}y^{32} + 288x^{20}y^{28} \\ + 264x^{16}y^{28} + 120nx^{20}y^{20} - 600x^{20}y^{20} + 216x^{16}y^{20} + 96x^{16}y^{16} + 144x^8y^{16})|_{x=y=1} \\ = 108n^2 - 372n + 336$$

$$M_2^*(\Gamma, x, y) = (D_x \cdot D_y)(NM(\Gamma; x, y))|_{x=y=1} \\ = (1944n^2x^{36}y^{36} - 25272nx^{36}y^{36} + 81648x^{36}y^{36} + 6912nx^{32}y^{36} - 41472$$

$$\begin{aligned} & x^{32}y^{36} + 3072 nx^{32}y^{32} - 15360 x^{32}y^{32} + 5376 x^{28}y^{32} + 3840 nx^{20}y^{32} - 19200 \\ & x^{20}y^{32} + 3360 x^{20}y^{28} + 2688 x^{16}y^{28} + 1200 nx^{20}y^{20} - 6000 x^{20}y^{20} + 1920 x^{16}y^{20} \\ & + \quad \quad \quad 768 \quad \quad \quad x^{16}y^{16} \quad \quad \quad + 768 \quad \quad \quad x^8y^{16})|_{x=y=1} \\ & = 1944 n^2 - 10248 n + 14496 \end{aligned}$$

$$\begin{aligned} F_N^*(\Gamma, x, y) &= (D_x^2 + D_y^2)(NM(\Gamma; x, y))|_{x=y=1} \\ &= (108 n^2 x^{36} y^{36} - 1404 nx^{36} y^{36} + 4536 x^{36} y^{36} + 408 nx^{32} y^{36} - 2448 x^{32} y^{36} \\ &+ 192 nx^{32} y^{32} - 960 x^{32} y^{32} + 360 x^{28} y^{32} + 312 nx^{20} y^{32} - 1560 x^{20} y^{32} + 288 \\ & x^{20} y^{28} + 264 x^{16} y^{28} + 120 nx^{20} y^{20} - 600 x^{20} y^{20} + 216 x^{16} y^{20} + 96 x^{16} y^{16} \\ &+ 144 x^8 y^{16})|_{x=y=1} \\ &= 108 n^2 - 372 n + 336 \end{aligned}$$

$$\begin{aligned} {}^{nm}M_2(\Gamma, x, y) &= (S_x S_y)(NM(\Gamma; x, y))|_{x=y=1} \\ &= (0.001 n^2 - 0.015 n + 0.049 + 0.005 n x^{32} y^{36} - 0.031 x^{32} y^{36} + 0.003 n x^{32} y^{32} \\ &- 0.015 x^{32} y^{32} + 0.007 x^{28} y^{32} + 0.009 n x^{20} y^{32} - 0.047 x^{20} y^{32} + 0.011 x^{20} y^{28} \\ &+ 0.013 x^{16} y^{28} + 0.008 n x^{20} y^{20} - 0.038 x^{20} y^{20} + 0.019 x^{16} y^{20} + 0.012 x^{16} y^{16} \\ &+ 0.047 x^8 y^{16})|_{x=y=1} \\ &= 0.001 n^2 + 0.01 n + 0.026 \end{aligned}$$

$$\begin{aligned} NR_\alpha(\Gamma, x, y) &= (D_x^\alpha + D_y^\alpha)(NM(\Gamma; x, y))|_{x=y=1} \\ &= 3 n^2 - 21 n + 36 32^\alpha + (12 n - 48) 20^\alpha + (-24 + 6 n) 36^\alpha \\ &+ 6 8^\alpha + 24 16^\alpha + 8 24^\alpha + 18 28^\alpha \end{aligned}$$

$$\begin{aligned} ND_3(\Gamma, x, y) &= D_x D_y (D_x + D_y)(NM(\Gamma; x, y))|_{x=y=1} \\ &= (139968 n^2 x^{36} y^{36} - 1819584 nx^{36} y^{36} + 5878656 x^{36} y^{36} + 470016 nx^{32} y^{36} \\ &- 2820096 x^{32} y^{36} + 196608 nx^{32} y^{32} - 983040 x^{32} y^{32} + 322560 x^{28} y^{32} \\ &+ 199680 nx^{20} y^{32} - 998400 x^{20} y^{32} + 161280 x^{20} y^{28} + 118272 x^{16} y^{28} \\ &+ 48000 nx^{20} y^{20} - 40000 x^{20} y^{20} + 69120 x^{16} y^{20} + 24576 x^{16} y^{16} \\ &+ 18432 x^8 y^{16})|_{x=y=1} \\ &= 139968 n^2 - 905280 n + 1551360 \end{aligned}$$

$$\begin{aligned} ND_5(\Gamma, x, y) &= (D_x S_y + D_y S_x)(NM(\Gamma; x, y))|_{x=y=1} \\ &= (3 n^2 - 1.3 n + 12.083 n x^{32} y^{36} + 6 n x^{32} y^{32} + 13.35 n x^{20} y^{32} + 6 n \\ & x^{20} y^{20} + 12.686 x^{20} y^{28} + 12.107 x^{28} y^{32} + 15 x^8 y^{16} + 6 x^{16} y^{16} + 12.3 x^{16} y^{20} \\ &+ 13.929 x^{16} y^{28} + 126 x^{36} y^{36} - 72.5 x^{32} y^{36} - 30 x^{32} y^{32} - 66.75 x^{20} y^{32} - \\ & 30 x^{20} y^{20})|_{x=y=1} \\ &= 3 n^2 - 1.567 n - 1.229 \end{aligned}$$

$$\begin{aligned} NH(\Gamma, x, y) &= 2(S_x)J(NM(\Gamma; x, y))|_{x=1} \\ &= (0.042 n^2 - 0.542 n + 1.75 x^{72} + 0.176 x^{68} n - 1.059 x^{68} + 0.094 x^{64} n \\ &- 0.469 x^{64} + 0.2 x^{60} + 0.231 x^{52} n - 1.154 x^{52} + 0.25 x^{48} + 0.273 x^{44} \\ &+ 0.15 x^{40} n - 0.75 x^{40} + 0.333 x^{36} + 0.188 x^{32} + 0.5 x^{24})|_{x=1} \\ &= 0.042 n^2 + 0.109 n + 0.062 \end{aligned}$$

$$\begin{aligned}
 NI(\Gamma, x, y) &= S_x J(D_x + D_y)(NM(\Gamma; x, y))|_{x=y=1} \\
 &= (1.5n^2 - 19.5n + 63x^{72} + 6x^{68}n - 36x^{68} + 3x^{64}n - 15x^{64} + 6x^{60} \\
 &\quad + 6x^{52}n - 30x^{52} + 6x^{48} + 6x^{44} + 3x^{40}n - 15x^{40} + 6x^{36} + 3x^{32} + 6 \\
 &\quad x^{24})|_{x=1} \\
 &= 1.5n^2 - 1.5n
 \end{aligned}$$

$$\begin{aligned}
 S(\Gamma, x, y) &= (S_x^3 Q_{-2} J D_x^3 D_y^3)(M(\Gamma; x, y))|_{x=1} \\
 &= (9519.456n^2 - 123752.932n + 399817.164x^{70} + 31906.332x^{66}n - \\
 &\quad 191437.992x^{66} + 13515.934x^{62}n - 67579.669x^{62} + 22120.315x^{58} \\
 &\quad + 12582.912x^{50}n - 62914.56x^{50} + 10825.347x^{46} + 7281.778x^{42} \\
 &\quad + 3499.052x^{38}n - 17495.262x^{38} + 5002.239x^{34} + 1864.135x^{30} + 1181.716 \\
 &\quad x^{22})|_{x=1} \\
 &= 9519.456n^2 - 62248.701n + 108665.21
 \end{aligned}$$

Star of Silicate Network SSL(n)

In the present subsection, we explore the degree-based topological descriptors for the star of silicate network [27]. We define the creation of a new star of a silicate network from the star of the David network in Figure 3.

Step 1: Construct a star of David graph H of dimension 1 (Figure3).

Step 2: By inserting $2n - 2$ vertices at every edge of H, divide each edge into $2n - 1$ edges.

Step 3: If one is the mirror image of the other and if they are at an odd distance $1, 3, 5, 7, \dots, (6n - 1)$ from one corner vertices except the pairs at a distance $(2n - 1)$, connect any two vertices u and v by an edge.

Step 4: At each new crossing of the edge, insert a new vertex. The resulting network is called the n -dimensional star of David network, denoted by $SD(n)$.

Step 5: Replacing each K_3 subgraph with a tetrahedron. This network is known as the n -dimension star silicate star or star of silicate network star and is denoted by $SSL(n)$. The graph for the $SSL(2)$ silicate network star is shown in Figure 4.

Throughout this section, we denote the graph of star silicate network $SSL(n)$ by G .

In the graph of star of silicate network, the 6 corner vertices and the central vertex of each tetrahedron are of degree 3. The vertices inserted in step two of the construction have degree 4. All the remaining vertices have

bdegree 6. Thus, the set of all distinct degrees d_u for $u \in V(SSL(n))$ is $\{3, 4, 6\}$. The following table gives the edge partition of G .

Table 4. Edge partition of Star of Silicate Network $SSL(n)$.

(δ_u, δ_v)	frequency
(11, 11)	6
(11, 14)	24
(14, 14)	6
(14, 17)	$(24n - 36)$
(14, 26)	$(12n - 24)$
(16, 19)	12
(16, 26)	12
(16, 28)	12
(17, 17)	$(24n - 60)$
(17, 19)	12
(17, 26)	$(24n - 48)$
(18, 26)	$(12n^2 - 48n + 48)$
(18, 28)	$(24n - 36)$
(18, 30)	$(24n^2 - 48n + 24)$
(19, 26)	12
(19, 28)	12
(26, 26)	$(6n^2 - 24n + 24)$
(26, 28)	12
(26, 30)	$(12n^2 - 48n + 48)$
(28, 28)	$(12n - 18)$
(28, 30)	$(24n - 36)$
(30, 30)	$(18n^2 - 36n + 18)$

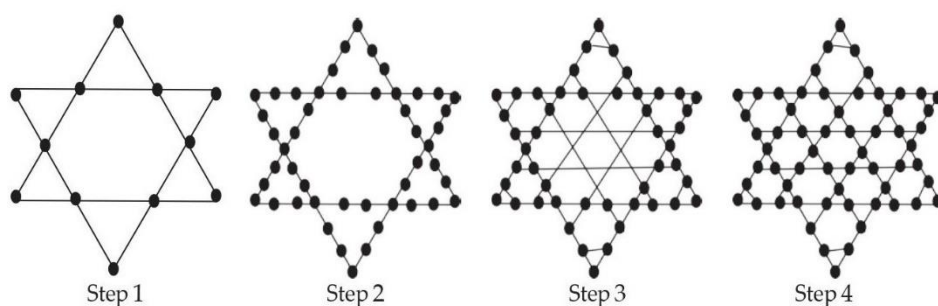


Figure 3. The construction of star of David graph of dimension 2.

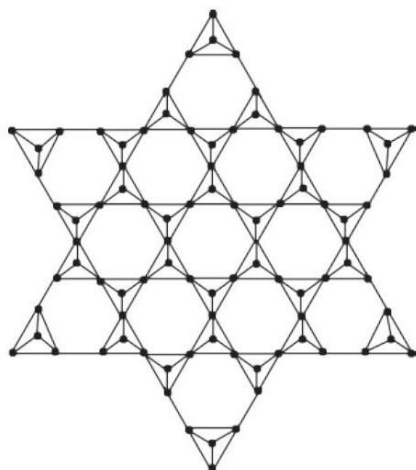


Figure 4. The graph of star of silicate network SSL(2).

NM-Polynomial of star of silicate network SSL(n)

In this section we will find the NM-Polynomial of silicate network SSL(n).

Theorem 3.5. Let Γ be the graph of star of silicate network SSL(n), then

$$\begin{aligned} NM(\Gamma, x, y) = & 6 x^{11} y^{11} + 24 x^{11} y^{14} + 6 x^{14} y^{14} + (24 n - 36) x^{14} y^{17} + (12 n \\ & - 24) x^{14} y^{26} + 12 x^{16} y^{19} + 12 x^{16} y^{26} + 12 x^{16} y^{28} + (24 n - 60) x^{17} y^{17} \\ & + 12 x^{17} y^{19} + (24 n - 48) x^{17} y^{26} + 12 n^2 - 48 n + 48 x^{18} y^{26} + (24 n \\ & - 36) x^{18} y^{28} + 24 n^2 - 48 n + 24 x^{18} y^{30} + 12 x^{19} y^{26} + 12 x^{19} y^{28} + 6 n^2 - \\ & 24 n + 24 x^{26} y^{26} + 12 x^{26} y^{28} + 12 n^2 - 48 n + 48 x^{26} y^{30} + (12 n - \\ & 18) x^{28} y^{28} + (24 n - 36) x^{28} y^{30} + 18 n^2 - 36 n + 18 x^{30} y^{30} \end{aligned}$$

Proof: Using Table 5 and definition of NM-polynomial, we have following computation

$$\begin{aligned} NM(\Gamma; x, y) &= \sum_{i \leq j} \Gamma_{i,j} x^i y^j \\ &= m(11,11)x^{11}y^{11} + m(11,14)x^{11}y^{14} + m(14,14)x^{14}y^{14} + m(14,17)x^{14}y^{17} \\ &+ m(14,26)x^{14}y^{26} + m(16,19)x^{16}y^{19} + m(16,26)x^{16}y^{26} + m(16,28)x^{16}y^{28} \\ &+ m(17,17)x^{17}y^{17} + m(17,19)x^{17}y^{19} + m(17,19)x^{17}y^{19} + m(17,26)x^{17}y^{26} \\ &+ m(18,26)x^{18}y^{26} + m(18,28)x^{18}y^{28} + m(18,30)x^{18}y^{30} + m(19,26)x^{19}y^{26} \\ &+ m(19,28)x^{19}y^{28} + m(26,26)x^{26}y^{26} + m(26,28)x^{26}y^{28} + m(26,30)x^{26}y^{30} \\ &+ m(28,28)x^{28}y^{28} + m(28,30)x^{28}y^{30} + m(30,30)x^{30}y^{30} \\ &= 6 x^{11} y^{11} + 24 x^{11} y^{14} + 6 x^{14} y^{14} + (24 n - 36) x^{14} y^{17} + (12 n - 24) x^{14} y^{26} \\ &+ 12 x^{16} y^{19} + 12 x^{16} y^{26} + 12 x^{16} y^{28} + (24 n - 60) x^{17} y^{17} + 12 x^{17} y^{19} + (24 n \\ &- 48) x^{17} y^{26} + 12 n^2 - 48 n + 48 x^{18} y^{26} + (24 n - 36) x^{18} y^{28} + 24 n^2 - 48 n \\ &+ 24 x^{18} y^{30} + 12 x^{19} y^{26} + 12 x^{19} y^{28} + 6 n^2 - 24 n + 24 x^{26} y^{26} + 12 x^{26} y^{28} \\ &+ 12 n^2 - 48 n + 48 x^{26} y^{30} + (12 n - 18) x^{28} y^{28} + (24 n - 36) x^{28} y^{30} + 18 \\ &n^2 - 36 n + 18 x^{30} y^{30} \end{aligned}$$

Neighborhood degree based topological indices of star of silicate network SSL(n)

□

In this section we will find the neighborhood degree based topological indices of Table 1 for the silicate network SSL(n).

Theorem 3.6. Let Γ be the graph of star of silicate network SSL(n), then

$$M'_1(\Gamma, x, y) = 3744 n^2 - 4272 n + 1884$$

$$M_2^*(\Gamma, x, y) = 48192 n^2 - 65160 n + 31470$$

$$F_N^*(\Gamma, x, y) = 0.114 n^2 + 0.034 n + 0.025$$

$$NR_\alpha(\Gamma, x, y) = 3 n^2 - 21 n + 36 \cdot 32^\alpha + (12 n - 48) 20^\alpha + (-24 + 6 n) 36^\alpha \\ + 6 \cdot 8^\alpha + 24 \cdot 16^\alpha + 18 \cdot 28^\alpha$$

$$ND_3(\Gamma, x, y) = 2576256 n^2 - 3820560 n + 1920348$$

$$ND_5(\Gamma, x, y) = 152.287 n^2 - 125.42 n + 46.714$$

$$NH(\Gamma, x, y) = 0.537 - 1.043 n + 2.805 n^2$$

$$NI(\Gamma, x, y) = 72 n^2 - 60 n + 24$$

$$S(\Gamma, x, y) = -257183.062 n + 130224.908 + 173674.325 n^2$$

Proof: Using Table 1 and Theorem 5.1, we have following computation

$$M'_1(\Gamma, x, y) = (D_x + D_y)(NM(\Gamma; x, y))|_{x=y=1} \\ = (1080 n^2 x^{30} y^{30} - 2160 n x^{30} y^{30} + 1080 x^{30} y^{30} + 1392 n x^{28} y^{30} + 672 n^2 x^{26} y^{30} \\ - 2088 x^{28} y^{30} + 672 n x^{28} y^{28} - 2688 n x^{26} y^{30} - 1008 x^{28} y^{28} + 2688 x^{26} y^{30} \\ + 312 n^2 x^{26} y^{26} + 648 x^{26} y^{28} - 1248 n x^{26} y^{26} + 1248 x^{26} y^{26} + 1152 n^2 x^{18} y^{30} \\ - 2304 n x^{18} y^{30} + 1152 x^{18} y^{30} + 1104 n x^{18} y^{28} + 564 x^{19} y^{28} + 528 n^2 x^{18} y^{26} \\ - 1656 x^{18} y^{28} - 2112 n x^{18} y^{26} + 540 x^{19} y^{26} + 1032 n x^{17} y^{26} + 2112 x^{18} y^{26} + 528 \\ x^{16} y^{28} - 2064 x^{17} y^{26} + 504 x^{16} y^{26} + 480 n x^{14} y^{26} - 960 x^{14} y^{26} + 432 x^{17} y^{19} + 816 \\ n x^{17} y^{17} + 420 x^{16} y^{19} - 2040 x^{17} y^{17} + 744 n x^{14} y^{17} - 1116 x^{14} y^{17} + 168 x^{14} y^{14} + \\ 600 x^{11} y^{14} + 132 x^{11} y^{11})|_{x=y=1} \\ = 3744 n^2 - 4272 n + 1884$$

$$M_2^*(\Gamma, x, y) = (D_x \cdot D_y)(NM(\Gamma; x, y))|_{x=y=1} \\ = (16200 n^2 x^{30} y^{30} - 32400 n x^{30} y^{30} + 16200 x^{30} y^{30} + 20160 n x^{28} y^{30} \\ + 9360 n^2 x^{26} y^{30} - 30240 x^{28} y^{30} + 9408 n x^{28} y^{28} - 37440 n x^{26} y^{30} - 14112 x^{28} y^{28} \\ + 37440 x^{26} y^{30} + 4056 n^2 x^{26} y^{26} + 8736 x^{26} y^{28} - 16224 n x^{26} y^{26} + 16224 x^{26} y^{26} \\ + 12960 n^2 x^{18} y^{30} - 25920 n x^{18} y^{30} + 12960 x^{18} y^{30} + 12096 n x^{18} y^{28} + 6384 \\ x^{19} y^{28} + 5616 n^2 x^{18} y^{26} - 18144 x^{18} y^{28} - 22464 n x^{18} y^{26} + 5928 x^{19} y^{26} + 10608 \\ n x^{17} y^{26} + 22464 x^{18} y^{26} + 5376 x^{16} y^{28} - 21216 x^{17} y^{26} + 4992 x^{16} y^{26} + 4368 \\ n x^{14} y^{26} - 8736 x^{14} y^{26} + 3876 x^{17} y^{19} + 6936 n x^{17} y^{17} + 3648 x^{16} y^{19} - 17340 x^{17} y^{17}$$

$$\begin{aligned}
 & + 5712 \, nx^{14}y^{17} - 8568 \, x^{14}y^{17} + 1176 \, x^{14}y^{14} + 3696 \, x^{11}y^{14} + 726 \, x^{11}y^{11})|_{x=y=1} \\
 & = 48192 \, n^2 - 65160 \, n + 31470
 \end{aligned}$$

$$\begin{aligned}
 F_N^*(\Gamma, x, y) &= (D_x^2 + D_y^2)(NM(\Gamma; x, y))|_{x=y=1} \\
 &= (1080 \, n^2x^{30}y^{30} - 2160 \, nx^{30}y^{30} + 1080 \, x^{30}y^{30} + 1392 \, nx^{28}y^{30} + 672 \, n^2x^{26}y^{30} \\
 &\quad - 2088 \, x^{28}y^{30} + 672 \, nx^{28}y^{28} - 2688 \, nx^{26}y^{30} - 1008 \, x^{28}y^{28} + 2688 \, x^{26}y^{30} \\
 &\quad + 312 \, n^2x^{26}y^{26} + 648 \, x^{26}y^{28} - 1248 \, nx^{26}y^{26} + 1248 \, x^{26}y^{26} + 1152 \, n^2x^{18}y^{30} \\
 &\quad - 2304 \, nx^{18}y^{30} + 1152 \, x^{18}y^{30} + 1104 \, nx^{18}y^{28} + 564 \, x^{19}y^{28} + 528 \, n^2x^{18}y^{26} \\
 &\quad - 1656 \, x^{18}y^{28} - 2112 \, nx^{18}y^{26} + 540 \, x^{19}y^{26} + 1032 \, nx^{17}y^{26} + 2112 \, x^{18}y^{26} \\
 &\quad + 528 \, x^{16}y^{28} - 2064 \, x^{17}y^{26} + 504 \, x^{16}y^{26} + 480 \, nx^{14}y^{26} - 960 \, x^{14}y^{26} + 432 \, x^{17}y^{19} \\
 &\quad + 816 \, nx^{17}y^{17} + 420 \, x^{16}y^{19} - 2040 \, x^{17}y^{17} + 744 \, nx^{14}y^{17} - 1116 \, x^{14}y^{17} \\
 &\quad + 168 \, x^{14}y^{14} + 600 \, x^{11}y^{14} + 132 \, x^{11}y^{11})|_{x=y=1} \\
 &= 3744 \, n^2 - 4272 \, n + 1884
 \end{aligned}$$

$$\begin{aligned}
 {}^{nm}M_2(\Gamma, x, y) &= (S_x S_y)(NM(\Gamma; x, y))|_{x=y=1} \\
 &= (0.044 \, n^2x^{18}y^{30} - 0.089 \, nx^{18}y^{30} + 0.048 \, x^{18}y^{28} + 0.026 \, n^2x^{18}y^{26} \\
 &\quad - 0.103 \, nx^{18}y^{26} + 0.054 \, nx^{17}y^{26} + 0.033 \, nx^{14}y^{26} + 0.083 \, nx^{17}y^{17} + 0.101 \, nx^{14}y^{17} \\
 &\quad - 0.04 \, x^{30}y^{30} + 0.029 \, x^{28}y^{30} + 0.015 \, n^2x^{26}y^{30} + 0.015 \, nx^{28}y^{28} - 0.062 \, nx^{26}y^{30} \\
 &\quad + 0.009 \, n^2x^{26}y^{26} - 0.036 \, nx^{26}y^{26} + 0.02 \, n^2x^{30}y^{30} - 0.109 \, x^{17}y^{26} + 0.016 \, x^{26}y^{28} \\
 &\quad + 0.023 \, x^{19}y^{28} + 0.024 \, x^{19}y^{26} + 0.037 \, x^{17}y^{19} + 0.039 \, x^{16}y^{19} + 0.029 \, x^{16}y^{26} \\
 &\quad + 0.027 \, x^{16}y^{28} + 0.05 \, x^{11}y^{11} + 0.156 \, x^{11}y^{14} + 0.031 \, x^{14}y^{14} + 0.02 \, x^{30}y^{30} \\
 &\quad - 0.043 \, x^{28}y^{30} - 0.023 \, x^{28}y^{28} + 0.062 \, x^{26}y^{30} + 0.036 \, x^{26}y^{26} + 0.044 \, x^{18}y^{30} \\
 &\quad - 0.066 \, x^{14}y^{26} - 0.208 \, x^{17}y^{17} - 0.151 \, x^{14}y^{17} + 0.103 \, x^{18}y^{26} - 0.071 \, x^{18}y^{28})|_{x=y=1} \\
 &= 0.114 \, n^2 + 0.034 \, n + 0.025
 \end{aligned}$$

$$\begin{aligned}
 NR_\alpha(\Gamma, x, y) &= (D_x^\alpha + D_y^\alpha)(NM(\Gamma; x, y))|_{x=y=1} \\
 &= 3 \, n^2 - 21 \, n + 36 \, 32^\alpha + (12 \, n - 48) \, 20^\alpha + (-24 + 6 \, n) \, 36^\alpha + 6 \, 8^\alpha \\
 &\quad + 24 \, 16^\alpha + 18 \, 28^\alpha
 \end{aligned}$$

$$\begin{aligned}
 ND_3(\Gamma, x, y) &= D_x D_y (D_x + D_y)(NM(\Gamma; x, y))|_{x=y=1} \\
 &= (972000 \, n^2x^{30}y^{30} - 1944000 \, nx^{30}y^{30} + 972000 \, x^{30}y^{30} + 1169280 \, nx^{28}y^{30} \\
 &\quad + 524160 \, n^2x^{26}y^{30} - 1753920 \, x^{28}y^{30} + 526848 \, nx^{28}y^{28} - 2096640 \, nx^{26}y^{30} \\
 &\quad - 790272 \, x^{28}y^{28} + 2096640 \, x^{26}y^{30} + 210912 \, n^2x^{26}y^{26} + 471744 \, x^{26}y^{28} \\
 &\quad - 843648 \, nx^{26}y^{26} + 843648 \, x^{26}y^{26} + 622080 \, n^2x^{18}y^{30} - 1244160 \, nx^{18}y^{30} \\
 &\quad + 622080 \, x^{18}y^{30} + 556416 \, nx^{18}y^{28} + 300048 \, x^{19}y^{28} + 247104 \, n^2x^{18}y^{26} - \\
 &\quad 834624 \, x^{18}y^{28} - 988416 \, nx^{18}y^{26} + 266760 \, x^{19}y^{26} + 456144 \, nx^{17}y^{26} \\
 &\quad + 988416 \, x^{18}y^{26} + 236544 \, x^{16}y^{28} - 912288 \, x^{17}y^{26} + 209664 \, x^{16}y^{26} \\
 &\quad + 174720 \, nx^{14}y^{26} - 349440 \, x^{14}y^{26} + 139536 \, x^{17}y^{19} + 235824 \, nx^{17}y^{17} \\
 &\quad + 127680 \, x^{16}y^{19} - 589560 \, x^{17}y^{17} + 177072 \, nx^{14}y^{17} - 265608 \, x^{14}y^{17} + 32928
 \end{aligned}$$

$$\begin{aligned} & x^{14}y^{14} + 92400 x^{11}y^{14} + 15972 x^{11}y^{11})|_{x=y=1} \\ & = 2576256 n^2 - 3820560 n + 1920348 \end{aligned}$$

$$\begin{aligned} ND_5(\Gamma, x, y) &= (D_x S_y + D_y S_x)(NM(\Gamma; x, y))|_{x=y=1} \\ &= (54.4 n^2 x^{18} y^{30} - 108.8 n x^{18} y^{30} + 52.762 n x^{18} y^{28} + 25.641 n^2 x^{18} y^{26} \\ &\quad - 102.564 n x^{18} y^{26} + 52.398 n x^{17} y^{26} + 28.747 n x^{14} y^{26} + 48 n x^{17} y^{17} \\ &\quad + 48.908 n x^{14} y^{17} - 72 n x^{30} y^{30} + 48.114 n x^{28} y^{30} + 24.246 n^2 x^{26} y^{30} + 24 \\ &\quad n x^{28} y^{28} - 96.985 n x^{26} y^{30} + 12 n^2 x^{26} y^{26} - 48 n x^{26} y^{26} + 36 n^2 x^{30} y^{30} - 104.796 \\ &\quad x^{17} y^{26} + 24.066 x^{26} y^{28} + 25.827 x^{19} y^{28} + 25.19 x^{19} y^{26} + 24.149 x^{17} y^{19} + 24.355 \\ &\quad x^{16} y^{19} + 26.885 x^{16} y^{26} + 27.857 x^{16} y^{28} + 12 x^{11} y^{11} + 49.403 x^{11} y^{14} + 12 x^{14} y^{14} \\ &\quad + 36 x^{30} y^{30} - 72.171 x^{28} y^{30} - 36 x^{28} y^{28} + 96.985 x^{26} y^{30} + 48 x^{26} y^{26} + 54.4 \\ &\quad x^{18} y^{30} - 57.495 x^{14} y^{26} - 120 x^{17} y^{17} - 73.361 x^{14} y^{17} + 102.564 x^{18} y^{26} - \\ &\quad 79.143 x^{18} y^{28})|_{x=y=1} \\ &= 152.287 n^2 - 125.42 n + 46.714 \end{aligned}$$

$$\begin{aligned} NH(\Gamma, x, y) &= 2(S_x)J(NM(\Gamma; x, y))|_{x=1} \\ &= (0.429 x^{28} + 0.828 x^{58} n + 1.043 x^{46} n + 1.116 x^{43} n + 0.6 x^{40} n + 1.412 x^{34} n \\ &\quad + 1.548 n x^{31} + 0.6 n^2 x^{60} - 1.2 n x^{60} + 0.429 n^2 x^{56} - 1.286 n x^{56} + 0.231 n^2 x^{52} \\ &\quad - 0.923 n x^{52} + n^2 x^{48} - 2 n x^{48} + 0.545 n^2 x^{44} - 2.182 n x^{44} - 2.323 x^{31} - 1.2 x^{40} \\ &\quad - 3.529 x^{34} - 2.233 x^{43} - 1.565 x^{46} + x^{48} + 0.923 x^{52} + 1.071 x^{56} - 1.241 x^{58} \\ &\quad + 0.6 x^{60} + 0.545 x^{22} + 1.92 x^{25} + 0.686 x^{35} + 0.571 x^{42} + 2.727 x^{44} + 0.667 x^{36} \\ &\quad + 0.533 x^{45} + 0.511 x^{47} + 0.444 x^{54})|_{x=1} \\ &= 0.537 - 1.043 n + 2.805 n^2 \end{aligned}$$

$$\begin{aligned} NI(\Gamma, x, y) &= S_x J(D_x + D_y)(NM(\Gamma; x, y))|_{x=y=1} \\ &= (18 n^2 x^{60} - 36 n x^{60} + 18 x^{60} + 24 x^{58} n + 12 n^2 x^{56} - 36 x^{58} - 36 n x^{56} \\ &\quad + 30 x^{56} + 6 n^2 x^{52} + 12 x^{54} - 24 n x^{52} + 24 x^{52} + 24 n^2 x^{48} - 48 n x^{48} + 24 x^{48} \\ &\quad + 24 x^{46} n + 12 x^{47} + 12 n^2 x^{44} - 36 x^{46} - 48 n x^{44} + 12 x^{45} + 24 x^{43} n + 60 x^{44} \\ &\quad - 48 x^{43} + 12 x^{42} + 12 x^{40} n - 24 x^{40} + 12 x^{36} + 24 x^{34} n + 12 x^{35} - 60 x^{34} + \\ &\quad 24 x^{31} n - 36 x^{31} + 6 x^{28} + 24 x^{25} + 6 x^{22})|_{x=1} \\ &= 72 n^2 - 60 n + 24 \end{aligned}$$

$$\begin{aligned} S(\Gamma, x, y) &= (S_x^3 Q_{-2} J D_x^3 D_y^3)(M(\Gamma; x, y))|_{x=1} \\ &= (-134507.36 x^{58} n - 77651.352 x^{46} n + 81000 n x^{56} + 36069.89 n x^{44} \\ &\quad - 21094.275 x^{38} + 9381.239 x^{33} - 44197.209 x^{32} - 19899.372 x^{29} + 2570.392 \\ &\quad x^{26} + 7204.269 x^{23} + 1328.671 x^{20} + 59311.829 x^{50} - 60139.038 x^{41} \\ &\quad + 67253.68 x^{58} n^2 + 36164.609 x^{54} n^2 - 107934.59 x^{54} n + 14827.957 x^{50} n^2 \\ &\quad - 59311.829 x^{50} n + 38825.676 x^{46} n^2 + 16602.402 x^{42} n^2 - 66409.609 x^{42} n \\ &\quad + 30069.519 x^{41} n + 10547.137 x^{38} n + 17678.884 x^{32} n + 13266.248 x^{29} n \\ &\quad + 13498.368 x^{40} + 10288.5 x^{34} + 18195.195 x^{43} + 38825.676 x^{46} + 32928 x^{52} \\ &\quad - 121500 x^{56} + 67253.68 x^{58} + 80973.165 x^{42} - 54104.835 x^{44} + 19827.986 x^{45} \end{aligned}$$

$$+ 89572.668 x^{54})|_{x=1}$$

$$= -257183.062 n + 130224.908 + 173674.325 n^2$$

Rhenium Trioxide Lattice $RO(m, n, r)$

We review the neighborhood degree-based topological descriptors for the $RO(p, q, r)$ rhenium trioxide lattice in this subsection [28]. It consists of rhenium atoms and oxygen atoms and is an inorganic compound. Rhenium trioxide is a red solid with a metallic cluster and a primitive cubic unit cell forming a crystal, that is, the ReO_3 unit cell. Rhenium atoms are the vertices marked in a hollow circle, and oxygen atoms are the vertices identified in the solid circles. The unit cell ReO_3 includes oxygen atoms of 12 and rhenium atoms of 8 (Figure 5).

By ReO_3 , we represent $p \times q \times rReO_3$ lattice. It is a three-dimensional sequence of p unit cell rows along the X-axis, q unit cell columns along the Y-axis, and r unit cell pages along the Z-axis.

The $RO(p, q, r)$ graph is the $RO(p, q, r)$ rhenium trioxide graph, which is constructed as follows:

Step 1: We draw a 3d-grid $M(p, q, r)$, which is described by the Cartesian product of paths $P_p \times P_q \times P_r$. Such vertices refer to atoms of rhenium.

Step 2: Subdivide each of the $M(p, q, r)$ edges in this step. Oxygen atoms correspond to the new vertices. We are now going to mark the vertices of $RO(p, q, r)$. The rhenium atoms will obtain the same 3d-grid mark as the vertices. Between two rhenium atoms (a', b', c') and (a'', b'', c'') , the oxygen atom will receive the label (a, b, c) , where $a \approx (a' + a'')/2$, $b \approx (b' + b'')/2$, and $c \approx (c' + c'')/2$. Two vertices (x', y', z') and (x'', y'', z'') are adjacent if $|(x' - x'') + (y' - y'') + (z' - z'')| \approx 1/2$. The number of vertices and edges in $RO(p, q, r)$ are $4pqr - pq - qr - pr$ and $6pqr - 2pq - 2qr - 2pr$, respectively. Throughout this section, G denotes the graph of rhenium trioxide $RO(p, q, r)$.

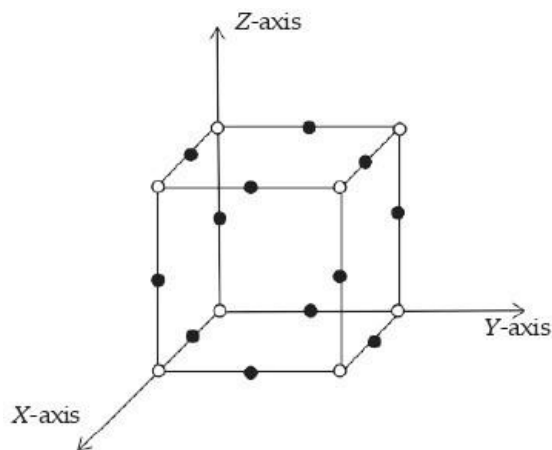


Figure 5. The unit cell of rhenium trioxide lattice ReO_3 .

Table 5. Edge partition of Rhenium Trioxide Lattice $RO(m, n, r)$.

(δ_u, δ_v)	frequency
(6, 7)	24
(7, 8)	24
(8, 8)	$8(m + n + r - 9)$
(8, 9)	$8(m + n + r - 6)$
(9, 10)	$8(m + n + r - 6)$
(10, 10)	$8(mn + nr + mr - 5m - 5n - 5r + 18)$
(10, 11)	$2(mn + nr + mr - 4m - 4n - 4r + 12)$
(12, 12)	$2(3mnr - 7mn - 7nr - 7mr + 16m + 16n + 16r - 36)$

NM-Polynomial of rhenium trioxide $RO(m, n, r)$

In this section we will find the NM-Polynomial of the rhenium trioxide.

Theorem 3.7. Let Γ be the graph of rhenium trioxide $RO(p, q, r)$, then

$$\begin{aligned}
 NM(\Gamma, x, y) = & 24 x^6 y^7 + 24 x^7 y^8 + 8(m + n + r - 9) x^8 y^8 + 8(m + n + r - 6) x^8 y^9 \\
 & + 8(m + n + r - 6) x^9 y^{10} + 8(mn + mr + nr - 5m - 5n - 5r + 18) x^{10} y^{10} \\
 & + 2(mn + mr + nr - 4m - 4n - 4r + 12) x^{10} y^{11} + 2(3mnr - 7mn - 7mr - 7nr + 16m + 16n + 16r - 36) x^{12} y^{12}
 \end{aligned}$$

Proof: Using Table 5 and definition of NM-polynomial, we have following computation

$$\begin{aligned}
 NM(\Gamma; x, y) &= \sum \Gamma_{i,j} x^i y^j \\
 &= m(6,7) x^6 y^7 + m(7,8) x^7 y^8 + m(8,8) x^8 y^8 + m(8,9) x^8 y^9 \\
 &+ m(9,10) x^9 y^{10} + m(10,10) x^{10} y^{10} + m(10,11) x^{10} y^{11} + m(12,12) x^{12} y^{12} \\
 &= 24 x^6 y^7 + 24 x^7 y^8 + 8(m + n + r - 9) x^8 y^8 + 8(m + n + r - 6) x^8 y^9 \\
 &+ 8(m + n + r - 6) x^9 y^{10} + 8(mn + mr + nr - 5m - 5n - 5r + 18) x^{10} y^{10} \\
 &+ 2(mn + mr + nr - 4m - 4n - 4r + 12) x^{10} y^{11} + 2(3mnr - 7mn - 7mr - 7nr + 16m + 16n + 16r - 36) x^{12} y^{12}
 \end{aligned}$$

$$7mn - 7mr - 7nr + 16m + 16n + 16r - 36)x^{12}y^{12}$$

□

4.4.2 Neighborhood degree based topological indices of rhenium trioxide $RO(m, n, r)$.

In this section we will find the neighborhood degree based indices listed in Table1 for the rhenium trioxide.

Theorem 3.8. Let Γ be the graph of rhenium trioxide $RO(m, n, r)$, then

$$M'_1(\Gamma, x, y) = 216m - 134mn + 144mnr - 134mr + 216n - 134nr + 216r - 552$$

$$M'_2(\Gamma, x, y) = 1536m - 996mn + 864mnr - 996mr + 1536n - 996nr + 1536r - 3360$$

$$F_N^*(\Gamma, x, y) = 216m - 134mn + 144mnr - 134mr + 216n - 134nr + 216r - 552$$

$${}^{nm}M_2(\Gamma, x, y) = 0.074n + 0.074r + 0.001mn + 0.001nr + 0.074m - 0.167 + 0.001mr + 0.042mnr$$

$$NR_\alpha(\Gamma, x, y) = 3n^2 - 21n + 36 \cdot 2^\alpha + (12n - 48) \cdot 20^\alpha + (-24 + 6n) \cdot 36^\alpha + 6 \cdot 8^\alpha + 24 \cdot 16^\alpha + 18 \cdot 28^\alpha$$

$$ND_3(\Gamma, x, y) = 43776m - 27764mn + 20736mnr - 27764mr + 43776n - 27764nr + 43776r - 86688$$

$$ND_5(\Gamma, x, y) = 16.127n + 16.127r - 7.982mn - 7.982nr + 16.127m - 47.982 - 7.982mr + 12mnr$$

$$NH(\Gamma, x, y) = 0.688n + 0.688r - 0.176mn - 0.176nr + 0.688m - 2.122 - 0.176mr + 12mnr$$

$$NI(\Gamma, x, y) = 8m - 4mn + 6mnr - 4mr + 8n - 4nr + 8r - 24$$

$$S(\Gamma, x, y) = 3398.591n + 3398.591r - 2166.129mn - 6896.939 - 2166.129nr + 3398.591m - 2166.129mr + 1682.56mnr$$

Proof: Using Table 1 and Theorem 6.1, we have following computation

$$\begin{aligned} M'_1(\Gamma, x, y) &= (D_x + D_y)(NM(\Gamma; x, y))|_{x=y=1} \\ &= (768mx^{12}y^{12} - 336mnx^{12}y^{12} + 144mnrx^{12}y^{12} - 336mr x^{12}y^{12} + 768nx^{12}y^{12} \\ &\quad - 336nr x^{12}y^{12} + 768rx^{12}y^{12} - 1728x^{12}y^{12} - 168mx^{10}y^{11} + 42mnx^{10}y^{11} + 42 \\ &\quad mrx^{10}y^{11} - 168nx^{10}y^{11} + 42nr x^{10}y^{11} - 168rx^{10}y^{11} - 800mx^{10}y^{10} + 160 \\ &\quad x^{10}y^{10}mn + 160x^{10}y^{10}mr - 800nx^{10}y^{10} + 160x^{10}y^{10}nr - 800x^{10}y^{10}r + 504 \\ &\quad x^{10}y^{11} + 152mx^9y^{10} + 152nx^9y^{10} + 152x^9y^{10}r + 2880x^{10}y^{10} - 912x^9y^{10} \\ &\quad + 136mx^8y^9 + 136nx^8y^9 + 136x^8y^9r + 128x^8y^8m + 128x^8y^8n + 128x^8y^8r \\ &\quad - 816x^8y^9 - 1152x^8y^8 + 360x^7y^8 + 312x^6y^7)|_{x=y=1} \\ &= 216m - 134mn + 144mnr - 134mr + 216n - 134nr + 216r - 552 \end{aligned}$$

$$\begin{aligned} M'_2(\Gamma, x, y) &= (D_x \cdot D_y)(NM(\Gamma; x, y))|_{x=y=1} \\ &= (4608mx^{12}y^{12} - 2016mnx^{12}y^{12} + 864mnrx^{12}y^{12} - 2016mr x^{12}y^{12} + \end{aligned}$$

$$\begin{aligned}
 & 4608 \, nx^{12}y^{12} - 2016 \, nrx^{12}y^{12} + 4608 \, rx^{12}y^{12} - 10368 \, x^{12}y^{12} - 880 \, mx^{10}y^{11} + \\
 & 220 \, mnx^{10}y^{11} + 220 \, mrx^{10}y^{11} - 880 \, nx^{10}y^{11} + 220 \, nrx^{10}y^{11} - 880 \, rx^{10}y^{11} - \\
 & 4000 \, mx^{10}y^{10} + 800 \, x^{10}y^{10}mn + 800 \, x^{10}y^{10}mr - 4000 \, nx^{10}y^{10} + 800 \\
 & x^{10}y^{10}nr - 4000 \, x^{10}y^{10}r + 2640 \, x^{10}y^{11} + 720 \, mx^9y^{10} + 720 \, nx^9y^{10} + 720 \\
 & x^9y^{10}r + 14400 \, x^{10}y^{10} - 4320 \, x^9y^{10} + 576 \, mx^8y^9 + 576 \, nx^8y^9 + 576 \, x^8y^9r + \\
 & 512 \, x^8y^8m + 512 \, x^8y^8n + 512 \, x^8y^8r - 3456 \, x^8y^9 - 4608 \, x^8y^8 + 1344 \, x^7y^8 + \\
 & 1008 \, x^6y^7)|_{x=y=1} \\
 & = 1536 \, m - 996 \, mn + 864 \, mnr - 996 \, mr + 1536 \, n - 996 \, nr + 1536 \, r - \\
 & 3360
 \end{aligned}$$

$$\begin{aligned}
 F_N^*(\Gamma, x, y) &= (D_x^2 + D_y^2)(NM(\Gamma; x, y))|_{x=y=1} \\
 &= (768 \, mx^{12}y^{12} - 336 \, mn \, x^{12}y^{12} + 144 \, mnr \, x^{12}y^{12} - 336 \, mr \, x^{12}y^{12} + 768 \\
 &nx^{12}y^{12} - 336 \, nrx^{12}y^{12} + 768 \, rx^{12}y^{12} - 1728 \, x^{12}y^{12} - 168 \, mx^{10}y^{11} + 42 \\
 &mnx^{10}y^{11} + 42 \, mrx^{10}y^{11} - 168 \, nx^{10}y^{11} + 42 \, nrx^{10}y^{11} - 168 \, rx^{10}y^{11} - 800 \, mx^{10}y^{10} \\
 &+ 160 \, mnx^{10}y^{10} + 160 \, mrx^{10}y^{10} - 800 \, nx^{10}y^{10} + 160 \, nrx^{10}y^{10} - 800 \, x^{10}y^{10}r \\
 &+ 504 \, x^{10}y^{11} + 152 \, mx^9y^{10} + 152 \, nx^9y^{10} + 152 \, x^9y^{10}r + 2880 \, x^{10}y^{10} - 912 \\
 &x^9y^{10} + 136 \, mx^8y^9 + 136 \, nx^8y^9 + 136 \, x^8y^9r + 128 \, x^8y^8m + 128 \, x^8y^8n + 128 \\
 &x^8y^8r - 816 \, x^8y^9 - 1152 \, x^8y^8 + 360 \, x^7y^8 + 312 \, x^6y^7)|_{x=y=1} \\
 &= 216 \, m - 134 \, mn + 144 \, mnr - 134 \, mr + 216 \, n - 134 \, nr + 216 \, r - 552
 \end{aligned}$$

$$\begin{aligned}
 {}^{nm}M_2(\Gamma, x, y) &= (S_x S_y)(NM(\Gamma; x, y))|_{x=y=1} \\
 &= (0.125x^8y^8m + 0.125x^8y^8n + 0.222mx^{12}y^{12} + 0.222nx^{12}y^{12} - \\
 &0.073mx^{10}y^{11} - 0.073nx^{10}y^{11} - 0.073rx^{10}y^{11} - 0.4mx^{10}y^{10} - 0.4nx^{10}y^{10} + \\
 &0.089mx^9y^{10} + 0.089nx^9y^{10} + 0.111mx^8y^9 + 0.111nx^8y^9 + 0.571x^6y^7 + \\
 &0.429x^7y^8 - 1.125x^8y^8 - 0.5x^{12}y^{12} - 0.533x^9y^{10} + 1.44x^{10}y^{10} - 0.667x^8y^9 + \\
 &0.222rx^{12}y^{12} + 0.125x^8y^8r + 0.111x^8y^9r + 0.089x^9y^{10}r - 0.4x^{10}y^{10}r - \\
 &0.097nrx^{12}y^{12} + 0.018mnx^{10}y^{11} + 0.018mrx^{10}y^{11} + 0.018nrx^{10}y^{11} + \\
 &0.08mnx^{10}y^{10} + 0.08mrx^{10}y^{10} + 0.08nrx^{10}y^{10} - 0.097mnx^{12}y^{12} \\
 &+ 0.042mnrx^{12}y^{12} - 0.097mrx^{12}y^{12} + 0.218x^{10}y^{11})|_{x=y=1} \\
 &= 0.074 \, n + 0.074 \, r + 0.001 \, mn + 0.001 \, nr + 0.074 \, m - 0.167 + 0.001 \, mr + \\
 &0.042 \, mnr
 \end{aligned}$$

$$\begin{aligned}
 NR_\alpha(\Gamma, x, y) &= (D_x^\alpha + D_y^\alpha)(NM(\Gamma; x, y))|_{x=y=1} \\
 &= 3 \, n^2 - 21 \, n + 36 \, 32^\alpha + (12 \, n - 48) \, 20^\alpha + (-24 + 6 \, n) \, 36^\alpha + 6 \, 8^\alpha \\
 &\quad + 24 \, 16^\alpha + 18 \, 28^\alpha
 \end{aligned}$$

$$\begin{aligned}
 ND_3(\Gamma, x, y) &= D_x D_y (D_x + D_y)(NM(\Gamma; x, y))|_{x=y=1} \\
 &= (110592 \, mx^{12}y^{12} - 48384 \, mn \, x^{12}y^{12} + 20736 \, mnr \, x^{12}y^{12} - 48384 \, mr \, x^{12}y^{12} \\
 &+ 110592 \, nx^{12}y^{12} - 48384 \, nr \, x^{12}y^{12} + 110592 \, rx^{12}y^{12} - 248832 \, x^{12}y^{12} - 18480 \\
 &mx^{10}y^{11} + 4620 \, mn \, x^{10}y^{11} + 4620 \, mr \, x^{10}y^{11} - 18480 \, nx^{10}y^{11} + 4620 \, nr \, x^{10}y^{11} \\
 &- 18480 \, rx^{10}y^{11} - 80000 \, mx^{10}y^{10} + 16000 \, mn \, x^{10}y^{10} + 16000 \, mr \, x^{10}y^{10} - 80000 \\
 &nx^{10}y^{10} + 16000 \, nr \, x^{10}y^{10} - 80000 \, x^{10}y^{10}r + 55440 \, x^{10}y^{11} + 13680 \, mx^9y^{10}
 \end{aligned}$$

$$\begin{aligned}
 & +13680 \, nx^9y^{10} + 13680 \, x^9y^{10}r + 288000 \, x^{10}y^{10} - 82080 \, x^9y^{10} + 9792 \, mx^8y^9 \\
 & +9792 \, nx^8y^9 + 9792 \, x^8y^9r + 8192 \, x^8y^8m + 8192 \, x^8y^8n + 8192 \, x^8y^8r - 58752 \\
 & x^8y^9 - 73728 \, x^8y^8 + 20160 \, x^7y^8 + 13104 \, x^6y^7)|_{x=y=1} \\
 & = 43776 \, m - 27764 \, mn + 20736 \, mnr - 27764 \, mr + 43776 \, n - 27764 \, nr + \\
 & 43776 \, r - 86688
 \end{aligned}$$

$$\begin{aligned}
 ND_5(\Gamma, x, y) &= (D_x S_y + D_y S_x)(NM(\Gamma; x, y))|_{x=y=1} \\
 &= (16 \, x^8y^8m + 16 \, x^8y^8n + 64 \, mx^{12}y^{12} + 64 \, nx^{12}y^{12} - 16.073 \, mx^{10}y^{11} \\
 &- 16.073 \, nx^{10}y^{11} - 16.073 \, rx^{10}y^{11} - 80 \, mx^{10}y^{10} - 80 \, nx^{10}y^{10} + 16.089 \, mx^9y^{10} \\
 &+ 16.089 \, nx^9y^{10} + 16.111 \, mx^8y^9 + 16.111 \, nx^8y^9 + 48.571 \, x^6y^7 + 48.429 \, x^7y^8 \\
 &- 144 \, x^8y^8 - 144 \, x^{12}y^{12} - 96.533 \, x^9y^{10} + 288 \, x^{10}y^{10} - 96.667 \, x^8y^9 + 64 \, rx^{12}y^{12} \\
 &+ 16 \, x^8y^8r + 16.111 \, x^8y^9r + 16.089 \, x^9y^{10}r - 80 \, x^{10}y^{10}r - 28 \, nrx^{12}y^{12} \\
 &+ 4.018 \, mnx^{10}y^{11} + 4.018 \, mrx^{10}y^{11} + 4.018 \, nrx^{10}y^{11} + 16 \, mnx^{10}y^{10} \\
 &+ 16 \, mrx^{10}y^{10} + 16 \, nr \, x^{10}y^{10} - 28 \, mnx^{12}y^{12} + 12 \, mnrx^{12}y^{12} - 28 \, mrx^{12}y^{12} \\
 &+ 48.218 \, x^{10}y^{11})|_{x=y=1} \\
 &= 16.127 \, n + 16.127 \, r - 7.982 \, mn - 7.982 \, nr + 16.127 \, m - 47.982 - 7.982 \, mr \\
 &+ 12 \, mnr
 \end{aligned}$$

$$\begin{aligned}
 NH(\Gamma, x, y) &= 2(S_x)J(NM(\Gamma; x, y))|_{x=1} \\
 &= (-9 \, x^{16} - 5.647 \, x^{17} - 5.053 \, x^{19} + 14.4 \, x^{20} - 6 \, x^{24} + 0.842 \, x^{19}m \\
 &+ 0.842 \, x^{19}n + 0.941 \, x^{17}m + 0.941 \, x^{17}n + x^{16}m + x^{16}n + 2.667 \, mx^{24} \\
 &+ 2.667 \, nx^{24} - 0.762 \, mx^{21} - 0.762 \, nx^{21} - 0.762 \, rx^{21} - 4 \, mx^{20} - 4 \, nx^{20} \\
 &+ 3.692 \, x^{13} + 3.2 \, x^{15} + 0.5 \, x^{24}mnr - 1.167 \, x^{24}mn - 1.167 \, x^{24}nr - 1.167 \, x^{24}mr \\
 &+ 0.19 \, x^{21}mn + 0.19 \, x^{21}nr + 0.19 \, x^{21}mr + 0.8 \, x^{20}mn + 0.8 \, x^{20}mr + \\
 &0.8 \, x^{20}nr + x^{16}r + 0.941 \, x^{17}r + 0.842 \, x^{19}r - 4 \, x^{20}r + 2.667 \, rx^{24} \\
 &+ 2.286 \, x^{21})|_{x=1} \\
 &= 0.688 \, n + 0.688 \, r - 0.176 \, mn - 0.176 \, nr + 0.688 \, m - 2.122 - 0.176 \, mr \\
 &+ 0.5 \, mnr
 \end{aligned}$$

$$\begin{aligned}
 NI(\Gamma, x, y) &= S_x J(D_x + D_y)(NM(\Gamma; x, y))|_{x=y=1} \\
 &= (32 \, mx^{24} - 14 \, x^{24}mn + 6 \, x^{24}mnr - 14 \, x^{24}mr + 32 \, nx^{24} - 14 \, x^{24}nr \\
 &+ 32 \, rx^{24} - 72 \, x^{24} - 8 \, mx^{21} + 2 \, x^{21}mn + 2 \, x^{21}mr - 8 \, nx^{21} + 2 \, x^{21}nr - 8 \, rx^{21} \\
 &- 40 \, mx^{20} + 8 \, x^{20}mn + 8 \, x^{20}mr - 40 \, nx^{20} + 8 \, x^{20}nr - 40 \, x^{20}r + 24 \, x^{21} + 8 \\
 &x^{19}m + 8 \, x^{19}n + 8 \, x^{19}r + 144 \, x^{20} - 48 \, x^{19} + 8 \, x^{17}m + 8 \, x^{17}n + 8 \, x^{17}r + 8 \\
 &x^{16}m + 8 \, x^{16}n + 8 \, x^{16}r - 48 \, x^{17} - 72 \, x^{16} + 24 \, x^{15} + 24 \, x^{13})|_{x=1} \\
 &= 8 \, m - 4 \, mn + 6 \, mnr - 4 \, mr + 8 \, n - 4 \, nr + 8 \, r - 24
 \end{aligned}$$

$$\begin{aligned}
 S(\Gamma, x, y) &= (S_x^3 Q_{-2} J D_x^3 D_y^3)(M(\Gamma; x, y))|_{x=1} \\
 &= (-7122.329 \, x^{17} + 4657.239 \, x^{19} - 1552.413 \, x^{19}m - 1552.413 \, x^{19}n + \\
 &1187.055 \, x^{17}m + 1187.055 \, x^{17}n - 20190.726 \, x^{22} + 24691.358 \, x^{18}
 \end{aligned}$$

$$\begin{aligned}
 &+ 8973.656 x^{22}m + 8973.656 x^{22}n - 6858.711 x^{18}m - 6858.711 x^{18}n \\
 &+ 884.736 x^{15}m + 884.736 x^{15}n + 764.268 x^{14}m + 764.268 x^{14}n + 1918.427 x^{13} \\
 &- 5308.416 x^{15} + 8973.656 x^{22}r - 6858.711 x^{18}r + 884.736 x^{15}r + 764.268 x^{14}r \\
 &- 6878.414 x^{14} + 1335.922 x^{11} + 1187.055 x^{17}r - 1552.413 x^{19}r - 3925.974 \\
 &x^{22}mn + 1682.56 x^{22}mnr - 3925.974 x^{22}mr - 3925.974 x^{22}nr + 388.103 x^{19}mn \\
 &+ 388.103 x^{19}mr + 388.103 x^{19}nr + 1371.742 x^{18}mn + 1371.742 x^{18}mr \\
 &+ 1371.742 x^{18}nr)|_{x=1} \\
 &= 3398.591 n + 3398.591 r - 2166.129 mn - 6896.939 - 2166.129 nr \\
 &+ 3398.591 m - 2166.129 mr + 1682.56 mnr
 \end{aligned}$$

Graphical representation and comparative study

In this section, we present the graphical representations and comparative analysis of the computed NM-polynomials and neighborhood degree sum-based topological indices for the four investigated structures. The NM-polynomials for all four structures are illustrated in Figures 6, 7, 8, and 9. These figures provide insights into the variations in NM-polynomial values, demonstrating how they evolve across different structural configurations.

Following this, Figures 10, 11, and 12 depict the graphical representations of neighborhood degree sum-based topological indices for the first three structures. These indices capture essential connectivity characteristics and local neighborhood influences within each molecular framework. To facilitate a comparative study, Figures 13, 14, and 15 present a detailed comparison of these indices, allowing for a deeper understanding of their relative behaviors across the examined structures.

A critical observation from the figures reveals that the computed indices exhibit diverse responses depending on the structural properties. By analyzing the vertical axes of the graphical representations, we can conclude that among all neighborhood degree sum-based indices, ND_3 demonstrates the most dominant nature across all structures, consistently yielding the highest values. This suggests that ND_3 is more sensitive to changes in the local connectivity patterns of the molecular structures. In contrast, the index F_N^* exhibits a relatively slow growth trend, indicating a less pronounced variation with respect to structural modifications.

Furthermore, the graphical trends indicate that the computed topological indices generally increase as the underlying graph parameters, such as vertex degree and edge connectivity, grow. This trend underscores the direct relationship between structural complexity and the magnitude of topological indices, reinforcing their potential application in characterizing and differentiating molecular structures. The observed patterns also provide

valuable insights into the impact of local and global connectivity features on the studied indices, making them useful for predictive modeling in chemical and materials sciences.

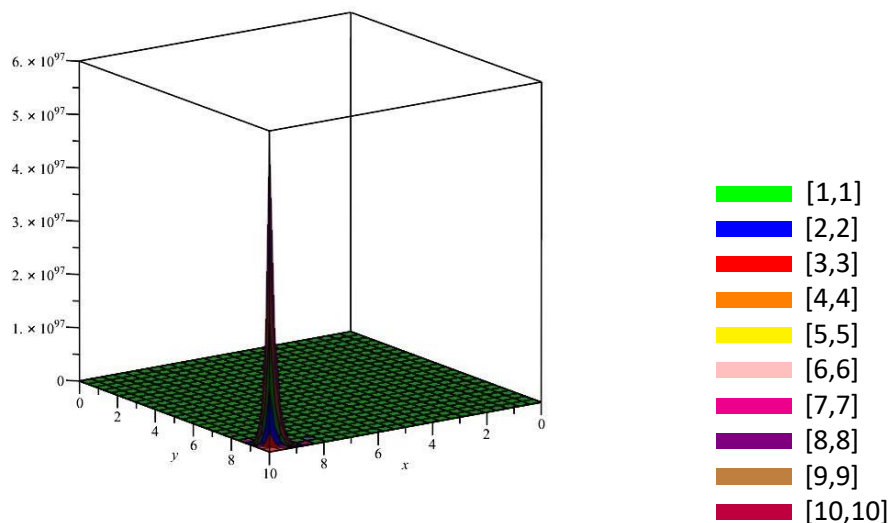


Figure 6. NM Polynomial of Enhanced mesh $M(m,n)$ network.

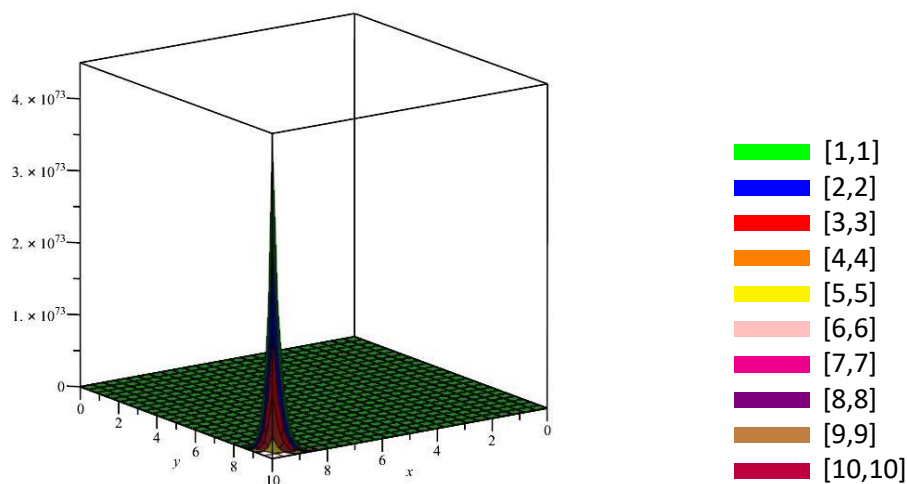


Figure 7. NM Polynomial of Triangular mesh T_n network.

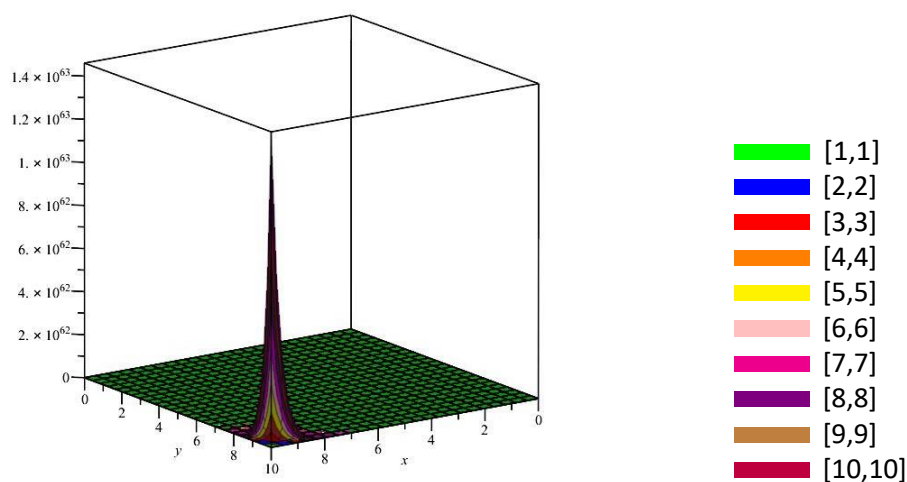


Figure 8. NM Polynomial of star of silicate network $SSL(n)$.

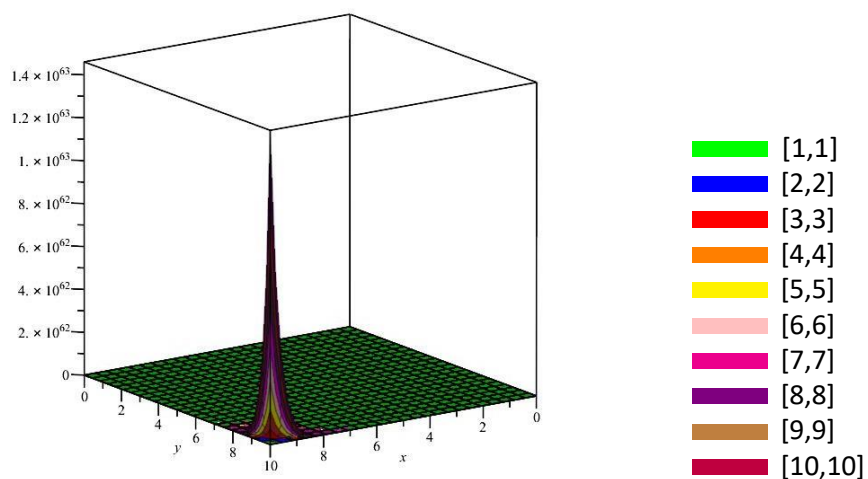


Figure 9. NM Polynomial of rhenium trioxide $RQ(m, n, r)$.

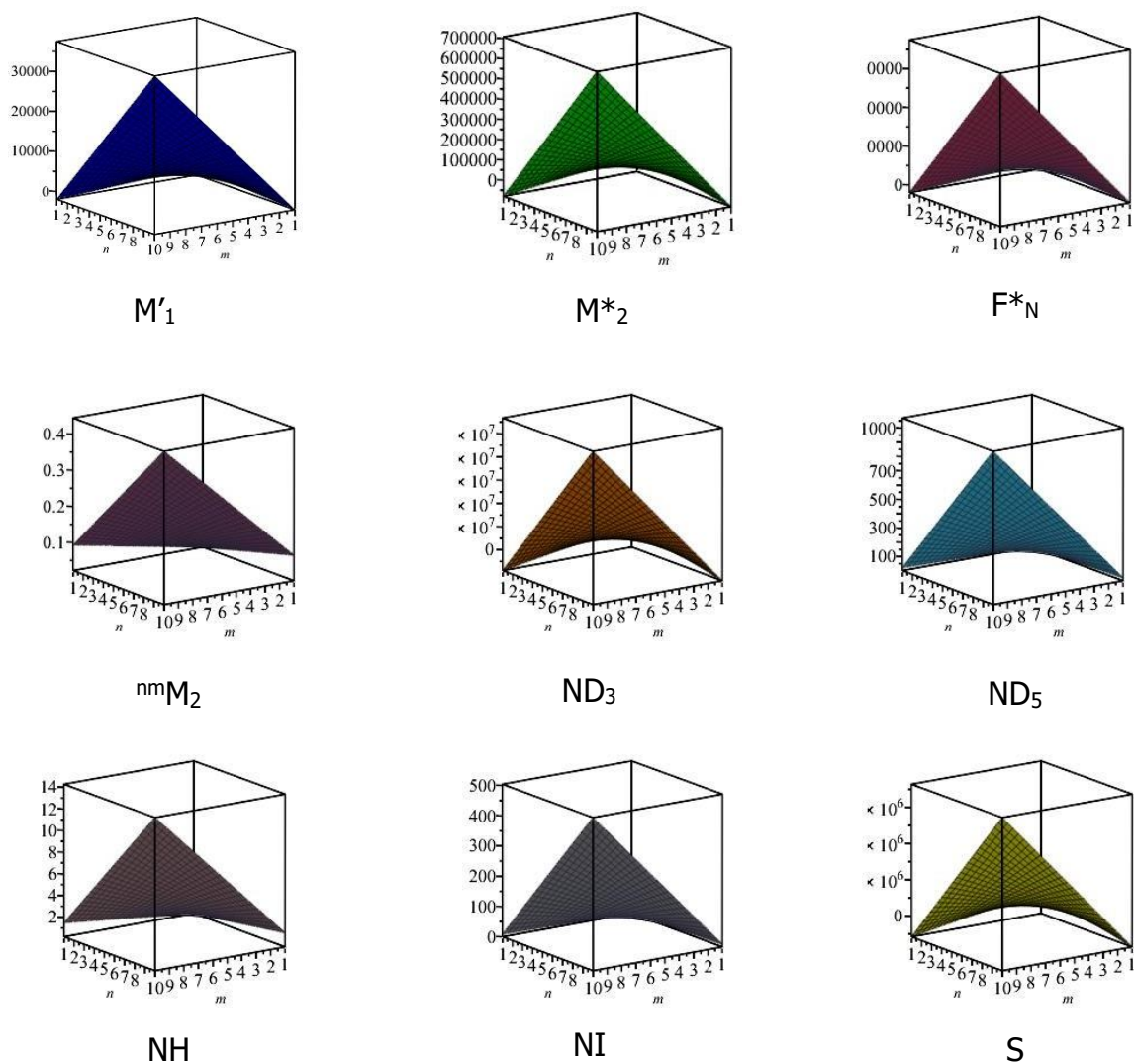


Figure 10. 3D graphical representation of topological indices of Enhanced mesh $M(5, 5)$ network.

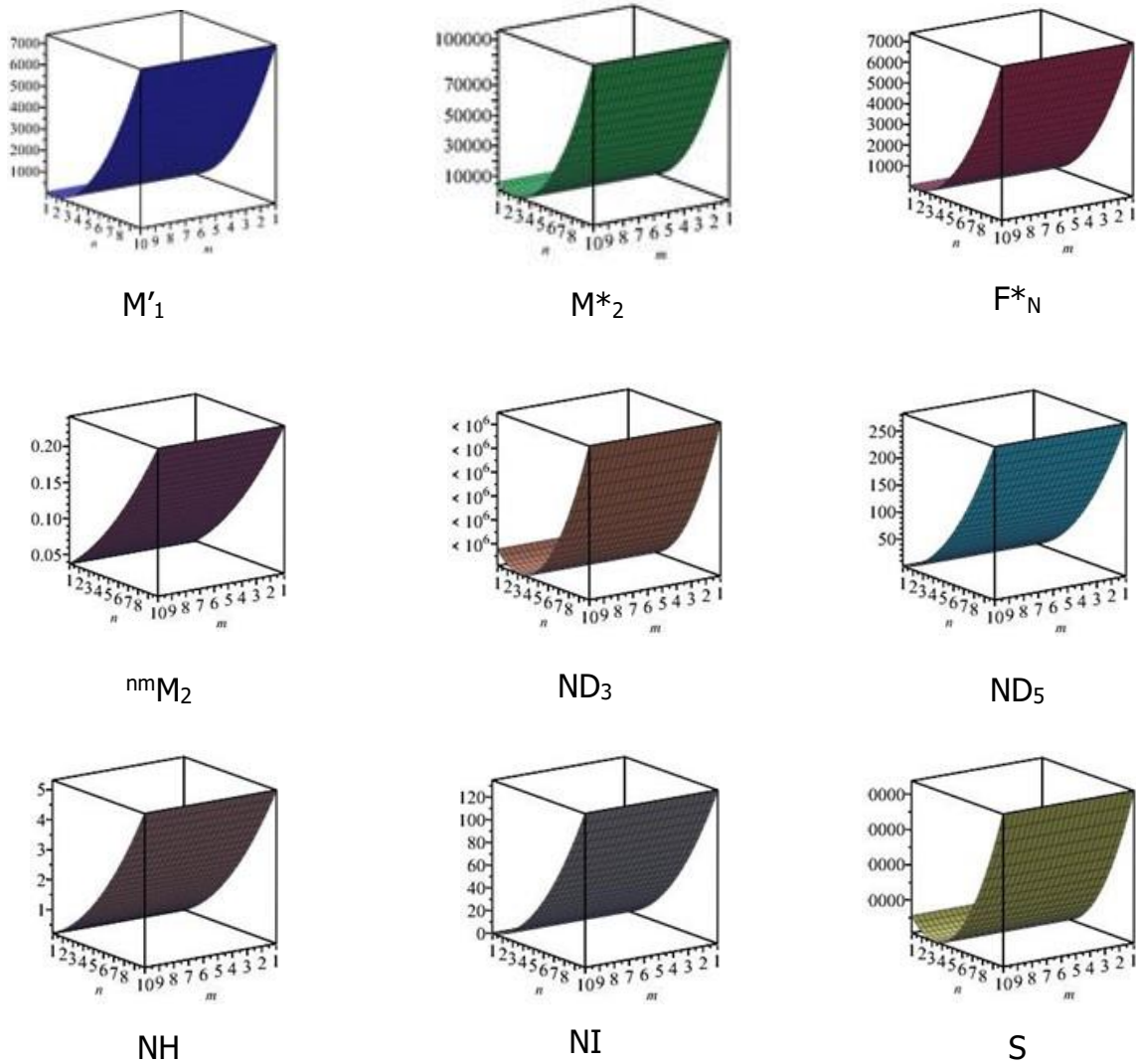


Figure 11. 3D graphical representation of topological indices of Triangular mesh T_n network.

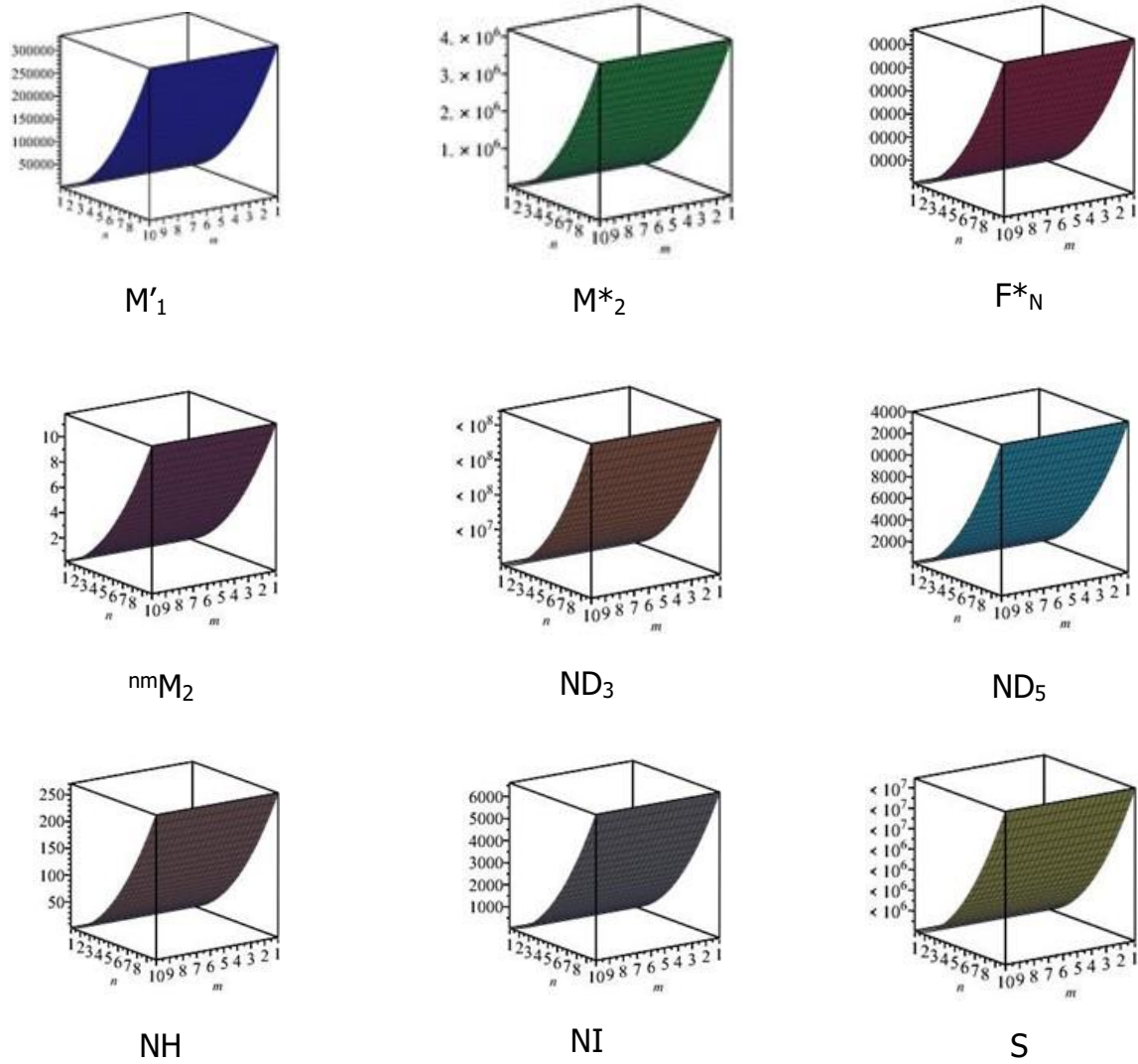


Figure 12. 3D graphical representation of topological indices of star of silicate network $SSL(n)$.

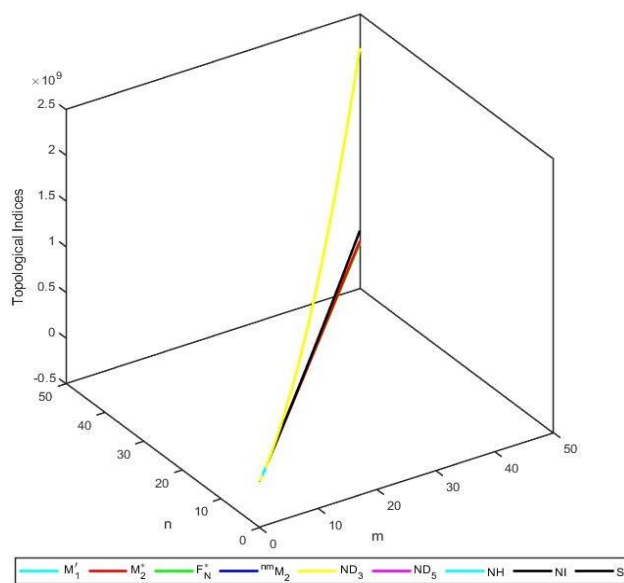
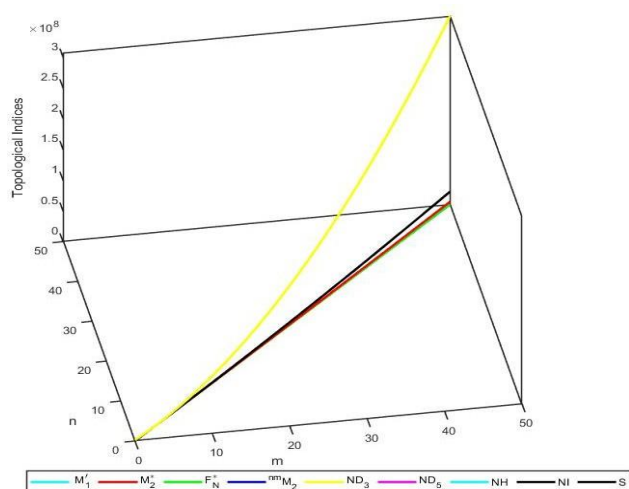
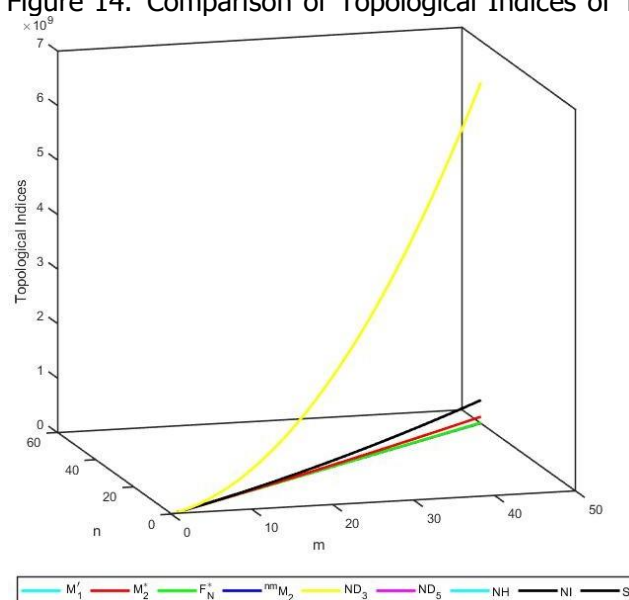


Figure 13: Comparison of Topological Indices of Enhanced mesh $M(m, n)$ network.

Figure 14. Comparison of Topological Indices of Triangular mesh T_n network.Figure 15. Comparison of Topological Indices of star of silicate network $SSL(n)$.

Conclusion

In this study, we have successfully applied neighborhood degree-based indices using NM-polynomials to analyze the structural features of four complex molecular networks. The results provide a quantitative framework for characterizing the unique graph-theoretical properties of these networks, offering valuable insights into their topological behavior.

We demonstrate that NM-polynomials serve as a powerful tool in uncovering previously unrecognized structural properties of molecular networks. While this work focuses on known molecular structures, the methodologies and indices presented here offer significant potential for extension to new and emerging molecular frameworks. Future research will explore the application of these indices in novel chemical and biological systems, facilitating the design of new materials and drug molecules with optimized structural and physicochemical properties. The adaptability of this approach suggests that it

could be instrumental in characterizing previously unexplored molecular topologies, making it a valuable tool in computational chemistry and materials science.

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