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Computing Topological Indices for Niobium Dioxide and Metal-Organic Frameworks via M-Polynomials

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Abstract

This paper investigates the topological properties of metal-organic frameworks and niobium dioxide using M-polynomials. The stability and wide range of bonding that the NbO_2 molecule exhibits make it a promising candidate for a number of uses, such as energy storage, gas detection, and catalysis. We use M-polynomials to calculate several degree-based topological indices for metal-organic frameworks and niobium dioxide. The M-polynomial is one such fundamental polynomial that provides a way to derive a multitude of degree-based topological indices. These indices are crucial for research in chemistry, biology, and physics and are derived from degree-based M-polynomials. This work develops a new M-polynomial algorithm for the computation and comparison of several degree-based molecular descriptors.

1 Introduction

Scientists and researchers have been fascinated to the optical characteristics of metallic nanoparticles [1]. The nanoparticles heat overwhelms cancer tissue while inflicting no harm to healthy cells [2]. K Banhatti and K hyper-Banhatti indices of nanotubes and circulant graphs have been examined [3, 4]. Niobium nanoparticles are suitable for optothermal cancer treatment because of their ability to attach to ligands fast. Chemical graph theory is a modern branch of applied chemistry that has remained an appealing subject of research for scientists throughout the last two decades, with notable contributions made by scientists including like [5, 6, 7].

To provide quantitative, thorough, and insightful insights into the properties of complex molecular structures and materials, it is necessary to use modern mathematical methods in their research and characterization. This has been demonstrated by numerous mathematical techniques, such as graph theory and polynomial models, which have been successfully used in materials research [8]. The

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use of M-polynomials to provide a thorough understanding of molecular structures and reactivity is one such strategy that has attracted interest [9]. One and oldest technique for analysing the properties and behaviour of chemical graphs is for finding their topological indices. Lots of work have been done, now further scientists and researchers are working for finding the reciprocal of topological indices. Gutmana et al. introduced this technique in a unique way [10]. A fascinating topic for research using M-polynomials is niobium oxide NbO_2, a transition metal oxide with special characteristics like better electrochemical performance and possible superconductivity [11]. Additionally, metal-organic frameworks $MOFs$ represent another significant group of materials that could considerably benefit from an indepth M-polynomial study because of their distinctive structural plasticity, high porosity, and tunable functionality [12].

The wide range of uses for NbO_2 and $MOFs$ including catalysis, gas storage, energy storage, environmental remediation, and even biomedicine [13], emphasizes the importance of thoroughly understanding their structures and properties. Designing new materials with specialized properties may result from a thorough examination of their features using M-polynomials [14]. This research will rigorously delve into their M-polynomials to gain a thorough grasp of the molecular structures, potential reactivity, and inherent qualities of NbO_2 and $MOFs$. We intend to identify distinctive structural and chemical behaviors by contrasting the M-polynomials of different materials, thereby shedding light on how these materials might interact in real-world applications. NbO_2 is well known for its exceptional capacity to engage as a member of the initial barrier [15].

Our current study uses M-polynomials to characterize the molecular structures of metal-organic frameworks $MOFs$ and niobium oxide NbO_2. Topological indices are frequently used in $QSPR$ and $QSAR$ investigations as straightforward numerical descriptors, allowing for a direct comparison with a molecule's physical, biological, or chemical properties. This benefit has inspired a lot of academics in recent years to study numerous chemical compounds and compute topological descriptors of various molecular graphs.

This study expands on those earlier studies by analyzing and contrasting the structural and chemical characteristics of NbO_2 and $MOFs$ using M-polynomials. The objective is to produce accurate, quantitative representations of their molecular structures, providing useful information about their potential reactivity and other crucial characteristics. This knowledge could direct the creation and improvement of these materials for various uses.

A molecular graph is a straightforwardly connected graph that captures the complex structure of chemical compounds like niobium oxide NbO_2 and metal-organic frameworks MOF in the context of chemical graph theory relevant to our investigation. Chemical atoms and bonds are included in this model; they are frequently identified as vertices and edges, respectively.

The connectedness of the vertex set V_G and edge set E_G is significant in this context. In such molecular graphs, the total number of atoms associated with a vertex v in the graph G, denoted by the notation dv, corresponds to an atom's valency. This aspect of chemical graph theory is crucial to understanding M-polynomials of NbO_2 and $MOFs$.

Gutman with Das praised the properties of first and second Zagreb polynomials for some chemical graphs of chemical compounds in 2004, which we explored in the [16] research articles. Hosoya polynomials, also called M-polynomials, are a class of polynomials first presented in 1988. They are discussed in [17] and [18], respectively. S Manzoor, et al. also studied and analysis of degree-based entropy measures for metal–organic super lattices [19]. Ghani, et al. also finding a

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Paradigmatic approach for finding the Valency-Based K-Banhatti and Redefined Zagreb Entropy for Niobium Oxide and a metal–organic framework [20]. These polynomials are similar to topological indices, which depend on atom valency. It is possible to use a network's M-polynomials in a specific way to derive topological properties. This M-polynomial with the following definition fits with x, y variables, $\alpha_{i,j}$ are number of edges, where $\lambda(u)$ represents vertex's degree and u the number of edges that make up the vertex. In keeping with it, the number of edges in a graph is determined by the function $i \leq j, \alpha_{i,j}(G)$

$$\Pi(G; x, y) = \sum_{i \leq j} \alpha_{i,j}(G) x^i y^j \quad (1)$$

Valency-based 1st Zagreb index, which dependent on the graph's topological description is provided G is

$$M_1(G) = \sum_{uv \in E(G)} (\tilde{\lambda}(u) + \tilde{\lambda}(v)) \quad (2)$$

Similarly, second Zagreb index graph G.

$$M_2(G) = \sum_{uv \in (G)} (\tilde{\lambda}(u) \cdot \tilde{\lambda}(v)) \quad (3)$$

M-polynomials correspond to above Zagreb indices are
The M-polynomials correspond to first and second Zagreb descriptors defined as [20]

$$\Pi_{M_1}(G) = \left(D_x + D_y\right)(\Pi(G; x, y)) \quad (4)$$

$$\Pi_{M_2}(G) = \left(D_x D_y\right)(\Pi(G; x, y)) \quad (5)$$

The M-polynomials that go along with the general Randić index based on atoms have a valency that is

$$R_\alpha(G) = \sum_{uv \in E(G)} (\tilde{\lambda}(u) \cdot \tilde{\lambda}(v))^\alpha, \quad (6)$$

$$\Pi_{R_\alpha}(G) = \left(D_x^\alpha D_y^\alpha\right)(\Pi(G; x, y)) \quad (7)$$

Operators are defined as

$$D_x(\Pi(G; x, y)) = x \frac{\partial(\Pi(G; xy))}{\partial x} \quad (8)$$

$$D_y(\Pi(G; x, y)) = y \frac{\partial(\Pi(G; xy))}{\partial y} \quad (9)$$

$$S_x(\Pi(G; x, y)) = \int_0^x \frac{(\Pi(G; z, y))}{z} \tilde{\lambda} z \quad (10)$$

$$S_y(\Pi(G; x, y)) = \int_0^y \frac{(\Pi(G; x, z))}{z} \tilde{\lambda} z \quad (11)$$

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In the study described here, we extend and adapt the Zagreb polynomials and Zagreb indices idea, which was first developed and used to silicate structures, to clarify the intricate structures of metal-organic frameworks $MOFs$ and niobium oxide NbO_2. This method offers a strong tool for analyzing these complex materials because it is based on atom-bond connectivity and partitioned according to the valences of its constituent atoms. Similar to earlier studies on the silicon tetrahedron SiO_4 in silicate structure research, our work primarily focuses on the deep investigation of the structural organization inside these compounds. Using the atom-bonds partitioning method, we derive exact formulas for NbO_2 and MOF s main valency-based Zagreb indices. The chemical complexity of these compounds can be better understood thanks to this methodology, which may also help with the compounds' optimization for different uses.

2 M-polynomials of Niobium dioxide

According to the theory of chemical graphs, a molecule is modeled as a graph with atoms acting as nodes (vertices) and chemical bonds acting as edges (lines). This simplification enables the theoretically tractable capture and quantification of complicated molecular structures. Niobium dioxide NbO_2 is a substance made up of one atom of niobium (Nb) and two atoms of oxygen (O). It is a crucial component of many industrial applications, including catalysis and lithium-ion batteries, and it crystallizes in the tetragonal system. It is critical to understand the precise bonding structure and the spatial arrangement of the atoms that make up Niobium dioxide NbO_2 to use chemical graph theory to understand its structure. Niobium (Nb) and oxygen (O) atoms are shown as vertices, and their bonds are shown as edges in the final graph representation see Figure 1.

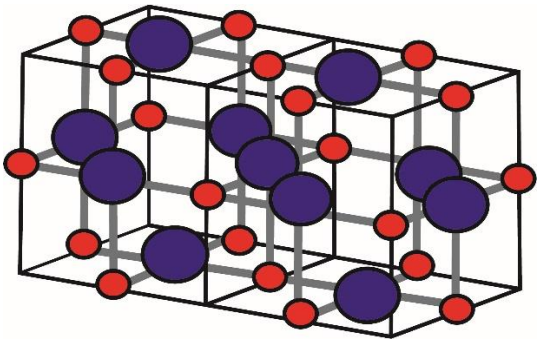

Figure 1: Niobium dioxide NbO_2 structure

Niobium Dioxide NbO_2 molecular structure and characteristics have been better understood because of our comparative analysis of M and MN polynomials for this substance. We obtained the M-polynomial for NbO_2 by mathematical and computer investigation. This polynomial provided valuable insights into the reactivity and stability of the compound by precisely representing atomic connections, bond types, and ring typologies within the NbO_2 molecule. The outcomes confirm the chemical graph theory reliability for describing and characterizing molecular structures. Additionally, they show how similar approaches might be utilized with additional molecular systems, paving the way for the future prediction and control of various substances physicochemical properties.

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Theorem 1. Let $\Upsilon(p,q)$ be a Niobium dioxide NbO_2 and $\Pi(\Upsilon(p,q);x,y)$ its M-polynomials

$$\Pi(\Upsilon(p,q));x,y) = 16x^2y^3 + (16q+16p-24)x^3y^3 + (12pq-8q-8p+8)x^3y^4 + (4pq-2q-2p)x^4y^4$$

Proof: According to the degree of both end vertices of each edge, the partitions is $|E(2,3)\Upsilon(p,q)| = 16, |E(3,3)(\Upsilon(p,q)| = 8(2q+2p-3)|E,(3,4)\Upsilon(p,q)| = 4(3qp-2q-2p+2)$ and $|E(4,4)\Upsilon(p,q)| = 2(2qp-q-p)$. By using the definition of M polynomial 1, on Niobium dioxide

$$\Pi(\Upsilon(p,q);x,y) = \sum_{i\leq j} m_{i,j}(\Upsilon(p,q))x^iy^j = 16x^2y^3 + (16q+16p-24)x^3y^3 + (12pq-8q-8p+8)x^3y^4 + (4pq-2q-2p)x^4y^4$$

Theorem 2. Let $\Upsilon(p,q)$ be Niobium dioxide $NbO_2 D_x(\Pi(\Upsilon(p,q);x,y))$ and $D_y(\Pi(\Upsilon(p,q);x,y))$ are the differential operators. Then

$$D_x((\Upsilon(p,q);x,y)) = (32)x^2y^3 + (48q+48p-72)x^3y^3 + (36qp-24q-24p+24)x^3y^4 + (16qp-8q-8p)x^4y^4$$
$$D_y(\Pi(\Upsilon(p,q);x,y)) = (48)x^2y^3 + (48qp+48p-72)x^3y^3 + (48qp-32p-32q+32)x^3y^4 + (16qp-8q-8p)x^4y^4$$

Proof: For the structure of $\Upsilon(p,q)$ be Niobium dioxide, this can achieve the desired function outcome $D_x(\Pi(\Upsilon(p,q);x,y))$.

$$D_x(\Pi(\Upsilon(p,q);x,y)) = x\frac{\partial\Pi(\Upsilon(p,q))}{\partial x}$$
$$= x\frac{\partial}{\partial x}(16)x^2y^3 + (16q+16p-24)x^3y^3 + (12pq-8q-8p+8)x^3y^4 + (4qp-2q-2p)x^4y^4$$
$$= x((32)xy^3 + (48q+48p-72)x^2y^3 + (36qp-24q-24p+24)x^2y^4 + (16qp-8q-8p)x^3y^4$$
$$= (32x^2y^3 + (48q+48p-72)x^3y^3 + (36qp-24q-24p+24)x^3y^4 + (16qp-8q-8p)x^4y^4$$

replace variable y with new parameter, multiply the result by parameter, The function's desired result, $D_y(\Pi(\Upsilon(p,q);x,y))$, can be obtained as

$$D_y((\Upsilon(p,q);x,y)) = y\frac{\partial\Pi(\Upsilon(p,q))}{\partial y}$$
$$= y\frac{\partial}{\partial y}((16)x^2y^3 + (16q+16p-24)x^3y^3 + (12qp-8q-8p+8)x^3y^4 + (4qp-2q-2p)x^4y^4$$
$$= y((48)x^2y^2 + (48q+48p-72)x^3y^2 + (48qp-32p-32q+32)x^3y^3 + (16qp-8q-8p)x^4y^3$$
$$= ((48)x^2y^3 + (48q+48p-72)x^3y^3 + (48qp-32p-32q+32)x^3y^4 + (16qp-8q-8p)x^4y^4$$

Theorem 3. Let $\Upsilon(p,q)$ be Niobium dioxide and $S_x(\Pi(\Upsilon(p,q);x,y))$ and $S_y(\Pi(\Upsilon(p,q);x,y))$ are integral operators.

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$$S_x((\Upsilon(p,q);x,y))$$
$$= 8x^3y^3 + y^4\left[\left(\frac{16q+16p-24}{3}\right)x^3 + \left(\frac{12qp-8q-8p+8}{3}\right)x^3 + \left(\frac{4pq-8q-8p+8}{4}\right)x^4\right]$$
$$S_y((\Upsilon(p,q);x,y))$$
$$= 4x^2y^4 + \left(\frac{16q+16p-24}{4}\right)x^3y^4 + \left(\frac{12pq-8q-8p+8}{5}\right)x^3y^5 + \left(\frac{4pq-2q-2p}{5}\right)x^4y^5$$

Proof: change variable x, with a newly defined parameter, In the case of $\Upsilon(p,q)$ Niobium dioxide structure, this can achieve the desired function outcome, $S_x(\Pi(\Upsilon(p,q);x,y))$

$$S_x(\Pi(\Upsilon(p,q);x,y)) = \int_0^z \frac{\Pi(\Upsilon(p,q);z,y)}{z}\tilde{\lambda}z$$
$$= \int_0^x \frac{1}{z}\big(((16)z^2y^3 + (16q+16p-24)z^3y^4 + (12qp-8q-8p+8)z^3y^4$$
$$+(4qp-2q-2p)z^4y^4\tilde{\lambda}z$$

apply integral on each component, we have

$$= \int_0^x (16)zy^3\tilde{\lambda}z + \int_0^x (16q+16p-24)z^2y^4\tilde{\lambda}z + \int_0^x (12qp-8q-8p+8)z^2y^4\tilde{\lambda}z$$
$$+\int_0^x (4qp-8q-8p+8)z^3y^4\tilde{\lambda}z$$

now applying limits on each component

$$= (16)\frac{z^2}{2}y^3\Big|_0^x + (16q+16p-24)\frac{z^3}{3}y^4\Big|_0^x + (12qp-8q-8p+8)\frac{z^3}{3}y^4\Big|_0^x$$
$$+(4qp-8q-8p+8)\frac{z^4}{4}y^4\Big|_0^2$$

Finally

$$= 8x^3y^3 + y^4\left[\left(\frac{16q+16p-24}{3}\right)x^3 + \left(\frac{12qp-8q-8p+8}{3}\right)x^3 + \left(\frac{4pq-8q-8p+8}{4}\right)x^4\right]$$

Substitute a new parameter for the variable y, divide the result by new parameter

$$S_y(\Pi(\Upsilon(p,q);x,y)) = \int_0^2 \frac{\Pi(\Upsilon(p,q);x,z)}{z}\tilde{\lambda}z$$
$$= \int_0^y \frac{1}{z}\big((16)x^2z^3 + (16q+16p-24)x^3z^3 + (12pq-8q-8p+8)x^3z^4 + (4pq-2q-2p)x^4z^4\tilde{\lambda}z$$

Implementing integral on each component

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$$= \int_0^y (16)x^2z^3\tilde{\lambda}z + \int_0^y (16q+16p-24)x^3z^3\tilde{\lambda}z + \int_0^y (12pq-8q-8p+8)x^3z^4\tilde{\lambda}z + \int_0^y (4pq-2q-2p)x^4z^4\tilde{\lambda}z$$

Implementing limits on each component

$$= (16)x^2\frac{z^4}{4}\Big|_0^z + (16q+16p-24)x^3\frac{z^4}{4}\Big|_0^y + (12pq-8q-8p+8)x^3\frac{z^5}{5}\Big|_0^y + (4pq-2q-2p)x^3\frac{z^5}{5}\Big|_0^y$$

After some algebraic calculations

$$= y^4\left[4x^2 + \left(\frac{16q+16p-24}{4}\right)x^3\right] + y^5\left[\left(\frac{12pq-8q-8p+8}{5}\right)x^3 + \left(\frac{4pq-2q-2p}{5}\right)x^3\right]$$

Theorem 4. Let $\Upsilon(p,q)$ be Niobium dioxide and $\Pi_{M_1}(\Upsilon(p,q);x,y)$ is the 1st Zagreb M-polynomial for Niobium dioxide.

$$\Pi_{M_1}(\Upsilon(p,q)))$$
$$= 80x^2y^3 + 2(48q+48p-72)x^3y^4 + 2(36pq-24q-24p+24)x^3y^4 + 2(16pq-8q-8p)x^4y^4$$

Proof:

$$\Upsilon(p,q)\cdot D_x(\Pi(\Upsilon(p,q);x,y)) = D_y(\Pi(\Upsilon(p,q);x,y))$$
$$\Pi_{M_1}(\Upsilon(p,q)) = (D_x+D_y)(\Pi(\Upsilon(p,q))) = D_x(\Pi(\Upsilon(p,q))) + D_y(\Pi(\Upsilon(p,q)))$$
$$= (32)x^2y^3 + (48q+48p-72)x^3y^3 + (36pq-24q-24p+24)x^3y^4 + (16qp-8q-8p)x^4y^4$$
$$+(48)x^2y^3 + (48qp+48p-72)x^3y^3 + (48qp-32p-32q+32)x^3y^4 + (16qp-8q-8p)x^4y^4$$
$$= 80x^2y^3 + 2(48q+48p-72)x^3y^4 + 2(36pq-24q-24p+24)x^3y^4 + 2(16pq-8q-8p)x^4y^4.$$

Theorem 5. Let $\Upsilon(p,q)$ be Niobium dioxide and $\Pi_{M_2}(\Upsilon(p,q);x,y)$ is the 2nd Zagreb M-polynomial for Niobium dioxide.

$$\Pi_{M_2}(\Upsilon(p,q)) = x^2y^3[18144 + 72(2q+2p-3)] + y^4[64(4pq-2p-2q+2)x^3 + 32(2p-q-p)x^4]$$

Proof:

$$\Pi_{M_2}(\Upsilon(p,q)) = (D_xD_y)(\Pi(\Upsilon(p,q))) = D_x(((48)x^2y^3 + (48pq+48p-72)x^2y^3$$
$$+(48pq-32p-32q+32)x^3y^4 + (16p-8q-8p)x^4y^4$$
$$= 144x^2y^3 + 72(2q+2p-3)x^2y^3 + 64(4pq-2p-2q+2)x^3y^4 + 32(2p-q-p)x^4y^4.$$

Theorem 6. Let $\Upsilon(p,q)$ be Niobium dioxide and $\Pi_{R_\alpha}(\Upsilon(p,q);x,y)$ is the general Randić M polynomial. Then

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$$\Pi_{R_\alpha}(\Upsilon(p,q)) = y^3[3^\alpha(16)x^2 + 9^\alpha(16q+16p-24)x^3] + y^4[16^\alpha(12pq-8q-8p+8)x^3 + 16^\alpha(4pq-2q-2p)x^4]$$

Proof:

$$\begin{aligned}
&\Pi_{R_\alpha}(\Upsilon(p,q)) = \left(D_x^\alpha D_y^\alpha\right)(\Pi(\Upsilon(p,q))) \\
=\ &\left[\left(D_x^\alpha D_y^\alpha\right)((16)x^2 + (16q+16p-24)x^3]y^3 + y^4[(12pq-8q-8p+8)x^3 + (4pq-2q-2p)x^4\right] \\
=\ &D_x^\alpha(3^\alpha(16)x^2y^3 + 3^\alpha(16q+16p-24)x^3y^3 + 4^\alpha(12pq-8q-8p+8)x^3y^4 + 4^\alpha(4pq-2q-2p)x^4y^4 \\
=\ &9^\alpha(16)x^2y^3 + 9^\alpha(16q+16p-24)x^3y^3 + 16^\alpha(12pq-8q-8p+8)x^3y^4 + 9^\alpha(4pq-2q-2p)x^4y^4
\end{aligned}$$

3 Topological Indices of Niobium Dioxide

The following are the topological indices corresponding to M-polynomials.

Name of the Index	Index Value
$M_1(G)$	$-8+24p+24q+116pq$
$M_2(G)$	$-15+16p+16q+208pq$
$MM_2(G)$	$\frac{2}{3}+\frac{167}{72}p+\frac{167}{72}q+\frac{5}{4}pq$
$R_{\alpha(G)}$	$\frac{16}{(6^\alpha)}16x^2y^3+\frac{1}{(9^\alpha)}(16p+16q-24)x^3y^3+\frac{1}{(12^\alpha)}(12pq-8p-8q+8)x^3y^4+\frac{1}{(16^\alpha)}(4pq-2p-2q)x^4y^3$
$RR_{\alpha(G)}$	$16(6^\alpha)16+\frac{1}{(9^\alpha)}(16p+16q-24)+\frac{1}{(12^\alpha)}(12pq-8p-8q+8)+\frac{1}{(16^\alpha)}(4pq-2p-2q)$
$SSD(G)$	$\frac{64}{3}+\frac{16}{3}p+\frac{16}{3}q+36pql$
$H(G)$	$\frac{164}{35}+\frac{224}{21}p+\frac{13}{7}pq+\frac{128}{21}q$
$IS(G)$	$\frac{93}{5}+\frac{116}{7}p+\frac{164}{7}pq+\frac{116}{7}q$

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$AZI(G)$	$\frac{680993}{4000}+\frac{1222197}{36288}p+\frac{6561604}{27145}pq+\frac{1222197}{36288}q$

Table 1: Topological Indices

Additionally, the table demonstrates that as N increases, the various indices show varying rates of increase. As an illustration, Randić indices rise more quickly than the first and second Zagreb indices. This implies that as networks get bigger, Randić indices become increasingly accurate indicators of their stability and complexity. Compared to the hexagon network, the honeycomb network has a higher and Randić index. This implies that compared to the hexagon network, the honeycomb network is more stable and complicated.

Table 2: Comparison among various parameters of $G = \mathrm{NbO}_2$ for $p, q \geq 2, p = q$

(p, q)	$M_1(G)$	$M_2(G)$	$MM_2(G)$	$R_\alpha(G)$	$RR_\alpha(G)$	$SSD(G)$	$H(G)$	$IS(G)$	$AZI(G)$
(2,2)	552	881	15	50	1543	187	46	179	402
(3,3)	1180	1953	26	58	1551	377	72	329	590
(4,4)	2040	3441	40	69	1562	640	101	526	826
(5,5)	3132	5345	56	82	1575	975	135	770	1111
(6,6)	4456	7665	73	98	1591	1381	172	1061	1445
(7,7)	6012	10401	94	116	1609	1860	213	1399	1826
(8,8)	7800	13553	118	136	1630	2411	258	1783	2256
(9,9)	9820	17121	144	160	1653	3033	-306	2215	2734
(10,10)	21105	21105	172	185	1679	3728	358	2693	3261

The NbO_2 molecule is a cluster molecule, meaning that it is made up of several NbO_2 units that are bound together, which explains these tendencies. The molecule gets larger and more complex as the number of NbO_2 units rises. As a result, the molecule's many topological indices—including complexity, connection, distance, and branching—increase. The high values of the Zagreb indices in

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the table further demonstrate the great degree of stability of the $G = NbO_2$ molecule. A molecule's connectedness is measured by the Zagreb indices, and molecules with high values of these indices are said to be well-connected. The $G = NbO_2$ molecule is hence less prone to break down.

4 M-polynomial of Metal-organic framework

Metal-organic frameworks MOF are a new family of porous materials made up of metal-containing nodes (frequently referred to as secondary building units, or SBUs) and organic linkers. MOFs have become one of the fastest developing topics in chemistry due to their structural and functional tunability. This virtually extraordinary boom in MOF research can be attributed advancements in cluster chemistry, maturation of organic synthesis relevant to ligand creation and post-synthetic modification, advancements in structure determination, particularly by X-ray crystallography, as well as the development of hardware and software for evaluating sorption qualities, MOF research transdisciplinary growth with neighbouring fields, and the ever-expanding application potential.[21]

Furthermore, the synthesis and characterization of the materials are briefly discussed from the industrial perspective [22]. Imran et al Computed of entropy measures for metal-organic frameworks.[23]. Metal organic frameworks are distinguished by their three-dimensional metallic ion frameworks. The metal-organic framework's molecular formula is $FeTPyP - Co$, where Fe denotes iron, TP_yP denotes tetrakis pyridyl porphyrin, and Co denotes cobalt [24]. The metal ions and organic molecules in the $\mathrm{MOF}_{(\mathrm{p,q})}$ network can all host a variety of guest molecules. Among their many applications are gas storage, heterogeneous catalysis, energy storage systems, and chemical analysis. Metal organic frameworks are also useful for these purposes. Mathrm The nomenclature of a $2D$ metal organic framework is $MOF_{(p,q)}$, where s and t are the unit cells in a row and column, respectively. The metal organic framework, or $MOF_{(2,2)}$ is shown in Figure 2. According to Figure 2 of $MOF_{(2,2)}$, the metal organic framework mathrm $MOF_{(p,q)}$ uses $2(44pq - p - q) + 1$ atom-bonds and has $74pq$ atoms.

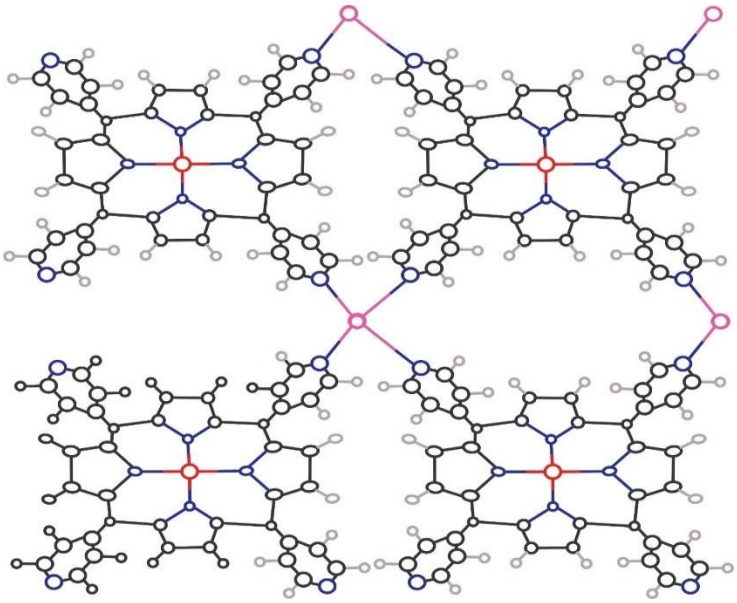

Figure 2: Structure of $MOF_{(2,2)}$

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Theorem 7. Let $\Omega(p,q)$ be a structure of $\mathrm{MOF}_{(p,q)}$ metal organic framework, and $\Pi(\Upsilon(p,q);x,y)$ is the general M-polynomials. Then

$$\Pi(\Upsilon(p,q));x,y) = (1+24pq)xy^3+6(p+q-1)x^2y^3+2(28pq-2p-2q+1)x^3y^3 +4(2pq-p-q+1)x^3y^4$$

Proof: According to the degree of both end vertices of each edge, the edge partitions is as $|E(1,3)\Upsilon(p,q)| = 1+24pq, |E(2,3)(\Upsilon(p,q)| = 6(p+q-1)|E,(3,3)\Upsilon(p,q)| = 2(28pq-2p-2q+1)$ and $|E(3,4)\Upsilon(p,q)| = 4(2pq-p-q+1)$. By using the definition 1

$$\Pi(\Upsilon(p,q);x,y) = \sum_{i\le j} m_{i,j}(\Upsilon(p,q))x^iy^j = (1+24pq)xy^3+6(p+q-1)x^2y^3 +2(28pq-2p-2q+1)x^3y^3+4(2pq-p-q+1)x^3y^4$$

Theorem 8. Let $\Omega(p,q)$ be a structure of $\mathrm{MOF}_{(p,q)}$ metal organic framework, $D_x(\Pi(\Omega(p,q);x,y))$ and $D_y(\Pi(\Omega(p,q);x,y))$ are the differential operators for $\Omega(p,q)$ then

$$D_x((\Pi(\Omega(p,q);x,y)) = (1+24pq)xy^3+6(2p+2q-2)x^2y^3 +6(32pq-2p-2q+1)x^2y^3+12(2pq-p-q+1)x^3y^3$$
$$D_y(\Pi(\Omega(p,q);x,y)) = 3(1+24pq)xy^3+9(2p+2q-2)x^2y^3 +6(32pq-2p-2q+1)x^2y^3+16(2pq-p-q+1)x^3y^3$$

Proof: These differential operators are used and demonstrated in this proof. Change the variable x, to a new parameter, multiply the result by the new parameter

$$D_x(\Pi(\Omega(p,q);x,y)) = x\frac{\partial\Pi(\Omega(p,q)}{\partial x}$$
$$= x\frac{\partial}{\partial x}(1+24pq)xy^3+6(p+q-1)x^2y^3+2(28pq-2p-2q+1)x^3y^3+4(2pq-p-q+1)x^3y^4$$
$$= x((1+24pq)xy^3+6(2p+2q-2)xy^3+6(32pq-2p-2q+1)x^2y^3+12(2pq-p-q+1)x^2y^4$$
$$= (1+24pq)xy^3+6(2p+2q-2)x^2y^3+6(32pq-2p-2q+1)x^3y^3+12(2pq-p-q+1)x^3y^3$$

Differential operators will be used in this proof to demonstrate their use. Change the variable y to a new parameter

$$D_y\Big((\Pi(\Omega(p,q);x,y)) = y\frac{\partial\Pi(\Pi(\Omega(p,q))}{\partial y}$$
$$= y\frac{\partial}{\partial y}((1+24pq)xy^3+6(p+q-1)x^2y^3+2(28pq-2p-2q+1)x^3y^3+4(2pq-p-q+1)x^3y^4$$
$$= y((3(1+24pq))xy^2+9(2p+2q-2)x^2y^2+6(32pq-2p-2q+1)x^3y^2+16(2pq-p-q+1)x^3y^3$$
$$= y((3(1+24pq))xy^3+9(2p+2q-2)x^2y^3+6(32pq-2p-2q+1)x^3y^3+16(2pq-p-q+1)x^3y^4$$

Theorem 9. Let $\Omega(p,q)$ be a γ-sheet of metal organic framework $S_x(\Pi(\Omega(p,q);x,y))$ and $S_y(\Pi(\Omega(p,q);x,y))$ are the integral operators. Then

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$$S_x((\Upsilon(p,q);x,y))$$
$$= (1+24pq)xy^3 + y^3\left[3(p+q-1)x^2\left(\frac{2(28pq-2p-2q+1)}{3}\right)x^3 + \left(\frac{4(2pq-p-q+1)}{3}\right)x^3x\right]$$
$$S_x((\Upsilon(p,q);x,y))$$
$$= (1+24pq)x^3y + y^3\left[(3(p+q-1))x^2 + \frac{2(28pq-2p-2q+1)}{3}y^3 + \left(\frac{4(2pq-p-q+1)}{3}\right)x^3y^3\right]$$

Proof: In this proof, the application of integral operators will be shown. Substitute a new parameter for the variable x

$$S_x\left((\Pi(\Omega(p,q);x,y)) = \int_0^z \frac{\Pi(\Upsilon(p,q);z,y)}{z}\tilde{\lambda}z\right.$$
$$= \int_0^x \left[\frac{1}{z}\left(((1+24pq)zy^3 + 6(p+q-1)z^2y^3 + 2(28pq-2p-2q+1)z^3y^3\right.\right.$$
$$\left.\left.+4(2pq-p-q+1)z^3y^4\right]\tilde{\lambda}z\right.$$

apply integral on each component, we have

$$= \int_0^x (1+24pq)y^3\tilde{\lambda}z + \int_0^x 6(p+q-1)zy^3\tilde{\lambda}z + \int_0^x 2(28pq-2p-2q+1)z^2y^3\tilde{\lambda}z$$
$$+\int_0^x 4(2pq-p-q+1)z^2y^4\tilde{\lambda}z$$

now applying limits on each component

$$= (1+24pq)zy^3|_0^x + 3(p+q-1)z^2y^3|_0^x + \frac{2(28pq-2p-2q+1)}{3}z^3y^3\Big|_0^x$$
$$+\left(\frac{4(2pq-p-q+1)}{3}\right)z^3y^4\Big|_0^x$$
$$= (1+24pq)xy^3 + y^3\left[3(p+q-1)x^2\left(\frac{2(28pq-2p-2q+1)}{3}\right)x^3 + \left(\frac{4(2pq-p-q+1)}{3}\right)x^3x\right]$$

The use of integral operators will be demonstrated in this proof. Substitute a new parameter for the variable y structure

$$S_y(\Pi(\Upsilon(p,q);x,y)) = \int_0^y \frac{\Pi(\Upsilon(p,q);x,z)}{z}\tilde{\lambda}z$$
$$= \int_0^y \frac{1}{z}\left[((1+24pq)x^3z + 6(p+q-1)x^3z^2 + 2(28pq-2p-2q+1)x^3z^3 + 4(2pq-p-q+1)x^4z^3\right]\tilde{\lambda}z$$

Implementing integral on each component

$$= \int_0^y (1+24pq)x^3\tilde{\lambda}z + \int_0^y 6(p+q-1)x^3z\tilde{\lambda}z + \int_0^y 2(28pq-2p-2q+1)x^3z^2\tilde{\lambda}z$$
$$+\int_0^y 4(2pq-p-q+1)x^4z^2\tilde{\lambda}z$$

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Implementing limits on each component

$$= (1+24pq)zx^3|_0^y + 3(p+q-1)x^3z^2|_0^y + \left(\frac{2(28pq-2p-2q+1)}{3}\right)x^3z^3\Big|_0^y + \left(\frac{4(2pq-p-q+1)}{3}\right)x^3z^3\Big|_0^y$$

$$= (1+24pq)x^3y + y^3\left[(3(p+q-1))x^2 + \frac{2(28pq-2p-2q+1)}{3}y^3 + \left(\frac{4(2pq-p-q+1)}{3}\right)x^3y^3\right]$$

Theorem 10. Let $\Omega(p,q)$ be a γ-sheet of metal organic framework network and $\Pi_{M_1}(\Omega(p,q);x,y)$ is 1st Zagreb M-polynomial.

$$\begin{aligned}&\Pi_{M_1}(\Upsilon(p,q))\big)\\ =\ & 4(1+24pq)xy^3 + 15(2p+2q-2)x^2y^3 + 12(32pq-2p-2q+1)x^2y^3 + 28(2pq-p+q+1)x^3y^3\end{aligned}$$

Proof:

$$\Upsilon(p,q)\cdot D_x(\Pi(\Upsilon(p,q);x,y)) = D_y(\Pi(\Upsilon(p,q);x,y))$$

$$\Pi_{M_1}(\Upsilon(p,q)) = \big(D_x+D_y\big)(\Pi(\Upsilon(p,q))) = D_x(\Pi(\Upsilon(p,q))) + D_y(\Pi(\Upsilon(p,q)))$$

$$\begin{aligned}=\ & (1+24pq)xy^3 + 6(2p+2q-2)x^2y^3 + 6(32pq-2p-2q+1)x^2y^3 + 12(2pq-p-q+1)x^3y^3\\ & 3(1+24pq)xy^3 + 9(2p+2q-2)x^2y^3 + 6(32pq-2p-2q+1)x^2y^3 + 16(2pq-p-q+1)x^3y^3\\ =\ & 4(1+24pq)xy^3 + 15(2p+2q-2)x^2y^3 + 12(32pq-2p-2q+1)x^2y^3 + 28(2pq-p-q+1)x^3y^3\end{aligned}$$

Theorem 11. Let $\Omega(p,q)$ be a γ-sheet of metal organic framework and $\Pi_{M_2}(\Omega(p,q);x,y)$ is the 2nd Zagreb M-polynomial for $\Omega(p,q)$. Then

$$\Pi_{M_2}(\Upsilon(p,q)) = (1+24pq)xy^3 + 12(p+q-1)x^2y^3 + 6(28pq-2p-2q+1)x^3y^3 + 12(2pq-p-q+1)x^3y^4$$

Proof:

$$\begin{aligned}&\Pi_{M_2}(\Omega(p,q)) = \big(D_xD_y\big)(\Pi(\Upsilon(p,q))) = D_x((1+24pq)xy^3 + 6(p+q-1)x^2y^3\\ &+2(28pq-2p-2q+1)x^3y^3 + 4(2pq-p-q+1)x^3y^4\\ &= (1+24pq)xy^3 + 12(p+q-1)x^2y^3 + 6(28pq-2p-2q+1)x^3y^3 + 12(2pq-p-q+1)x^3y^4.\end{aligned}$$

Theorem 12. Let $\Omega(p,q)$ be a γ-sheet of metal organic framework and $\Pi_{R_\alpha}(\Omega(p,q);x,y)$ is the general Randić index for $\Omega(p,q)$. Then

$$\begin{aligned}&\Pi_{R_\alpha}(\Omega(p,q))\\ =\ & (3^\alpha(1+24pq)xy^3 + 6^\alpha(6(p+q-1))x^2y^3 + 9^\alpha 2(28pq-2p-2q+1)x^3y^3 + 12^\alpha 4(2pq-p-q+1)x^3y\end{aligned}$$

Proof:

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$$\Pi_{R_\alpha}(\Upsilon(p,q)) = \left(D_x^\alpha D_y^\alpha\right)(\Pi(\Upsilon(p,q)))$$
$$= \left(D_x^\alpha D_y^\alpha\right)((1+24pq)xy^3 + 6(p+q-1)x^2y^3 + 2(28pq-2p-2q+1)x^3y^3 + 4(2pq-p-q+1)x^4y^4$$
$$= D_x^\alpha(3^\alpha(1+24pq)xy^3 + 3^\alpha(6(p+q-1))x^2y^3 + 3^\alpha 2(28pq-2p-2q+1)x^3y^3 + 4^\alpha 4(2pq-p-q+1)x^3y^4$$
$$= (3^\alpha(1+24pq)xy^3 + 6^\alpha(6(p+q-1))x^2y^3 + 9^\alpha 2(28pq-2p-2q+1)x^3y^3 + 12^\alpha 4(2pq-p-q+1)x^3y^4$$

5 Topological Indices of Metal-organic Framework

The following are the topological indices corresponding to M-polynomials.

Name of the Index	Index Value
$M_1(G)$	$488pq - 22p - 22q + 14$
$M_2(G)$	$672pq - 48p - 48q + 33$
$MM_2(G)$	$(82/3)pq - p - q + 1$
$R_{\alpha(G)}$	$6^\alpha 16 + 9^\alpha(16p + 16q - 24) + 12^\alpha(12pq - 8p - 8q + 8) + 16^\alpha(4pq - 2p - 2q)$
$RR_{\alpha(G)}$	$\frac{6}{3^\alpha}(1+24pq) + \frac{12}{6^\alpha}(p+q-1) + \frac{18}{3^\alpha}(12pq - 8p - 8q + 8) + \frac{48}{3^\alpha}(4pq - 2p - 2q)$
$SSD(G)$	$70pq - 3p - 3q + 2$
$H(G)$	$\frac{5984}{100}pq - \frac{4}{105}p - \frac{4}{105}q + \frac{43}{105}$
$IS(G)$	$\frac{710}{21}pq + \frac{4}{105}p + \frac{4}{105}q + \frac{1}{2}$
$AZI(G)$	$\frac{21300}{250}pq - \frac{204}{625}p + \frac{204}{625}q + \frac{1211}{1032}p$

Table 3: Topological Indices

Table 4: Comparison among various parameters of $G_1 = \mathrm{MOF}_{(p,q)}$, for $p, q \geq 2, s = t$ is shown in Table

(p, q)	$M_1(G_1)$	$M_2(G_1)$	$MM_2(G_1)$	$R_\alpha(G_1)$	$RR_\alpha(G_1)$
(2,2)	1878	2529	106	872	472

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(3,3)	4274	5793	241	1944	1236
(4,4)	7646	10401	430	3432	2368
(5,5)	11994	16353	674	5336	3868
(6,6)	17318	23649	973	7656	5736
(7,7)	23618	32289	1326	10392	7972
(8,8)	30894	42273	1734	13544	10576
(9,9)	39146	53601	2197	17112	13548
(10,10)	48374	66373	2714	21096	16888

Table 5: Comparison among various parameters of $G_1 = \mathrm{MOF}_{(\mathrm{p,q})}$, for $p, q \geq 2, s = t$

(p, q)	$SSD(G_1)$	$H(G)$	$IS(G)$	$AZI(G)$
(2,2)	270	239.36	178	401
(3,3)	4274	5793	241	1944
(4,4)	7646	10401	430	3432
(5,5)	11994	16353	674	5336
(6,6)	17318	23649	973	7656
(7,7)	23618	32289	1326	10392
(8,8)	30894	42273	1734	13544
(9,9)	39146	53601	2197	17112
(10,10)	48374	66373	2714	21096

The table indicates that as the values of p and q rise, so do the different topological indices of the MOF

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metal organic framework. This is because as the number of atoms rises, the framework gets bigger and more intricate.

Conclusion

Using M-polynomials, we have discovered unique topological indices for niobium oxide and metal-organic frameworks. For every network, we extracted nine topological indices using M-polynomial methods. We then plotted these indexes' behaviours graphically and performed a comparison analysis. The outcomes derived from these indices provide insightful information about several facets of the structures, reducing the necessity for lengthy laboratory experiments. All in all, our research advances our knowledge of the characteristics and actions of these substances.

Data Availability

In this article, no data were utilized.

Authors Contributions

All authors contributed equally.

Conflicts of Interest

Authors have no conflict of interest.

References

[1] Alam, Ashraful, et al. "Degree-Based Entropy for a Non-Kekulean Benzenoid Graph." Journal of Mathematics 2022 (2022): 25-30
[2] Ali, Akbar, et al. "Atom-bond sum-connectivity index." Journal of Mathematical Chemistry (2022): 1-13.
[3] Anjum, Muhammad Shahzad, and Muhammad Usman Safdar. "K Banhatti and K hyper Banhatti indices of nanotubes." Engineering and applied science letters 2.1 (2019): 19-37.
[4] Asghar, Adnan, et al. "K Banhatti and K hyper Banhatti indices of circulant graphs." International Journal of Advanced and Applied Sciences 5.5 (2018): 107-109.
[5] Boustani, Ihsan. Systematic ab initio investigation of bare boron clusters: Determination of the geometry and electronic structures of B_n(n = 214). Physical Review B 55.24 (1997): 16426.
[6] Chu, Yu-Ming, et al. "Computation of Zagreb Polynomials and Zagreb Indices for Benzenoid Triangular & Hourglass System." Polycyclic Aromatic Compounds (2022): 1-10.
[7] Vukičević, Damir and Gašperov, Marija. "Bond additive modeling 1. Adriatic indices." Croatica chemica acta 83.3 (2010): 243-260.
[8] N. Trinajsti, S. Nikoli, Z. Mihali, and I. Trinajsti. (1991). The Use of the Vertex-Distance Function in the Theory of Molecular Descriptors, Chemical Physics Letters, vol. 186(6), 481-484.
[9] M. Ghorbani and M. A. Hossein-Zadeh, (2017) New Insight into Modeling of M-polynomials of Nanotubes. Physica E: Low-dimensional Systems and Nanostructures, vol. 93, pp. 250-254.
[10] Gutmana, I., Furtulaa, B., Redzepovicb, I. (2024). On Topological Indices and Their Reciprocals.

Power System Technology
ISSN:1000-3673

Received: 13-02-2024 Revised: 16-03-2024 Accepted: 06-04-2024

Match Communications in Mathematical and in Computer Chemistry.

[11] D. Weber, C. Korte, D. Hesse, and J. Janek, (2018) High temperature phases of niobium (V) oxide. An in situ study, Dalton Transactions, vol. 47(24), pp. 8124-8134.

[12] H. Furukawa, K. E. Cordova, M. O'Keeffe, and O. M. Yaghi (2013) The Chemistry and Applications of Metal-Organic Frameworks, Science, vol. 341(6149), 120-128.

[13] M. J. Katz, S. Y. Moon, J. E. Mondloch, M. H. Beyzavi, C. J. Stephenson, J. T. Hupp, and O. K. Farha, (2018) Exploiting parameter space in MOFs a 20-fold enhancement of phosphate-ester hydrolysis with UiO-66-NH2, Chemical Science, vol. 6(4), pp. 2286-2291.

[14] L. Wang, Y. Han, X. Feng, J. Zhou, P. Qi, and B. Wang (2020) Metal-Organic Frameworks for Energy Storage and Conversion, Energy Storage Materials, vol. 24, pp. 492-516.

[15] Nico, C.; Monteiro, T.; Graça, M.P. (2016) Niobium oxides and niobates physical properties: Review and prospects. Prog. Mater. Sci.15-25, 80, 137. [CrossRef]

[16] Trinajstic, Nenad. Chemical graph theory. 2018 Vol. 1. 25-38.

[17] H. Hosoya, (2021) Discrete Appl. Math. 19 (1-3), 239-257.

[18] Manzoor, S., Siddiqui, M. K., & Ahmad, S. (2021). On physical analysis of degree-based entropy measures for metal-organic superlattices. The European Physical Journal Plus, 136(3), $1-22$.

[19] Ghani, M. U., Sultan, F., Tag El Din, E. S. M., Khan, A. R., Liu, J. B., Cancan, M. (2022). A Paradigmatic Approach to Find the Valency-Based K-Banhatti and Redefined Zagreb Entropy for Niobium Oxide and a Metal-Organic Framework. Molecules, 27(20), 6975.

[20] E. Deutsch and S. Klavzar (2015) Iran. J. Math. Chem. 6, 93-102 2015.

[21] Kitagawa, S. (2014). Metal-organic frameworks MOFs. Chemical Society Reviews, 43(16), 5415-5418.

[22] Czaja, A. U., Trukhan, N., Müller, U. (2009). Industrial applications of metal-organic frameworks. Chemical Society Reviews, 38(5), 1284-1293.

[23] Wurster, Benjamin, et al. "Driving the oxygen evolution reaction by nonlinear cooperativity in bimetallic coordination catalysts." Journal of the American Chemical Society 138.11 (2016): 3623-3626.

[24] Imran, M., Khan, A. R., Husin, M. N., Tchier, F., Ghani, M. U., Hussain, S. (2023). Computation of Entropy Measures for Metal-Organic Frameworks. Molecules, 28(12), 4726.