On computation of the topological invariants of metal-organic networks

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Abstract

Metal-Organic Networks (MON's) is the central bone for the chemical compounds of the latest study for the energy department. The study of MON's structure provides us numerous benefits in different fields related to chemical sciences, electrical and civil sectors. The MON's structure is also used to restore different chemical compounds, especially those elements which can be used for the energy purpose such as hydrogen and carbon. Topological indices of the MON's structure provide relationships between physical and chemical characteristics of the this compound such as melting points, boiling points, chemically stability, pressure, chemical reaction factors and many other basic properties. In this paper we calculate different topological indices based on first, second and third distances for two different metal-organic networks with expanding number of layers consisting on both organic ligands and metal vertices. A comparison between the calculated different kinds of the Topological Indices with the help of the numerical values and their graphical representation is also included.

On computation of the topological invariants of metal-organic networks

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In this paper we calculate different topological indices based on first, second and third distances for two different metal-organic networks with expanding number of layers consisting on both organic ligands and metal vertices. A comparison between the calculated different kinds of the Topological Indices with the help of the numerical values and their graphical representation is also included.

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Index Term

Metals-Organic Networks (MON), Chemical Compounds and Topological Invariants.

1 Introduction

According to the Chemistry, every substance is made up of different chemical element and every element has its own properties. Every element change the chemical, physical properties of that substance with respect to the its properties as well as its appearance too. Besides this, in the world of the chemistry some element are found in every substance in form of some order or bond and these element are are hydrogen, carbon oxygen and nitrogen. Almost every substance is made of these elements combination. As we know that hydrogen is the flame catching element and it help in combustion. Hydrogen is one of the next-source supply of energy [32, 34]. Hydrogen is such gas which is odourless and colourless and as a gas, it cannot be detected by ordinary means. So, it is the focus of the energy sector that low percentage of hydrogen can be detected by some sort of tool in less than a minute [25, 27, 31, 43].

Many scientist are working on the some method or device that can detect hydrogen as fast as it can. So, a group of scientist are give some progress in this regard. Won-Tea et al. [41] are successful in formation of a device that consist of Metal Organic Network (MON) in the palladium nano-wires which told the presence of molecular hydrogen(H_2) in less than seven seconds. Moreover, besides recognization and sensing, the MONs possess a large number of chemical and physical properties that are define in impregnating suitable active materials [2, 3, 5], ion exchange and post synthetic ligand [28], changing organic ligands [30], grafting active groups [18] and formation of composites with useful substance [11, 28]. The relation between solvents, molar ration, pH, temperature and architectures of MON's are proposed by the Seetharaj et al.[32]. MON's are very helpful and useful for the purification, storage and separation of molecules [17, 38]and gate path for the construction of nano-structures[29].

Now a days, a lot of important computational tools are used to compare certain type of chemical compounds in modern chemistry that come from graph theory. These tools are used to investigate several structural properties including physical and chemical properties of these compounds. A topological invariant (or simply denoted by TI) is one of the most important and basic tool which is used for the calculation of several types of properties of the organic materials such as heat of formation, heat of evaporation, melting point, temperature, tension, flash point,retention times in density and chromatography, boiling point, density, pressure, partition coefficient [9, 14, 24, 26, 37]. For the evaluation of paraffin's boiling point Wiener (1947) used a distance-based formula [42, 36]. Gutman and Trinajsti [12] (1972) defined some topological indices to evaluate a conjugated molecules' total energy of the π-electrons.

Furthermore, TI's show a fantastic results within the QSAR/QSPR research to narrate the systems with some chemical and biological property. This relation is mathematically expressed. Wasson [27] (2019) delivered the idea of linker opposition with a Metal Organic Network (MON) for topological invariants. The TI's of numerous networks which incorporates honeycomb structures, oxide networks consisting of C_6 and C_8 cycles, icosahedral, futtball like chemical structures called fullerene and large cylindrical type nanostructures known as carbon nanotubes are studied in [4, 6, 7, 8, 15, 16, 19, 21, 35, 39, 40, 20, 22]. The degree based indices for Eulerian graph [52, 54] for Zagreb indices, Sierpinski networks [53, 56] for topological descriptors and structural property and for lattices [55] have also been studied.

In the current study, we have investigated various topological indices that can be expressed in terms of the degrees of vertices of graphs with focus on parameters that describe the number of vertices lying at short distances from a given vertex in a graph. We have considered first second and third degrees of every vertex in this work. We consider metal organic networks of two kinds denoted by MON_1(t) and MON_2(t), where $t \geq 2$ represent the growth stage of these networks. When t increases, tehse networks grow in the outwards direction. Interestingly, both of these metal organic networks are structurally different but the order and size of these networks remains same for at all growth stages. We consider both organic ligands and metal nodes as well. The rest of the sections discuss the computation of the leap Zagreb indices and Wiener polarity indices for these graphs.

2 PRELIMINARIES

We consider a graph G to be a graph $G = (V(G), E(G))$, where the set $V(G)$ represents the vertex set of G and defined as $V(G) = \{v_1, v_2, ..., v_n\}$ and similarly the set $E(G)$ denotes the edge set of G respectively. The $|V(G)| = n$ is the order of the graph and $|E(G)| = m$ is the size of graph G. When there exists a path between every pair of vertices in G, we say that the graph G is connected graph. The distance $d(u, v)$ between two vertices u, v of graph G is defined as the length of the shortest path between u and v.

The first, second and third leap Zagreb indices of a graph have been introduced by Naji et al. and these are define as " the sum of squares of second degrees of vertices of G" is called first degree, "the sum of products of second degrees of pairs of adjacent vertices in G" is define as second degree and "the sum of products of first and second degrees of vertices of G" is called third leap Zagreb indices, respectively. For a MON graph, the first kind (LM_1), second kind (LM_2) and third kind (LM_3) leap Zagreb indices are defined as:

$$LM_1 = \sum_{v_i=1}^{n} d_2(v_i) \tag{1}$$

$$LM_2 = \sum_{i=1}^{n} d_2(v_i)d_2(v_j) \tag{2}$$

$$LM_3 = \sum_{i=1}^{n} d_1(v_i)d_2(v_i) \tag{3}$$

The concept of co-indices was invented by Doslic in 2008 and was first applied to the two Zagreb indices. Thus, in the co-induce of leap zagreb, we take those edges who found in the complement of any graph. we have to take a vertex and then take all the edges that are in the complement of that graph. Then repeat for every vertex and take sum of all the vertices. Definition: For any MON graph, second ($\overline{LM}_2$) and third ($\overline{LM}_3$) version of leap Zagreb Co-indices are

$$\overline{LM_2} = \sum_{(u,v)\notin E(G)} d_2(u)d_2(v) \tag{4}$$

$$\overline{LM_3} = \sum_{(u,v)\notin E(G)} d_2(u) + d_2(v) \tag{5}$$

As earlier we discussed about the structure of the leap Zagreb Co-indices, that it is an edge-based formula that take those edges which are in the complement of the graph. So, in rebuttal of above mention formula, we drive a formula that gave same result and work in the same manner but it is a vertex based formula and define on the neighborhood of that vertex. It is very useful for those graph which are symmetry on some point in any direction. As follow:

$$\begin{aligned}
\overline{LM}_2 &= \sum_{v\epsilon V(G)} f_v d_2(v_i)\Big\{\sum_{i=1}^{n} d_2(v_i) - d_2\big(N(v_i)\big)\Big\} \\
\overline{LM}_3 &= \sum_{v\epsilon V(G)} f_v \Big[\Big\{\sum_{i=1}^{n} d_2(v_i) - d[N(v_i)]\Big\} \\
&\quad + \Big\{d_2(v_i)\big(|V| - |N(v_i)|\big)\Big\}\Big]
\end{aligned}$$

The Wiener polarity index W_P(G) of a graph G is define as, the sum of the number of unordered pairs of vertices u, v of G such that the distance of u and v is equal to 3."
"The Harold Wiener introduced Wiener Polarity Index in 1947 for quantity. To calculate boiling points (BF) t_B of the paraffin, Wiener used a linear formula of W(G) and W_P(G). The Wiener Polarity index formula is define as:

$$W(G) = \sum_{i=1}^{n} \frac{1}{2} d_3(v_i) \tag{6}$$

3 Metal Organic Network (MON)

In this section, we study about structure of the metal-organic network (MON) that is made up of metals and organic molecules due to chemical bonding as shown in Figure 1 and Figure 2. The metal is zeolite imidazole which is shown as bigger vertex and organic element is shown as smaller vertex [41]. The networks (MON_1) and (MON_2) is formed by the combination of the basic Metal Organic structure. In the (MON_1), the bigger vertex which are zeolite imidazole are joined with each other. Similarly, In the (MON_2), the smaller vertex which are organic metal are joined with each other. In this way, the metal organic structure are increasing. Both (MON_1) and (MON_2) are the primary structure with different physical, chemical and all other properties. For these networks we have $|V(MON_1(t))| = 48t = |V(MON_2(t))|$ and $|E(MON_1(t))| = 72t - 12 = |E(MON_2(t))|$, where $t \geq 2$.

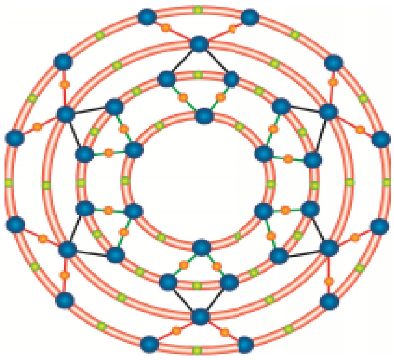

Figure 1: $MON_1(t)$ for t=2

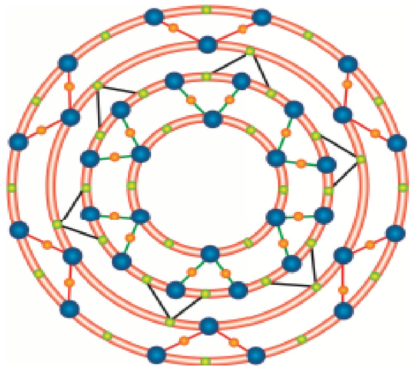

Figure 2: $MON_2(t)$ for t=2

4 Basic Results on MON$_1$ and MON$_2$

First we discussed some basic results for both of the MON's structure, that is, the order and size of both MON's, in the previous section. Now we discuss some properties of the $MON_1(t)$ graphs in details. The number of distinct types of vertices in $MON_1(t)$ can be identified as four, and they belong to the set $\{2, 3, 4, 6\}$. So we have the following vertex partitioning with respect to these types.

$$\begin{aligned} V_1 &= [v\epsilon V(MON_1(t))|V(v) = 2] \\ V_2 &= [v\epsilon V(MON_1(t))|V(v) = 3] \\ V_3 &= [v\epsilon V(MON_1(t))|V(v) = 4] \\ V_4 &= [v\epsilon V(MON_1(t))|V(v) = 6] \end{aligned}$$

On the same lines, we have four different types of edge partition depending upon the degrees on end-vertices of all edges in MON$_1$(t) that belong to the set $\{(2, 3), (2, 4), (2, 6), (4, 6)\}$. Thus, we have Table 1 and Table 2.

Table 1: Partition of edges with respect degree of end-vertices

$d(u), d(v)$	Frequency
$(2, 3)$	36
$(2, 4)$	$12(3t - 1)$
$(2, 6)$	$24(t - 1)$
$(4, 6)$	$12(t - 1)$

Now, we define the vertex/edge partitions of $MON_2(t)$. The number of distinct types of vertices in $MON_2(t)$ can be identified as three, which are in the set $\{2, 3, 4\}$. So, we have

$$\begin{aligned} V_1 &= [v\epsilon V(MON_1(t))|V(v) = 2] \\ V_2 &= [v\epsilon V(MON_1(t))|V(v) = 3] \\ V_3 &= [v\epsilon V(MON_1(t))|V(v) = 4] \end{aligned}$$

We have five different types of edges that are based on the degrees of end vertices in $MON_2(t)$ that are define as $(2, 3), (2, 4), (3, 3), (3, 4)$ and $(4, 4)$. Thus, we have

Table 2: Partition of edges with respect degree of end-vertices

$d(u), d(v)$	Frequency
$(2, 3)$	$12(t + 2)$
$(2, 4)$	$12(t + 1)$
$(3, 3)$	$24(t - 1)$
$(3, 4)$	$12(t - 1)$
$(4, 4)$	$12(t - 1)$

5 Tables Of First,Second and Third Degree Of MON's(t)

Before going on toward to the main results of our paper, we have to discuss the first, second and third degree of the MON's because we are using in the above mentioned result. Similarly, in this section we study the partition of the vertices and edges with respect to the first, second and third degrees.

5.1 Tables Of MON_1

"In this section, tables of MON_1 are discussed with respect to the vertex and edge partition. We discuss the vertex and edge partition of MON_1 with respect to the first, second and third degrees in Tables 3–7 which are used in the main results that provide us application in many fields.".

Table 3: Partition of Vertex with respect to the 1^{st} distance of Vertices

$d_1(v)$	Frequency
2	$30n$
3	12
4	$12n - 6$
6	$6n - 6$

Table 4: Partition of Vertices with respect 2^{nd} distance of Vertices

$d_2(v)$	Frequency
3	12
4	18
6	$12n - 6$
7	12
8	$24n - 36$
10	$12n - 12$

Table 5: Partition of Vertex with respect to the 3^{rd} distance of Vertices

$d_3(v)$	Frequency
4	12
6	6
9	12
10	12
11	12
12	6
14	$12n - 12$
16	$12n - 12$
18	$18n - 30$
20	6
22	$6n - 12$

Table 6: Partition of Edges with respect to 2^{nd} distance of degrees of end Vertices

$d_2(u,v)$	Frequency
$(3,4)$	24
$(3,7)$	12
$(4,6)$	24
$(6,8)$	$24n - 12$
$(7,10)$	12
$(8,10)$	$24n - 36$
$(8,8)$	$12n - 24$
$(10,10)$	$12n - 12$

Table 7: Partition of Vertices with respect to sum of the degrees of Neighbourhood

$d_2(v)$	S_v	Frequency
3	18	12
4	10	12
4	28	6
6	14	6
6	18	12
6	22	$12n-12$
7	20	12
8	26	$12n-24$
8	36	12
8	38	$12n-24$
10	30	$6n-6$
10	38	$6n-12$
10	60	6

5.2 Tables Of MON_2

This section is giving us the edge and vertex partition of the MON_2 with respect to the first, second and third degree partition in Tables 8–12. It is also important for our main results for Metal organic Network like structures, so head toward our tables.

Table 8: Partition of Vertex with respect to the 1^{st} distance of Vertices

$d_1(v)$	Frequency
2	$12n+18$
3	$24n-12$
4	$12n-6$

Table 9: Partition of Vertices with respect 2^{nd} distance of Vertices

$d_2(v)$	Frequency
3	12
4	18
5	$24n-12$
6	6
7	$12n-12$
8	$6n-6$
10	$6n-6$

Table 10: Partition of Vertex with respect to the 3^{rd} distance of Vertices

$d_3(v)$	Frequency
4	12
6	6
7	24
9	12
10	6
11	$12n-24$
13	$12n-12$
14	$12n-12$
18	$12n-12$

Table 11: Partition of Edges with respect to 2^{nd} distance of degrees of end Vertices

$d_2(u,v)$	Frequency
$(3,4)$	24
$(3,5)$	12
$(4,5)$	12
$(4,6)$	12
$(5,5)$	$12n-12$
$(5,7)$	$24n-24$
$(5,8)$	$12n-12$
$(7,10)$	$12n-12$
$(8,10)$	$12n-12$

Table 12: Partition of Vertices with respect to sum of the degrees of Neighbourhood

$d_2(v)$	S_v	Frequency
3	16	12
4	10	12
4	26	6
5	14	12
5	16	12
5	18	$12n-24$
6	14	6
7	27	$12n-12$
8	38	$6n-6$
10	40	$6n-6$

6 Results for the Metal Organic Networks

In this section, we are going towards our main result. This section contains the results on leap Zagreb Indices of first, second and third kind and their respective co-indices of 2^{nd} and 3^{rd} kind for both of the MON's. Moreover, in this section we also find results on the Wiener polarity index for both MON's structures.

6.1 Leap Zagreb Indices Of $\mathrm{MON}_1(t)$

First we discuss the Leap Zagreb indices of first kind of MON structure with the help of tables that are presented in previous section.

Theorem 6.1. *Let G be a graph of 48n vertices and 72m-12 edges then the* $1st$ *Leap Zegreb Index of graph is*

$$LM_1 = 3168n - 2304.$$

Proof: $1st$ Leap Zegreb is the vertex based index whose formula is

$$\begin{aligned} LM_1 &= \sum_{v_i=1}^{n} d_2(v_i) \\ LM_1 &= d_2(v_1) + d_2(v_2) + ... + d_2(v_n) \end{aligned}$$

By using values from Table 4, we get

$$\begin{aligned} LM_1 &= 3^2(12) + 4^2(18) + 6^2(12n - 6) \\ &\quad +7^2(12) + 8^2(24n - 36) \\ &\quad +10^2(12n - 12) \\ .LM_1 &= 3168n - 2304 \end{aligned}$$

Theorem 6.2. *Let G be a graph of 48n vertices and 72m-12 edges then the* $2nd$ *Leap Zegreb Index of graph is*

$$LM_2 = 5040n - 4236.$$

Proof: $2nd$ Leap Zegreb is the edge based index whose formula is

$$\begin{aligned} LM_2 &= \sum_{i=1}^{n} d_2(u_i) d_2(v_i) \\ LM_2 &= d_2(u_1)d_2(v_1) + d_2(u_2)d_2(v_2)... + d_2(u_n)d_2(v_n) \end{aligned}$$

By using values from Table 6, we get

$$\begin{aligned} LM_2 &= (3.4)(24) + (3.7)(12) + (4.6)(24) + (6.8)(24n - 12) \\ &\quad +(7.10)(12) + (8.10)(24n - 36) + (8.8)(12n - 24) \\ &\quad +(10.10)(12n - 12) \\ LM_2 &= 5040n - 4236 \end{aligned}$$

Theorem 6.3. *Let G be a graph of 48n vertices and 72m-12 edges then the $3rd$ Leap Zegreb Index of graph is*

$$LM_3 = 1200n - 708.$$

Proof: $3rd$ Leap Zegreb is the vertex based index whose formula is

$$\begin{aligned} LM_3 &= \sum_{i=1}^{n} d_1(v_i)d_2(v_i) \\ LM_3 &= d_1(v_1)d_2(v_1) + d_1(v_2)d_2(v_2) + ... + d_1(v_n)d_2(v_n) \end{aligned}$$

By using values from Table 3and Table 4, we get

$$\begin{aligned} LM_3 &= (2.4)(12) + (2.6)(12n + 6) + (2.7)(12) \\ &\quad +(2.8)(12n - 24) + (2.10)(6n - 6) + (3.3)(12) \\ &\quad +(4.4)(6) + (4.8)(12n - 12) + (6.10)(6n - 6) \\ LM_3 &= 1200n - 708 \end{aligned}$$

6.2 Leap Zagreb Indices Of MON$_2$(t)

Now, we discuss the Leap Zagreb indices of second kind of MON structure with the help of tables that are presented in previous section.

Theorem 6.4. *Let G be a graph of 48n vertices and 72m-12 edges then the $1st$ Leap Zegreb Index of graph is*

$$LM_1 = 2172n - 1260.$$

Proof: $1st$ Leap Zegreb is the vertex based index whose formula is

$$\begin{aligned} LM_1 &= \sum_{v_i=1}^{n} d_2(v_i) \\ LM_1 &= d_2(v_1) + d_2(v_2) + ... + d_2(v_n) \end{aligned}$$

By using values from Table 9, we get

$$\begin{aligned} LM_1 &= 3^2(12) + 4^2(18) + 5^2(24n - 12) + 6^2(6) + 7^2(12n \\ &\quad -12) + 8^2(6n - 6) + 10^2(6n - 6) \\ LM_1 &= 2172n - 1260. \end{aligned}$$

Theorem 6.5. *Let G be a graph of 48n vertices and 72m-12 edges then the $2nd$ Leap Zegreb Index of graph is*

$$LM_2 = 3420n - 2424.$$

Proof: $2nd$ Leap Zegreb is the edge based index whose formula is

$$\begin{aligned} LM_2 &= \sum_{i=1}^{n} d_2(u_i)d_2(v_i) \\ LM_2 &= d_2(u_1)d_2(v_1) + d_2(u_2)d_2(v_2)....... + d_2(u_n)d_2(v_n) \end{aligned}$$

By using values from Table 10, we get

$$\begin{aligned} LM_2 &= (3.4)(24) + (3.5)(12) + (4.5)(12) + (4.6)(12) \\ &\quad +(5.5)(12n - 12) + (5.7)(24n - 24) \\ &\quad +(5.8)(12n - 12) + (7.10)(12n - 12) \\ &\quad +(8.10)(12n - 12) \\ LM_2 &= 3420n - 2424. \end{aligned}$$

Theorem 6.6. *Let G be a graph of 48n vertices and 72m-12 edges then the $3rd$ Leap Zegreb Index of graph is*

$$LM_3 = 982n - 492.$$

Proof: $3rd$ Leap Zegreb is the vertex based index whose formula is

$$\begin{aligned} LM_3 &= \sum_{i=1}^{n} d_1(v_i)d_2(v_i) \\ LM_3 &= d_1(v_1)d_2(v_1) + d_1(v_2)d_2(v_2) + ... + d_1(v_n)d_2(v_n) \end{aligned}$$

By using values of first and second degree values from Table 8 and Table 9 to obtain the Leap Zagreb of third kind as follows, so we get

$$\begin{aligned} LM_3 &= (2.4)(12) + (2.5)(12n) + (2.6)(6) + (3.3)(12) \\ &\quad +(3.5)(12n - 12) + (3.7)(12n - 12) + (4.4)(6) \\ &\quad +(4.8)(6n - 6) + (10.12)(6n - 6) \\ LM_3 &= 982n - 492. \end{aligned}$$

7 Co-Indices of Leap Zagreb

The graph have the following co-indice of leap Zagreb index. The formula for co-indices of leap Zagreb are edge based which are following

$$\overline{LM_2} = \sum_{(u,v)\notin E(G)} d_2(u)d_2(v)$$

$$\overline{LM_3} = \sum_{(u,v)\notin E(G)} d_2(u) + d_2(v)$$

Now we suggest a vertex based formula that gives the same results.

$$\overline{LM_2} = \sum_{v\epsilon V(G)} f_v \times d_2(v_i)\left\{\sum_{i=1}^{n} d_2(v_i) - d_2\big(N(v_i)\big)\right\}$$

$$\begin{aligned}\overline{LM}_3 &= \sum_{v\epsilon V(G)} f_v\left[\left\{\sum_{i=1}^{n} d_2(v_i) - d[N(v_i)]\right\}\right. \\ &\quad \left.+\left\{d_2(v_i)\big(|V| - |N(v_i)|\big)\right\}\right]\end{aligned}$$

7.1 Co-Indices Of Leap Zegreb Of MON_1(t)

In this section, we are deriving Co-indices of Leap Zagreb of MON_1 by using the new formula's which are we derive. So,

Theorem 7.1. *Let G be a graph of 48n vertices and 72m-12 edges then the co-indice of the Leap Zegreb is*

$$\overline{LM}_2 = 120147456n^2 - 151488n + 43176.$$

Proof: As we Know that, Co-indice of Leap Zagreb is edge based and we are now using the edge based formula which we define in the above lines. So, we have

$$\overline{LM}_2 = \sum_{v\epsilon V(G)} f_v \times d_2(v_i)\left\{\sum_{i=1}^{n} d_2(v_i) - d_2\big(N(v_i)\big)\right\}$$

From the Fig 1, we have sum of degree of vertices as $\sum d(v_i) = 384n - 180$. Now put the values from the Table 7 we get

$$\begin{aligned}
\overline{LM_2} &= 12.3\big(384n - 198\big) + 12.4\big(384n - 190\big) \\
&\quad +6.4\big(384n - 208\big) + 6.(12n - 12)\big(384n - 202\big) \\
&\quad +6.12\big(384n - 198\big) + 6.6\big(384n - 194\big) \\
&\quad +7.12\big(384n - 200\big) + 8.12\big(384n - 216\big) \\
&\quad +8(12n - 24)\big(384n - 218\big) + 8(12n - 24)\big(384n \\
&\quad -206\big) + 10.6\big(384n - 240\big) + 10.6\big(384n - 210\big) \\
&\quad +10.(6n - 12)\big(384n - 218\big) \\
\overline{LM_2} &= 147456n^2 - 151488n + 43176.
\end{aligned}$$

Theorem 7.2. *Let G be a graph of 48n vertices and 72m-12 edges then the co-indice of the Leap Zegreb is*

$$\overline{LM_3} = 36864n^2 - 20448n + 1776.$$

Proof: As we Know that, Co-indice of Leap Zagreb is edge based and we are now using the edge based formula which we define in the above lines. So, we have

$$\begin{aligned}
\overline{LM_3} &= \sum_{v\epsilon V(G)} f_v \Bigg[\Bigg\{\sum_{i=1}^{n} d_2(v_i) - d[N(v_i)]\Bigg\} \\
&\quad + \Bigg\{ d_2(v_i)\big(|V| - |N(v_i)|\big)\Bigg\}\Bigg]
\end{aligned}$$

From the Fig 1 we have sum of degree of vertices= $\sum_{i=1}^{n} d(v_i) = 384n - 180$.

Now put the values from the Table 7 we obtain

$$\begin{aligned}
\overline{LM}_3 = \quad & 12[(384n-180-18)+3.(48n-4)] \\
& +12[(384n-180-10)+4.(48n-3)] \\
& +6[(384n-180-28)+4(48n-5)] \\
& +12n-12[(384n-180-28)+6(48n-3)] \\
& +12[(384n-180-18)+6(48n-3)] \\
& +6[(384n-180-14)+6(48n-3)] \\
& +12[(384n-180-20)+7(48n-3)] \\
& +12[(384n-180-36)+8(48n-5)] \\
& +12n-24[(384n-180-38)+8(48n-5)] \\
& +12n-24[(384n-180-26)+8(48n-3)] \\
& +6[(384n-180-60)+10(48n-7)] \\
& +6n-6[(384n-180-30)+10(48n-3)] \\
& +6n-12[(384n-180-38)+10(48n-7)]. \\
\overline{LM}_3 \;=\; & 36864n^2-20448n+1776.
\end{aligned}$$

7.2 Co-Indices Of Leap Zegreb Of MON_2(t)

In this section, we are deriving Co-indices of Leap Zagreb of MON_2 by using the new formula's which are derive from the following theorems.

Theorem 7.3. *Let G be a graph of 48n vertices and 72m-12 edges then the co-indice of the Leap Zegreb is*

$$\overline{LM_2} = 97344n^2 - 76404n + 17772.$$

Proof: As we Know that, Co-indice of Leap Zagreb is edge based and we are now using the edge based formula which we define in the above lines. So, we have

$$\overline{LM}_2 = \sum_{v\epsilon V(G)} f_v \times d_2(v_i)\left\{\sum_{i=1}^{n} d_2(v_i) - d_2\big(N(v_i)\big)\right\}.$$

From the Fig 2 we have sum of degree of vertices= $\sum_{i=1}^{n} d(v_i) = 312n - 108$. Now put the values from the Table12, we get

$$\begin{aligned}
\overline{LM_2} &= 12.3(312n - 108 - 16) + 12.4(312n - 108 \\
&\quad -10) + 6.4(312n - 108 - 26) + 12.5(312n \\
&\quad -108 - 14) + 12.5(312n - 124) + 5(12n \\
&\quad -24)(312n - 108 - 18) + (12n - 12)5(312n \\
&\quad -132) + 66(312n - 108 - 14) + 7(12n \\
&\quad -12)(312n - 135) + (6n - 6)8(312n - 146) \\
&\quad +(6n - 6)10(312n - 108 - 40) \\
\overline{LM_2} &= 97344n^2 - 76404n + 17772.
\end{aligned}$$

Theorem 7.4. *Let G be a graph of MON_2 with 48n vertices and 72m-12 edges then the co-indice of the Leap Zegreb is*

$$\overline{LM_3}(G) = 29952n^2 - 12960n + 1200.$$

Proof: As we Know that, Co-indice of Leap Zagreb is edge based and we are now using the edge based formula which we define in the above lines. So, we have

$$\begin{aligned}
\overline{LM_3} &= \sum_{v \epsilon V(G)} f_v \left[\left\{ \sum_{i=1}^{n} d_2(v_i) - d[N(v_i)] \right\} \right. \\
&\quad \left. + \left\{ d_2(v_i) \big(|V| - |N(v_i)| \big) \right\} \right]
\end{aligned}$$

From the Fig 2, we have sum of degree of vertices= $\sum_{i=1}^{n} d(v_i) = 312n - 108$. Now putting the values from the Table 12 and we get

$$\begin{aligned}
\overline{LM_3} &= 12[(312n - 124) + 3(48n - 4)] \\
&\quad +12[(312n - 128) + 4(48n - 3)] \\
&\quad +6[(312n - 108 - 26) + 4(48n - 5)] \\
&\quad +12[(312n - 108 - 14) + 5(48n - 3)] \\
&\quad +12[(312n - 108 - 16) + 5(48n - 3)] \\
&\quad +(12n - 24)[(312n - 108 - 18) + 5(48n - 3)] \\
&\quad +(12n - 12)[(312n - 108 - 24) + 5(48n - 4)] \\
&\quad +6[(312n - 108 - 14) + 6(48n - 3)] \\
&\quad +(12n - 12)[(312n - 108 - 27) + 7(48n - 4)] \\
&\quad +(6n - 6)[(312n - 108 - 38) + 8(48n - 5)] \\
&\quad +(6n - 6)[(312n - 108 - 40) + 10(48n - 5)] \\
\overline{LM_3} &= 29952n^2 - 12960n + 1200.
\end{aligned}$$

8 Wiener Polarity Index of MON Networks

"To find Wiener polarity, we study the vertices at distance 3. In this section, we find the Wiener polarity index of MON's by using the above tables."

8.1 Wiener Polarity Index of MON_1

First, we are acknowledge the MON_1 and find the Wiener polarity index of MON_1.

Theorem 8.1. *Let G=MON_1 be a graph of 48n vertices and 72m-12 edges then the Wiener Polarity Index of graph is*

$$W(G) = 408n - 264.$$

Proof: Wiener Polarity is the vertex based index whose formula is

$$\begin{aligned} W(G) &= \sum_{i=1}^{n} \frac{1}{2} d_3(v_i) \\ W(G) &= \frac{1}{2} d_3(v_1) + \frac{1}{2} d_3(v_2) + ... + \frac{1}{2} d_3(v_n) \end{aligned}$$

By using values from Table 6, we get

$$\begin{aligned} W(G) &= \frac{1}{2}(4.12) + \frac{1}{2}(6.6) + \frac{1}{2}(9.12) + \frac{1}{2}(10.12) \\ &\quad + \frac{1}{2}(11.12) + \frac{1}{2}(12.6) + \frac{1}{2}(14.12n - 12) \\ &\quad + \frac{1}{2}(16.12n - 12) + \frac{1}{2}(18.18n - 30) + \frac{1}{2}(20.6) \\ &\quad + \frac{1}{2}(22.6n - 12) \\ W(G) &= 408n - 264. \end{aligned}$$

8.2 Wiener Polarity Index of MON_2

First, we are acknowledge the MON_2 and find the wiener polarity index to MON_2.

Theorem 8.2. *Let G=MON_1 be a graph of 48n vertices and 72m-12 edges then the wiener Polarity Index of graph is*

$$W(G) = 336n - 192.$$

Proof: Wiener Polarity is the vertex based index whose formula is

$$\begin{aligned} W(G) &= \sum_{i=1}^{n} \frac{1}{2} d_3(v_i) \\ W(G) &= \frac{1}{2} d_3(v_1) + \frac{1}{2} d_3(v_2) + \ldots + \frac{1}{2} d_3(v_n) \end{aligned}$$

By using values from Table 10, we get

$$\begin{aligned} W(G) &= \frac{1}{2}(4.12) + \frac{1}{2}(6.6) + \frac{1}{2}(7.24) + \frac{1}{2}(9.12) \\ &+ \frac{1}{2}(10.6) + \frac{1}{2}(11.12n - 24) + \frac{1}{2}(13.12n - 12) \\ &+ \frac{1}{2}(14.12n - 12) + \frac{1}{2}(18.12n - 12) \\ W(G) &= 336n - 192. \end{aligned}$$

9 Graphical Representation and Comparison

In this section, we are differentiate the outcomes of the topological invariants for the MON's through the graphical representation that clearly shows that how the invariants are increasing monotonically.

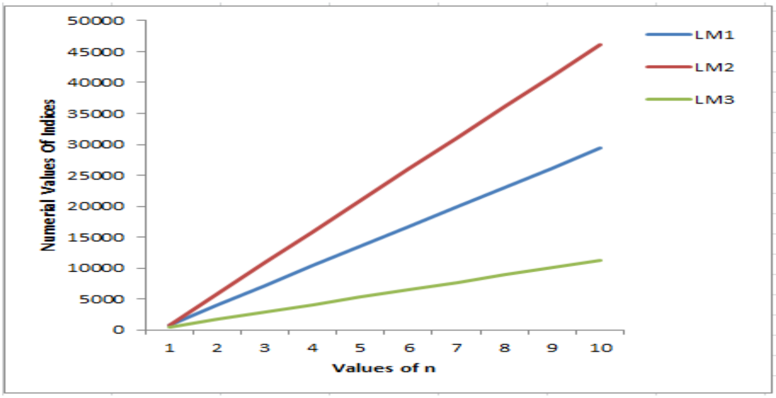

Figure 3: Comparison of leap Zagreb indices.

To make differentiation between the values of Leap Zagreb indices numerically for MON_1, for different values of n. Now, through graphical representation, we can easily configure that all values of Leap Zagreb indices escalate as the values of n increase. Moreover, the values of leap Zagreb index of second type increase more rapidly than the values of the leap Zagreb index of first kind. Similarly, the values of leap Zagreb index of third kind can be observed to grow with the least pace. For different values of n, the graphs of these indices are shown in Figure 3.

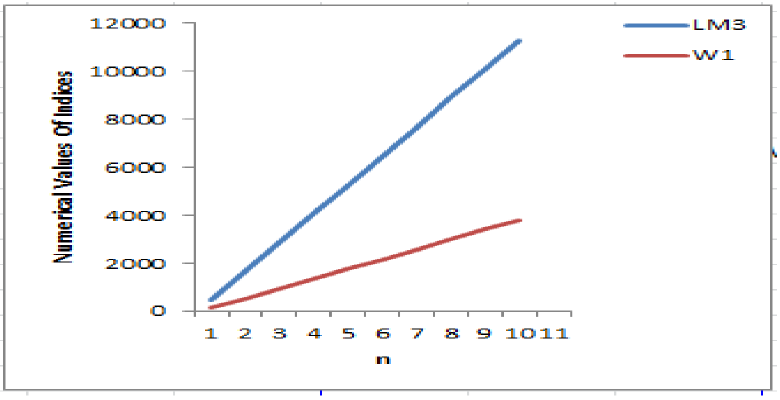

Figure 4: Comparison of leap Zagreb and Wiener polarity Indices.

Now, consider the comparison of leap Zagreb index of third kind and Wiener polarity indices numerically for MON_1, for different values of n. Now, we can easily observe that all values of leap Zagreb index of third kind and Wiener polarity indices increase monotonically with the values of n but the leap Zagreb index (third kind) increases with a quite higher slope. As the values of n increase, the graphic comparison pf these indices is presented in Figure 4.

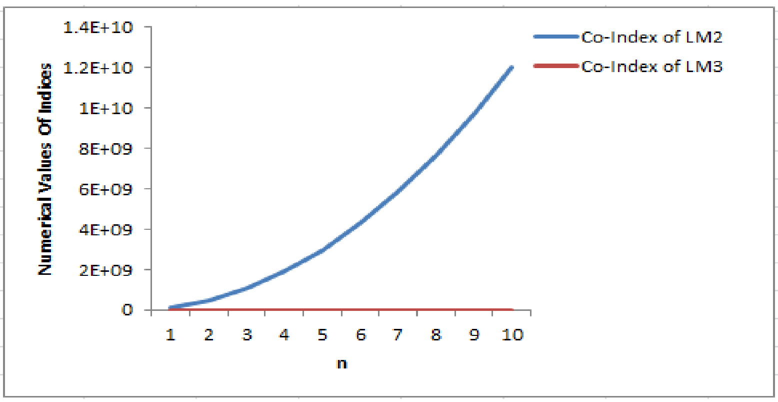

Figure 5: Comparison of co-Indices of leap Zagreb indices.

For the comparison of co-Indices of leap Zagreb numerically for MON_1, for different values of n. Now, we can easily see that all values of co-Indices of Leap Zagreb indices increase monotonically with the values of n. It can be observed that the graph of the second leap Zagreb coindex increases quadraticly but the graph of third leap Zagreb coindex increase linearly. As the values of n increase, the graphic comparison pf these indices is presented in Figure 5.

For the comparison of Leap Zagreb Indices numerically for MON_2, for different values of n. Now, through graphical representation, we can easily configure that all values of Leap Zagreb indices increase monotonically with values of n. For different values of n, the graphs of these topological indices are drawn in the same plot for comparison and shown in Figure 6.

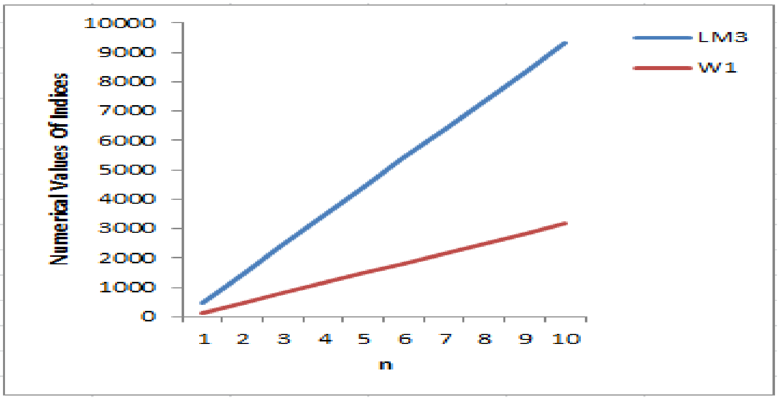

Figure 6: Comparison of leap Zagreb and Wiener polarity indices.

For the comparison of Leap Zagreb of third kind and Wiener Polarity Indices numerically for MON_2, for different values of n. Through Graphical representations, we can easily configure that all the values of n, Leap Zagreb of third kind and Wiener polarity indices increase monotonically as the values of n increase. The graphs of these indices are drawn in Figure 7 for detailed comparison.

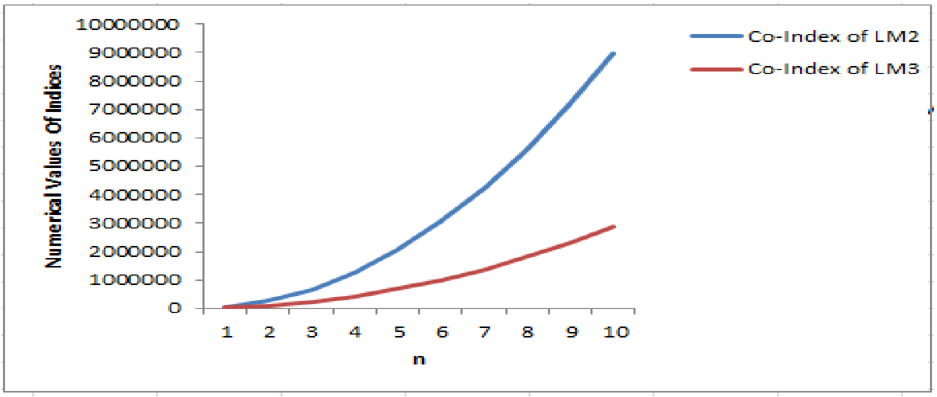

Figure 7: Comparison of co-indices of leap Zagreb indices.

Now we discuss the graphical misrepresentation of the paper of Hong et al [1]. Figure 6 in [1] depict the graphical comparison of $AZI(N)$, $S(N)$ and $AZI_M(N)$ which is not similar to the values of Table 9 of MON_1. The values of the graph presented in [1] are decreasing which is totally against the numerical values of the Table 9 in [1].

10 Conclusion

In this paper, we calculate Leap Zagreb Indices, Wiener Polarity Indices and Co-indices of Leap Zagreb Indices for MON_1 and MON_2. Also, we give a comparison by graphical representation for the different kind of the topological invariants by using numerical values in the above define Tables. We are also suggested a new formula's for the calculation of the Co-indices of Leap Zagreb which is vertex based and also provide the same results. Moreover, in this paper, we also point out the graphical misrepresentation in [1] by defining that topological invariants are monotone increasing when compared with the values of n.

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