

Mathematical Study of Zinc Oxide and Zinc Silicate Metal Organic Networks Via Reduce Reverse Degree Based Topological Indices

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In this article, some reduced reverse topological indices ((RR)TIs) are calculated based on edge partitions associated with the atomic structures of the Zinc Oxide (" ZNOX " ("h") and zinc silicate ("ZNSL " ("h") metal organic networks (MON's) respectively. I have calculated the reduced reverse degree-based topological indices associated with these metal organic networks like: "RRM1" ("G")",RRM2" ("G")",RRH M1 " ("G")",RRH M2 " ("G")",RRF" ("G")", RRABC(G), RRGA(G)"respectively. I have also discussed the numerical and graphical behavior of these metal organic networks. At the end, the mathematical results obtained are compared.

Keywords: Topological Indices; Reduce Reverse Indices, Chemical Graph Theory, Metal Organic Networks.































Introduction:

A large variety of chemical compounds exists in the field of chemistry. The most famous chemical compounds are known as metal organic network (MON') which are formed of all metal ions and organic molecules. In 1957, [1] were the first ones to study MONs'. After this in 1989, [2] again gave attention to MONsdue to their design and synthesis. MON's' like Zn as a chemical sensor could be transformed into devices for the purpose of luminescent characteristics [3]. Those electrons which have abundant of T-conjugated fluorescent molecules are very friendly to prepare Zn MON's' with nucleophilic characteristics in systematic luminescent sensors [4]. The small toxicity of zinc ions as a valuable character is supposed to suggest Zn-associated MON's' into the biological domains, particularly in the field of drug carries. Actually, Zn^{2+} is an endogenous small toxic change metal cation which is abundantly used in dermatology as a cicatrizing agent and skin moisturizer with astringent, antibacterial, and anti-inflammatory agents [5]. Furthermore, the toxicology, biomedical applications, and their biocompatibility are newly described making procedures of zinc-associated MON's'. [6] align the isoreticular series (IRMOF-1 to IRMOF-16) of 16 tremendous crystalline materials. Thus, so many IRMOF structures can be expand by applying zinc oxide octahedral clusters (Zn4O(CO)2) as the metal corners associated via diverse organic dicarboxylate linkers and so many others different 3-dimensional cubic networks are created. MON's' are mostly used to known the physicochemical properties like: grafting active groups [7], impregnating appropriate active material [8], ion interchange [9], producing composites with distinct substances [10], exchanging organic molecules reply time, and selectivity [11]. Recently, [12] and [13] give the progress in on the composing of many nanostructures and MON-associated applications like: electrocatalysis, sensing, photocatalysis, catalyst for manufacturing of first-class chemicals, and lithium-ion batteries. The subject of graph theory has proven to be a very effective tool in the field of modern chemistry which indicate the chemical and physical characteristics of the chemical compounds like: heat of formation, heat of evaporation, flash point, melting point, boiling point, temperature, pressure, density, and tension and partition coefficient [14][15][16].

Zinc oxide network (ZNOX (h)) is a chemical compound which is in fact insoluble in water and it is considered as an inorganic compound in the form of a white powder with density $5.61 g/cm^3$. ZNOX (h) when heated with carbon that decreases to the metal vapor to compress the liquid from which the solid metal freezes $ZnO_{(s)} + C_{(s)} \longrightarrow Zn_{(g)} + CO_{(g)}$. Zinc acts as a reactive metal to construct zinc ion (Zn^{2+}) and hydrogen gas. Likely "reduces those metal ions whose reduction potentials are higher than Zn^{2+}. ZNOX (h) is usually used in the manufacturing of rubber, enamels, pigment in white paint, photo-conductive surfaces, and protective coating for other metals. Figure 1 indicates the zinc oxide related MON' of dimension 3.

Zinc silicate network (ZNSL (h): silicate (SiO_4) lies in very attractive class of minerals. Silicate is in fact the chemical mixture of metal oxide with sand. The fundamental unit of SiO_4 is tetrahedron. Thus, all silicates get SiO_4 tetrahedron. Oxygen ions and silicon ions are denoted by the corner vertices and center vertices of SiO_4. In field of graph theory, we denote corner vertices and center vertices of SiO_4 with oxygen nodes and silicon nodes. Figure 2 indicates the ZNSL(h) related MON' of dimension 3. For more information, see Figure 2.

In the research of [17], 40], the precise prescription of topological indices of a certain synthetic structure has been enumerated and displayed. Using the reduced reverse degree based edge partitions, the reduced reverse degree based versions of the Zagreb indices, atom bond connectivity index, and geometric arithmetic index of the first and second metal organic frameworks in [18]. [19], [20][21][22][23][24][25] are references for the contributions

in Zagreb indices in recent years. A mathematically written assertion R(v) = Δ(G) – d(v)+1, is the notion of the reverse degree of a vertex was first introduced by [26]. Where Δ(G) is the largest degree of vertex and the notation dv is the number of edges attached to a vertex. Inspired from the above ideas regarding reduced reverse degree based topological indices of different chemical compounds. I would like to introduce the concept of calculating reduced reverse degree based topological indices for the chemical compound of Zinc Oxide and Zinc Silicate Metal Organic networks.

In this article, I computed new results for reduced reverse degree based topological indices (RR)TIs for the molecular structure of metal organic networks like ZNOX(h) and ZNSL(h) in the form of theorems (see section 3.1 and 3.2). It is worth highlighting that my study marks a pioneering effort, as I am the first one to calculate (RR)TIs of these networks. For the more detail about these reduce reverse (RR)TIs and TIs see references [26][27][28][29][30][31][32][33][34][42] [43] [44][45][46]].

Material and Methods:

In this study, let $G(V,E)$ be the graph of a given chemical compound with vertex set V and edge set E of a connected graph G. The number of edges attached with a vertex is known as degree of that vertex. The degree of a vertex e and f are represented by $d(e)$ and $d(f)$ and edge of a graph G by $ef \in E(G)$ respectively. The edges and vertices for the networks of $ZNOX\ (h)$ and $ZNSL\ (h)$ are determined and then the number of rows and columns is increased. In Figure1, $|V(G)| = 70\mathrm{h} + 46$ and $|E(G)| = 85\mathrm{h} + 55$ represent the number of vertices and edges in a graph G. In Figure 2, cardinality of vertex $|V(G)| = 82\mathrm{h} + 50$ and edge $|E(G)| = 103\mathrm{h} + 61$ respectively (for more detail see table 1 to 4). After this, some reduced reverse topological indices of the above indicated structures are determined. Finally, the graph of these structures is sketched by using excel.

The reduced reverse Zagreb indices [35][36][37] which are defined as:

$$RRM_1(G) = \sum_{kl \in E} [RR(h) + RR(k)] \text{ Eq } 2.1$$

$$RRM_2(G) = \sum_{ij \in E} [RR(h) \times RR(k)] \text{ Eq } 2.2$$

The reduced reverse hyper-Zagreb indices [38], which are represented as:

$$RRHM_1(G) = \sum_{ij \in E} [RR(h) + RR(k)]^2 \text{ Eq } 2.3$$

$$RRHM_2(G) = \sum_{ij \in E} [RR(h) \times RR(k)]^2 \text{ Eq } 2.4$$

Furtula and Gutman [39] is defined the reduced reverse forgotten index as:

$$RRF(G) = \sum_{ij \in E} [RR(h)^2 + RR(k)^2] \text{ Eq } 2.5$$

The reduced reverse atom bond connectivity index [40], is described as:

$$RRABC(G) = \sum_{ij \in E} \left[\frac{RR(h) + RR(k) - 2}{RR(h) \times RR(k)}\right] \text{Eq } 2.6$$

The reduced reverse Geometric-arithmetic index [41] is represented as:

$$RRGA(G) = \sum_{ij \in E} \left[\frac{2\sqrt{RR(h) \times RR(k)}}{RR(h) + RR(k)}\right] \text{ Eq } 2.7$$

Mathematical Results & Discussion for Computed Results:

Reduce Reverse Degree Based Topological Indices of Zinc Oxide Network

Let $G1(h,k)$ be the 3-dimensional graph of $ZNOX\ (h)$ MON's', where 'h' and 'k' are the unit cells in a row and column respectively. The molecular graph of $G1(2,2)$ is shown below in Figure In this section, some reduced reverse (RR)TIs for the MON's'of $ZNOX\ (h)$ are determined.

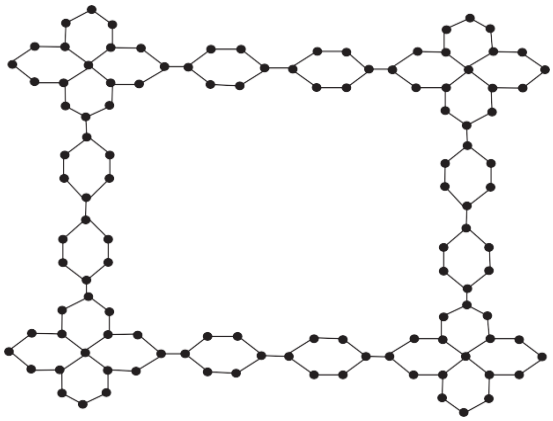


Figure 1. Zinc oxide network (ZNOX(h) ≅T) for h =3.

By using some mathematical techniques on the above Figure1 the constructed table is shown below.

Table 1. Edge partitions of Zinc oxide network

E_j	Types of edges (d(h),d(k))	Total No. of edges
E_1	(2,2)	6h+16
E_2	(2,3)	52h+28
E_3	(3,3)	9h+3
E_4	(3,4)	8h+8

By using table 1 and the formula of (RR)TIs $RR(h) = \Delta(G) - d(h) + 2$, where $\Delta(G)$ denote the maximum degree of the graph G and $d(h)$ represent the degree of the vertex h [26]. I have constructed the following table for the reduce reverse degree-based TIs.

Table 2. Edge partitions of Zinc oxide network

E_j	Types of edges (RR(h), RR(k))	Total No. of edges
E_1	(4,4)	6h+16
E_2	(4,3)	52h+28
E_3	(3,3)	9h+3
E_4	(3,2)	8h+8

Theorem:

Let $T \cong ZNOX(h)$ be the graph of Zinc oxide network for $h \geq 3$. Then the (RR)TIs of $ZNOX(h)$ are given below:

1. $RRM_1(ZNOX(h)) = 506h + 382$
2. $RRM_2(ZNOX(h)) = 849h + 667.$

Proof: By using Eq2.1, Eq 2.2 and Table 2.

$$1.\ RRM_1(ZNOX(h)) = \sum_{hk \in E(ZNOX(h))} [RR(h) + RR(k)]$$

$$= (6h + 16)(4 + 4) + (52h + 28)(4 + 3) + (9h + 3)(3 + 3) + (8h + 8)(3 + 2)$$

$$= 506h + 382\ .$$

$$2.\ RRM_2(ZNOX(h)) = \sum_{hk \in E(ZNOX(h))} [RR(h) \times RR(k)]$$

$$= (6h + 16)(4 \times 4) + (52h + 28)(4 \times 3) + (9h + 3)(3 \times 3)$$

$+(8h+8)(3\times 2)$
$=849h+667$.

Theorem:

Let $T\cong ZNOX(h)$ be the graph of Zinc oxide network for $h\geq 3$. Then the (RR)TIs of $ZNOX(h)$ are computed as given below:

1. $RRHM_1(ZNOX(h))=1162h+2704$
2. $RRHM_2(ZNOX(h))=10041h+8659$
3. $RRHF(ZNOX(h))=1758h+370.$

Proof: I will prove the theorem by using Eq 2.3, Eq 2.4, Eq 1.5 and Table 2.

1. $RRHM_1(ZNOX(h))=\sum_{hk\in E(ZNOX(h))}[RR(h)+RR(k)]^2$

$=(6h+16)(4+4)^2+(52h+28)(4+3)^2+(9h+3)(3+3)^2$
$+(8h+8)(3+2)^2$
$=1162h+2704$.

2. $RRHM_2(ZNOX(h))=\sum_{hk\in E(ZNOX(h))}[RR(h)\times RR(k)]^2$

$=(6h+16)(4\times 4)^2+(52h+28)(4\times 3)^2+(9h+3)(3\times 3)^2$
$+(8h+8)(3\times 2)^2$
$=10041h+8659$.

3. $RRF(ZNOX(h))=\sum_{hk\in E(ZNOX(h))}[RR(i)^2+RR(j)^2]$

$=(6h+16)(4^2+4^2)+(52h+28)(4^2+3^2)+(9h+3)(3^2+3^2)$
$+(8h+8)(3^2+2^2)$
$=1758h+370$

3.1.3 Theorem:

Let $T\cong ZNOX(h)$ be the graph of Zinc oxide network for $h\geq 3$. Then the following (RR)TIs of $ZNOX(h)$ are given below:

1. $RRABC(ZNOX(h))=\frac{98}{3}h+23$
2. $RRGA(ZNOX(h))=\left(\frac{75+1040\sqrt{3}+112\sqrt{6}}{35}\right)h+\left(95+80\sqrt{3}+16\sqrt{6}\right)$.

Proof: I will prove the theorem by using Eq2.6, Eq 2.7 and Table 2.

1. $RRABC(ZNOX(h))=\sum_{hk\in E(ZNOX(h))}\left[\frac{RR(h)+RR(k)-2}{RR(h)\times RR(k)}\right]$

$=(6h+16)\left(\frac{4+4-2}{(4\times 4)}\right)+(52h+28)\left(\frac{4+3-2}{(4\times 3)}\right)+(9h+3)\left(\frac{3+3-2}{(3\times 3)}\right)$
$+(8h+8)\left(\frac{3+2-2}{(3\times 2)}\right)$
$=\frac{98}{3}h+23$.

2. $RRGA(ZNOX(h))=\sum_{hk\in E(ZNOX(h))}\left[\frac{2\sqrt{RR(i)\times RR(j)}}{RR(i)+RR(j)}\right]$

$=(6h+16)\left(\frac{2\sqrt{4+4}}{(4+4)}\right)+(52h+28)\left(\frac{2\sqrt{4+3}}{(4+3)}\right)+(9h+3)\left(\frac{2\sqrt{3+3}}{(3+3)}\right)$

$$+(8h+8)\left(\frac{2\sqrt{3}+2}{(3+2)}\right)$$

$$=\left(\frac{75+1040\sqrt{3}+112\sqrt{6}}{35}\right)h+\left(95+80\sqrt{3}+16\sqrt{6}\right).$$

Reduce Reverse Degree Based Topological Indices of Zinc Silicate Network:

Let $G1(h,k)$ be the 3-dimensional graph of $ZNSL(h)$ MON's', where 'h' and 'k' are the unit cells in a row and column respectively. The molecular graph of $G1(2,2)$ is shown below in Figure 2. In this section, some reduced reverse (RR)TIs for the MON's' of ZNSL(h) are computed

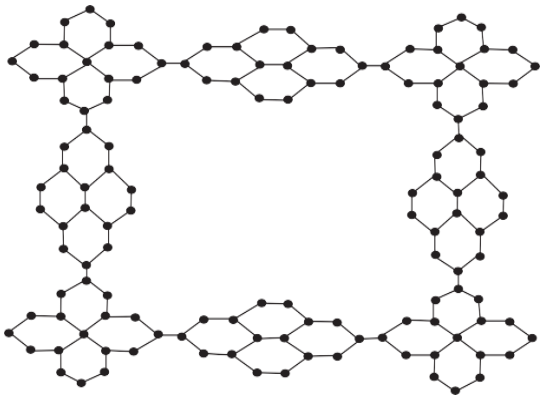


Figure 2. Zinc silicate network (ZNSL(h) ≅ W) for h = 3.

By using some mathematical techniques (relating to counting the degree of a vertex etc.) on the above Figure 2. The constructed table of above structure is given below.

Table 3: Edge partitions of zinc silicate network

E_j	Types of edges (d(h),d(k))	Total No. of edges
E_1	(2,2)	10h+14
E_2	(2,3)	64h+32
E_3	(3,3)	21h+7
E_4	(3,4)	8h+8

By using table 3 and the formula of (RR)TIs $RR(h)=\Delta(G)-d(h)+2$, where $\Delta(G)$ denote the maximum degree of the graph G and $d(h)$ represent the degree of the vertex h [26]. I have the following table for the reduced reverse degree based TIs.

Table 4. Edge partitions of zinc silicate network

E_j	Types of edges (RR(h), RR(k))	Total No. of edges
E_1	(4,4)	10h+14
E_2	(4,3)	64h+32
E_3	(3,3)	21h+7
E_4	(3,2)	8h+8

Theorem. Let $W \cong \mathrm{ZNSL(h)}$ be the graph of zinc silicate network for $h \geq 3$. Then the following (RR)TIs of $\mathrm{ZNSL(h)}$ are given below:

1. $RRM_1(\mathrm{ZNSL(h)}) = 694h + 418$
2. $RRM_1(\mathrm{ZNSL(h)}) = 1165h + 719.$

Proof: By using Eq2.1, Eq2.2 and Table 4.

1. $$RRM_1(\mathrm{ZNSL(h)}) = \sum_{hk\in E(\mathrm{ZNSL(h)})} [RR(h)+RR(k)]$$

$$=(10h+14)(4+4)+(64h+32)(4+3)+(21h+7)(3+3)$$
$$+(8h+8)(3+2)$$

$= 694h + 418$.

2. $RRM_2(\text{ZNSL(h)}) = \sum_{hk \in E(\text{ZNSL(h)})} [RR(h) \times RR(k)]$

$= (10h + 14) \times (64h + 32)(4 \times 3) + (21h + 7)(3 \times 3)$
$+(8h + 8)(3 \times 2)$
$= 1165h + 719$.

3.2.2 Theorem

Let $W \cong \text{ZNSL(h)}$ be the graph of Zinc oxide network for $h \geq 3$. Then the following (RR)TIs of ZNSL(h) are given below:

1. $RRHM_1(\text{ZNSL(h)}) = 4752h + 2916$
2. $RRHM_2(\text{ZNSL(h)}) = 12631h + 9047$
3. $RRHF(\text{ZNSL(h)}) = 2402h + 1478.$

Proof: I will prove the theorem by using Eq 2.3, Eq 2.4 , Eq2.5 and Table 4.

1. $RRHM_1(\text{ZNSL(h)}) = \sum_{hk \in E(\text{ZNSL(h)})} [RR(h) + RR(k)]^2$

$= (10h + 14)(4 + 4)^2 + (64h + 32)(4 + 3)^2 + (21h + 7)(3 + 3)^2$
$+(8h + 8)(3 + 2)^2$
$= 4752h + 2916$.

2. $RRHM_2(\text{ZNSL(h)}) = \sum_{hk \in E(\text{ZNSL(h)})} [RR(h) \times RR(k)]^2$

$= (10h + 14)(4 \times 4)^2 + (64h + 32)(4 \times 3)^2 + (21h + 7)(3 \times 3)^2$
$+(8h + 8)(3 \times 2)^2$
$= 2402h + 1478$.

3. $RRF(\text{ZNSL(h)}) = \sum_{hk \in E(\text{ZNSL(h)})} [RR(h)^2 + RR(k)^2]$

$= (10h + 14)(4^2 + 4^2) + (64h + 32)(4^2 + 3^2) + (21h + 7)(3^2 + 3^2)$
$+(8h + 8)(3^2 + 2^2)$
$= 9450h + \frac{925}{36}$.

Theorem:

Let $W \cong \text{ZNSL(h)}$ be the graph of Zinc oxide network for $h \geq 3$. Then the following (RR)TIs of ZNSL(h) are given below:

1. $RRABC(\text{ZNSL(h)}) = 9450h + \frac{925}{36}$
2. $RRGA(\text{ZNSL(h)})$

$$= \left(\frac{90\sqrt{8} + 768\sqrt{7} + 192\sqrt{5} + 336\sqrt{6}}{72}\right)h + \left(\frac{63\sqrt{2} + 96\sqrt{7} + 48\sqrt{5} + 28\sqrt{6}}{18}\right).$$

Proof: By using Eq2.6, Eq2.7 and Table 4.

1. $RRABC(\text{ZNSL(h)}) = \sum_{hk \in E(\text{ZNSL(h)})} \left[\frac{RR(h) + RR(k) - 2}{RR(h) \times RR(k)}\right]$

$= (10h + 14)\left(\frac{4 + 4 - 2}{(4 \times 4)}\right) + (64h + 32)\left(\frac{4 + 3 - 2}{(4 \times 3)}\right) + (21h + 7)\left(\frac{3 + 3 - 2}{(3 \times 3)}\right)$

$$+(8h+8)\left(\frac{3+2-2}{(3\times 2)}\right)$$

$$=9450h+\frac{925}{36}.$$

2. $$RRGA(\text{ZNSL(h)})=\sum_{hk\in E(\text{ZNSL(h)})}\left[\frac{2\sqrt{RR(h)\times RR(k)}}{RR(h)+RR(k)}\right]$$

$$=(10h+14)\left(\frac{2\sqrt{4+4}}{(4+4)}\right)+(64h+32)\left(\frac{2\sqrt{4+3}}{(4+3)}\right)+(21h+7)\left(\frac{2\sqrt{3+3}}{(3+3)}\right)$$

$$+(8h+8)\left(\frac{2\sqrt{3+2}}{(3+2)}\right)$$

$$=\left(\frac{90\sqrt{8}+768\sqrt{7}+192\sqrt{5}+336\sqrt{6}}{72}\right)h+\left(\frac{63\sqrt{2}+96\sqrt{7}+48\sqrt{5}+28\sqrt{6}}{18}\right).$$

Numerical and Graphical Discussion on Mathematical Results:

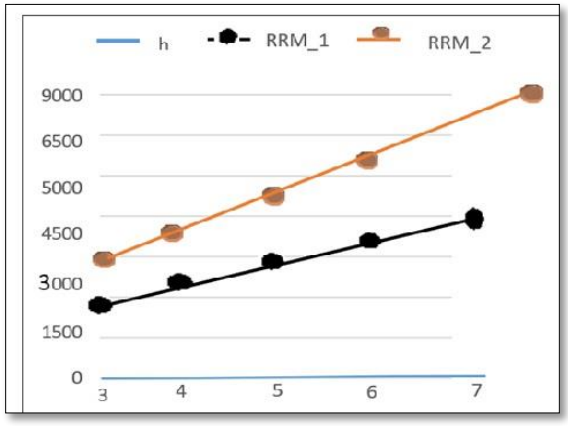
For the MON's' of $ZNOX(h)\ and\ ZNSL(h)$ some (RR)TIs are computed. The comparison of these (RR)TIs **gives** us insights into their many structural and chemical properties. In Tables 5 and 6, all the (RR)TIs in fact indicates the connectivity of atoms for the given graphs. The maximum value of the (RR)TIs indicates **strong connectivity** while the minimum value represents weak connectivity. Among all (RR)TIs the value of $RRHM_2(G)$ is maximum than all other (RR)TIs. This shows that $RRHM_2(G)$ gives us stronger connectivity for both graphs than other (RR)TIs as shown in Tables 5 and 6.

Table 5. Numerical results for the Zinc oxide

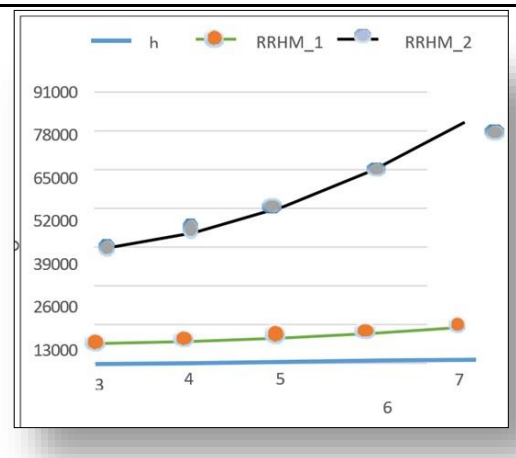
For h=	Reduced reverse first Zagreb index RRM_1	Reduced reverse second Zagreb index RRM_2	Reduced reverse first hyper Zagreb Index $RRHM_1$	Reduced reverse second hyper Zagreb index $RRHM_2$	Reduced reverse Forgotten index RRF	Reduced reverse atom bond index RRABC	Reduced reverse geometric index RRGA
3	1900	3214	6190	38782	5644	121	457.04
4	2406	4063	7352	48823	7402	153.64	518.47
5	2912	4912	8514	58864	9160	186.3	579.8
6	3418	5761	9676	68905	10918	218.96	641.33
7	3924	6610	10838	78946	12676	251.61	702.76
8	4430	7459	12000	88987	14434	284.28	764.19

Table 6. Numerical results for the Zinc Silicate

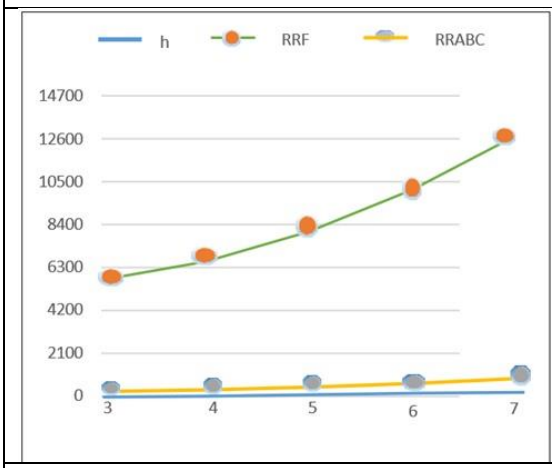
For h=	Reduced reverse first Zagreb index RR M_1	Reduced reverse second Zagreb index RR M_2	Reduced reverse first hyper Zagreb RRH M_1	Reduced reverse second hyper Zagreb index RRH M_2	Reduced reverse Forgotten index RRF	Reduced reverse atom bond index RRABC	Reduced reverse geometric index RRGA
3	2500	4214	17172	46940	8684	28375.69	176.28
4	3194	5379	21924	59571	11086	37825.69	225.43
5	3888	6544	26676	72202	13488	47275.69	274.58
6	4582	7709	31428	84833	15890	56725.69	323.73
7	5276	8874	36180	97464	18292	66175.69	372.88
8	5970	10039	40932	110095	20694	75625.69	427.47



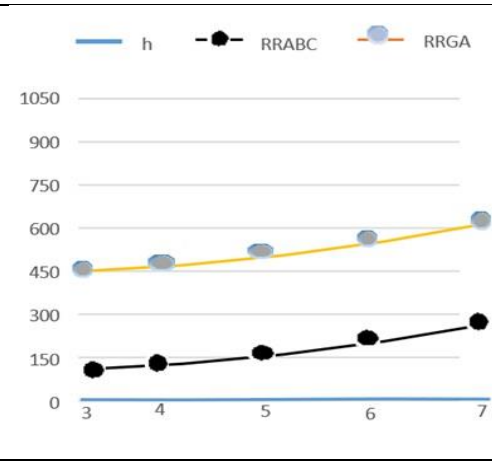
Graphical comparison of RRM_1 & RRM_2 for Zinc Oxide



Graphical comparison of RRHM_1 & RRHM_2 for Zinc Oxide.

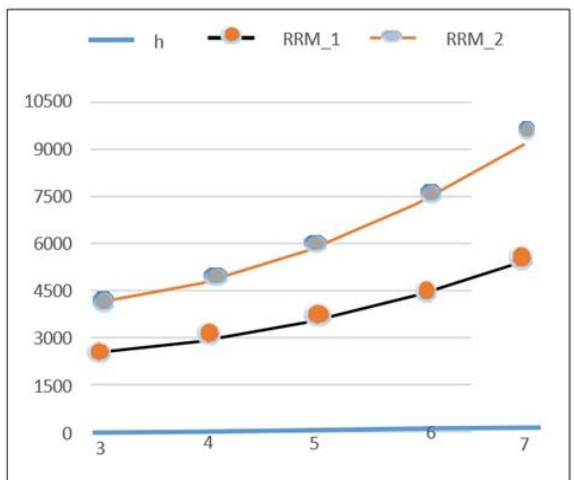


Graphical comparison of RRF & RRABC & RRGA for Zinc Oxide.

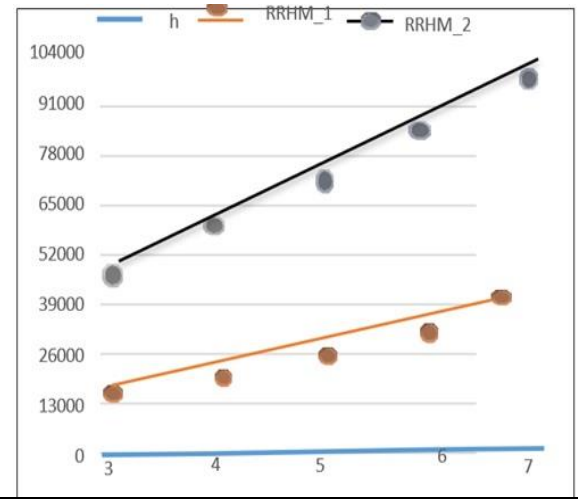


Graphical comparison of RRABC and For Zinc Oxide.

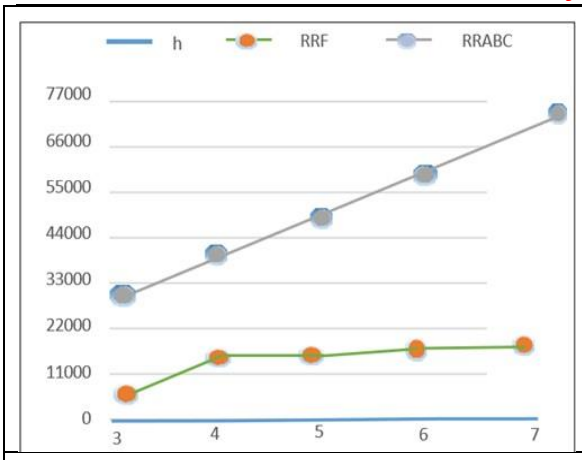
Figure 3: Graphical comparison of reduced reverse topological indices of Zinc Oxide



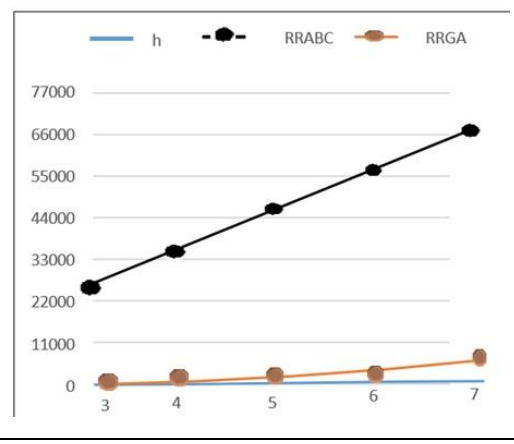
Graphical comparison of RRM_1 and RRM_2 for Zinc Silicate.



Graphical comparison of RRM_1 and RRM_2 for Zinc Silicate.



Graphical comparison of RRF and RRABC for Zinc Silicate.



Graphical comparison of RRABC and RRGA for Zinc Silicate.

Figure 4: Graphical comparison of reduced reverse topological indices of Zinc Silicate

Conclusion:

Topological indices are widely used as graph theoretical measures to determine the physicochemical properties like: grafting active groups, impregnating appropriate active material, ion interchange, producing composites with distinct substances, and selectivity of the given metal organic networks. The chemical structure of a given molecular graph is used to find the topological indices, which are widely used in the field of theoretical chemistry, environmental chemistry, toxicology, engineering and many other fields for the purpose of correlation analysis. Moreover, reduce reverse(RR)TIs and the topology of a molecule play a fundamental role in characterizing the shaping properties like: melting point, boiling point, enthalpy, and entropy of the given molecular graph. In this article, (RR)TIs of two important metal organic networks (MON's') such as Zinc oxide $(ZNOX\,(h))$ and Zinc silicate $(ZNSL\,(h))$ are computed. Also the numerical and graphical behaviors of these MON's' via (RR)TIs are discussed.

Limitations: The formula subtract the local vertex degree from the graph's over all maximum degree $\Delta(G)$, a single structural change or a peripheral heteroatom altering $\Delta(G)$ shifts the $RR(v)$ values for every single vertex in the entire molecular graph.

Future Work: In future study, I will apply these indices to some different MON's' and determine the physical chemical properties of these structures.

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Ethical Consideration: I consider all ethical considerations while conducting this study.

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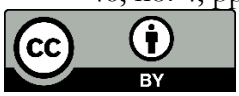
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