# Computing Novel Multiplicative Zagreb Connection Indices of Metal Organic Networks

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This article has been accepted for publication and undergone full peer review but has not been through the copyediting, typesetting, pagination and proofreading process, which may lead to differences between this version and the Version of Record. Please cite this article as doi: https://doi.org/10.32350/sir.51.03

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#### Abstract

Metal organic networks (MONs) are defined as one, two and three dimensional unique complex structures of porous material and subclass of polymer's coordination. These networks also show extreme surface area, morphology, excellent chemical stability, large pore volume, highly crystalline materials. The major advantages of MONs are tailorability, structural diversity, versatile applications, highly controllable nano-structures and functionality. So, the multi-functional applications of these MONs are made them more helpful tools in many fields of science in recent decade. In this paper, we light on the two different MONs with respect to the number of increasing layers of metal and organic ligands together. We define the novel multiplicative Zagreb connection indices (ZCIs) such that multiplicative fourth ZCI and multiplicative fifth ZCI. We also compute the main results for multiplicative Zagreb connection indices of two different MONs (zinc oxide and zinc silicate).

Keywords: Connection number, multiplicative Zagreb indices, metal organic networks

### 1. Introduction

Metal organic networks (MONs) are most popular chemical compounds which consist of metal ions and organic ligands. These networks have large pore diameters, intensive surface areas and giant pore volumes. A variety of MONs is presented in modern chemistry. Therefore, zinc based MONs could be modified into devices for luminescent characteristics, see [1]. The electron-rich T-conjugated fluorescent ligands are friendly to construct Zn based MONs through nucleophilic properties in efficient luminescent sensors, see [2]. MONs are widely used in gas and energy storage devices, assessment of chemicals, separation and purification of different gasesm, sensing, , heterogeneous catalysis, environmental hazard, adsorption analysis, toxicology, biomedical applications and biocompatibility. The cancer imaging, drug delivery and biosensing have been cured with the help of biomedical applications of zinc based MONs. So, the physical stability and mechanical properties of these networks have become a theme of useful content due to the abovementioned specifications.

In non-linear optically active MON  $Zn^{2+}$  is commonly used as a connecting point to prevail undesired d-d transitions in the visible region. The toxicology, biomedical applications and their biocompatibility are currently reported production procedures of zinc based MONs, see [3]. Eddaoudi et al. [4] discussed the isoreticular series (IRMOF-1 to IRMOF-16) of 16 highly crystalline materials. The fixed and free diameter of pores from IRMOF-1 to IRMOF-16 varies in the range of 3.8-19.1  $A^0$  and 12.8-28.8  $A^0$ , respectively. All the IRMOFs considered as the ordinary topology of  $CaB_6(13)$  and happened through the prototype IRMOF-1 which exists oxide-centered  $Zn_4O$  tetrahedron. Some IRMOF such as IRMOF- (8, 10, 12 and 16) have been seen in non-crystalline porous networks for  $SiO_2$  xerogels and aerogels (16). For more informations, we refer to [5-7].

MONs also predicts the physico-chemical properties such as impregnating suitable active material [8], grafting active groups [9], ion exchange [10], post synthetic ligand [11], changing organic ligands and biosensors enhancing sensitivity, response time and selectivity [12]. Lin et al. [13] (2009) presented the MONs related applications such as photo-catalysis, sensing, electro-catalysis, catalyst for production of fine chemicals and super-capacitors. The versatile applications of MONs are delivery of drugs [14], adsorption [15], storage of gases [16-18], sensing [19], catalysis for the separation and purification [20-21].

Graph theory provides beneficial tools in the field of moderm chemistry and pharmacology which depict the physical and chemical properties of chemical compounds such as heat of evaporation, flash point, heat of formation, boiling point, melting point, temperature, pressure, tention, partition coefficient, density, and retention in chromatography, see [22-24]. The very famous degree based TI was firsly discussed by Gutman and Trinajstić in 1972 to check the chemical physibility for the total  $\pi$ -electron energy of the chemical compound [25]. So, these topological indices (TIs) are one of the tabular (or numeric) tools which show biological, chemical and physical properties of chemical compounds. Awais et al. [26] (2020) studied two different MONs  $MON_1(p)$  and  $MON_2(p)$ , where  $p \ge 2$  with the help of generalized indices and their connection indices. Hong et al. [27] used these MONs to compare for chemical suitability among some well-known degree based TIs. Recently, Nadeem et al. [28], Haoer [29] and Kashif et al. [30] also used thses MONs in the shape of line graphs & studied some physical properties of these MONs of line graphs for different TIs, computing neighborhood and M-polynomials for different TIs. For more knowledge about MONs insight of TIs, we prefer to [31-33].

Tang et al. [34] (2009) used the concept of connection number which defined Gutman and Trinajstić in [25] to compute Zagreb connection indices of the subdivision based operations on networks. Nowa-days, these degree and connection number based TIs are abundantely used in the topological properties of four-layered neural networks, see [35]. Javaid et al. [36] and Liu et al. [37] computed these TIs of rhombus silicate & rhombus oxide networks and cellular neural networks. Javaid & Jung [38] and Raheem et al. [39] computed M-polynomial based TIs of silicate & oxide networks and 2Dlattice of three-layered single-walled titania nanotubes. Moreover, Zhao et al. [40] computed reverse degree based TIs of zinc based MONs. Moreover, a variety of networks has been defined by using connection number (or leap degree) based TIs, see [41-47].

In this paper, we define the multiplicative fourth ZCI and multiplicative fifth ZCI. We also discuss multiplicative first ZCI, multiplicative second ZCI and multiplicative third ZCI. We compute abovementioned multiplicative ZCIs of two different MONs such as zinc oxide (ZNOX (p) =IRMOF-10) and zinc silicate (ZNCL(p)=IRMOF-14) networks with respect to the increasing layers  $p \ge 1$ , taking both metal nodes and linkers together. The rest of the paper is designed as: section II gives the preliminaries and definitions, Section III gives the main results for different MONs (zinc oxide and zinc silicate) and Section IV gives conclusions.

#### 2. Preliminaries

The vertex and edge sets are V(G) and E(G) for simple and connected network G. A network is connected if their exists no loops and multiple edges. |V(G)| and |E(G)| are the cardinalities of vertex set and edge set which are equal to u and v, respectively. A path between two vertices generates a connected network. The distance between two vertices m and n is the shortest path between them. It is denoted by  $d_G(m,n)$ . The length of shortest and longest paths between m and n is called m-n geodesic and detour respectively. In general [48],  $N_G(n/q) = \{m \in V(G); d(m,n) = q\}$  is the open q-neighborhood set of n, where q represents a positive integer and  $|N_G(n/q)| = d_G(n/q)$  is called q-distance degree of a vertex n. In particular , If q = 1,  $d_G(n/1) = |N_G(n/1)| = d_G(n) = \text{degree of n}$  (number of vertices at distance one from particular vertex n). If q = 2,  $d_G(n/2) = |N_G(n/2)| = \tau_G(n) = \text{connection number of n}$  (number of vertices at distance two from particular vertex n). A network becomes chemical if it holds graphical terms vertex and edge equal to chemical terms atom and bond, respectively. In chemical networks, the degree of any vertex is at most 4. For more chemical terminologies, we suggest to see [49].

**Definition 2.1.** For a (molecular) network G, the first Zagreb index  $(M_1(G))$ , second Zagreb index  $(M_2(G))$  and third Zagreb index  $(M_3(G))$  are defined as

(a) 
$$M_1(G) = \sum_{n \in V(G)} [d_G(n)]^2 = \sum_{mn \in E(G)} [d_G(m) + d_G(n)]$$
  
(b)  $M_2(G) = \sum_{mn \in E(G)} [d_G(m) \times d_G(n)],$ 

(c) 
$$M_3(G) = \sum_{n \in V(G)} [d_G(n)]^3 = \sum_{mn \in E(G)} [d_G^2(m) + d_G^2(n)].$$

These degree based TIs are introduced by Gutman, Trinajstić, Ruscic and Furtula, see [25], [50-51]. These are abundantely used to predict better findings in molecular networks such as ZE-isomerism, absolute value of correlation coefficient, entropy, acentric factor, heat capacity, density, volume, temperature, boiling point, accentric factor and entropy [52-53].

**Definition 2.2** (see [54]). For a (molecular) network G, the first multiplicative Zagreb index  $(MZ_1(G))$  and second multiplicative Zagreb index  $(MZ_2(G))$  are defined as

(a) 
$$MZ_1(G) = \prod_{n \in V(G)} [d_G(n)]^2$$
,  
(b)  $MZ_2(G) = \prod_{mn \in E(G)} [d_G(m) \times d_G(n)]$ 

**Definition 2.3** (see [55]). For a (molecular) network G, the first multiplicative Zagreb index  $(MZ_1(G))$  is also defined as

$$MZ_1(G) = \prod_{mn \in E(G)} \left[ d_G(m) + d_G(n) \right].$$

**Definition 2.4.** For a (molecular) network G, the first Zagreb connection index  $(ZC_1(G))$ , second Zagreb connection index  $(ZC_2(G))$  and modified first Zagreb connection index  $(ZC_1^*(G))$  are defined as

(a) 
$$ZC_1(G) = \sum_{n \in V(G)} [d_G(n)]^2$$
,  
(b)  $ZC_2(G) = \sum_{mn \in E(G)} [\tau_G(m) \times \tau_G(n)]$ ,  
(c)  $ZC_1^*(G) = \sum_{n \in V(G)} [d_G(n) \times \tau_G(n)] = \sum_{mn \in E(G)} [\tau_G(m) + \tau_G(n)]$ 

These connection based TIs are defined by Ali and Trinajstić [56] (2018). They also reported that these connection based TIs are more correlated among the thirteen physicochemical properties of octane isomers than classical Zagreb indices.

**Definition 2.5.** For a (molecular) network G, the first multiplicative ZCI ( $MZC_1(G)$ ), second multiplicative ZCI ( $MZC_2(G)$ ), third multiplicative ZCI ( $MZC_3(G)$ ) are defined as

(a) 
$$MZC_1(G) = \prod_{n \in V(G)} [\tau_G(n)]^2$$
,

(b) 
$$MZC_2(G) = \prod_{mn \in E(G)} [\tau_G(m) \times \tau_G(n)],$$
  
(c)  $MZC_3(G) = \prod_{n \in V(G)} [d_G(n) \times \tau_G(n)].$ 

These connection based multiplicative Zagreb indices are defined by Haoer et al. [57]. They used these multiplicative versions by the same sense which named as multiplicative leap Zagreb indices.

**Definition 2.6.** For a (molecular) network G, the fourth multiplicative ZCI ( $MZC_4(G)$ ) and fifth multiplicative ZCI ( $MZC_5(G)$ ) are defined as

(a) 
$$MZC_4(G) = \prod_{mn \in E(G)} [\tau_G(m) + \tau_G(n)],$$
  
(b)  $MZC_5(G) = \prod_{n \in V(G)} [d_G(n) + \tau_G(n)].$ 

**Definition 2.7. Zinc Oxide Network (ZNOX(n)):** A chemical compound zinc oxide (ZnO) is insoluble in water which is inorganic compound of white powder shape and density 5.61 g/c  $m^3$ . The zinc oxide is heated with carbon (coke) who reduces to the metal vapor to condense the liquid from which the solid metal freezes.

$$ZnO_{(s)} + C_{(s)} \rightarrow Zn_{(g)} + CO_{(g)}$$

Zinc is a reactive metal to produce hydrogen gas and zinc ion  $(Zn^{2+})$ . It also reduces those metal ions whose reduction potentials are greater than  $Zn^{2+}$ . Zinc oxide is mostly used in making glazes, rubher, enamels, photoconductive surfaces, pigment in white paint, and protective coating for other metals. Zinc oxide related MON is  $Zn_4O(BPDC)_3$  which is also known as IRMOF-10. IRMOF-9 is a catenated

version of IRMOF-10. IRMOF-10 is three dimensional cubic networks with pore size  $16.7/20.2 A^0$  in diameter, see [58]. The MON of zinc oxide of dimension 1 is presented in Figure 1.



#### **Figure 1**: Metal Organic Network (ZNOX(p) $\cong R$ ). In particular p=1.

Let  $R \cong ZNOX(p)$  be the metal organic (zinc oxide) network of dimention p in the plane, see Figure 1. The partition of R with respect to vertex set V(R) and edge set E(R). We can easily see that each vertex of degrees and connection numbers sets are  $\{2,3,4\}$  and  $\{2,3,4,5,8\}$  respectively. We have  $V_1 = \{n \in V(R) | d_n = 2\}$ ,  $V_2 = \{n \in V(R) | d_n = 3\}$  and  $V_3 = \{n \in V(R) | d_n = 4\}$ , where  $|V_1| = 42p + 30$ ,  $|V_2| = 26p + 14$  and  $|V_3| = 2p + 2$ . So,  $|V(R)| = |V_1| + |V_2| + |V_3| = 70p + 46$ . The partition of vertices with respect to connection number are  $V_1 = \{n \in V(R) | , \tau_n = 2\}$ ,  $V_2 = \{n \in V(R) | , \tau_n = 3\}$ ,  $V_3 = \{n \in V(R) | \tau_n = 4\}$ ,  $V_4 = \{n \in V(R) | \tau_n = 5\}$  and  $V_5 = \{n \in V(R) | \tau_n = 8\}$ , where  $|V_1| = 2p+6$ ,  $|V_2| = 28p+20$ ,  $|V_3| = 30p+10$ ,  $|V_4| = 8p+8$  and  $|V_5| = 2p+2$ . So,  $|V(R)| = |V_1| + |V_2| + |V_3| + |V_4| + |V_5| = 70p + 46$ . Now, the partition of vertices with respect to degrees and connection numbers are  $V_1 = V_{1,\tau} = V_{2,2} = \{n \in V(R) | d_n = 2, \tau_n = 2\}$ ,  $V_2 = V_{2,3} = \{n \in V(R) | d_n = 2, \tau_n = 3\}$ ,  $V_3 = V_{2,4} = \{n \in V(R) | d_n = 2, \tau_n = 4\}$ ,  $V_4 = V_{3,4} = \{n \in V(R) | d_n = 3, \tau_n = 4\}$ ,  $V_5 = V_{3,5} = \{n \in V(R) | d_n = 3, \tau_n = 5\}$  and  $V_6 = V_{4,8} = \{n \in V(R) | d_n = 4, \tau_n = 8\}$ , where  $|V_1| = 8p$ ,  $|V_2| = 50p + 1$ ,  $|V_3| = 14p$ ,  $|V_4| = 22p + 1$ ,  $|V_5| = 16p$  and  $|V_6| = 4p$ , So,  $|V(R)| = |V_1| + |V_2| + |V_3| + |V_4| + |V_5| + |V_6| = 114p + 2$ . These vertex partitions are presented in Tables 2.1, 2.2 and 2.3.

Table 2.1: Partitions of *R*'s vertices with respect to degree.

| $V_{d}$ | 2      | 3      | 4    |
|---------|--------|--------|------|
| $ V_d $ | 42p+30 | 26p+14 | 2p+2 |

Table 2.2: Partitions of *R*'s vertices with respect to connection number.

| V <sub>τ</sub> | 2    | 3      | 4      | 5    | 8    |
|----------------|------|--------|--------|------|------|
| $ V_{	au} $    | 2p+6 | 28p+20 | 30p+10 | 8p+8 | 2p+2 |

Table 2.3: Partitions of *R*'s vertices with respect to degree and connection number.

| $V_{d,	au}$   | 2,2 | 2,3   | 2,4 | 3,4   | 3,5 | 4,8 |
|---------------|-----|-------|-----|-------|-----|-----|
| $ V_{d,	au} $ | 8p  | 50p+1 | 14p | 22p+1 | 16p | 4p  |

Now, There are four types partitions of edge sets of R with respect to degree as  $|E(R)| = |E_{2,2}^d| + |E_{2,3}^d| + |E_{3,4}^d| = 85p + 55$  and there are seven types partitions of edge sets of R with respect to

connection number of vertices as  $|\mathbf{E}(R)| = |E_{2,3}^c| + |E_{3,3}^c| + |E_{3,4}^c| + |E_{3,5}^c| + |E_{4,4}^c| + |E_{4,5}^c| + |E_{5,8}^c| = 85p + 55$ . These edge partitions are shown in Tables 2.4 and 2.5.

|                                  | e           | 1 0         |             |             |
|----------------------------------|-------------|-------------|-------------|-------------|
| $E^d_{d(m),d(n)}$                | $E^d_{2,2}$ | $E^d_{2,3}$ | $E^d_{3,3}$ | $E^d_{3,4}$ |
| $\left E_{d(m),d(n)}^{d}\right $ | 6p+16       | 52p+28      | 9p+3        | 8p+8        |

**Table 2.4**: Partitions of R's edges with respect to degree.

| <b>Table 2.5</b> : Partition of <i>R</i> 's edges with respect to connection nun |
|--|
|--|

| $E^c_{	au(m),	au(n)}$               | $E^{c}_{2,3}$ | $E^{c}_{3,3}$ | $E^{c}_{3,4}$ | $E^{c}_{3,5}$ | $E^{c}_{4,4}$ | $E^{c}_{4,5}$ | $E^{c}_{5,8}$ |
|-------------------------------------|---------------|---------------|---------------|---------------|---------------|---------------|---------------|
| $\left E^{c}_{	au(m),	au(n)} ight $ | 4p+12         | 4p+12         | 24p+12        | 4p+12         | 21p+7         | 12p+4         | 8p+8          |

**Definition 2.8. Zinc Silicate Network (ZNSL(n)):** Silicate ( $SiO_4$ ) is the most wonderful class of minerals. Silicate is the chemical mixture of metal carbonate or metal oxide with sand. Tetrahedra is used as the basic unit of silicate. So, all silicates gain  $SiO_4$  tetrahedral. In chemistry, silicon ions and oxygen ions are represented by the centre vertices and corner vertices of  $SiO_4$  respectively. In graph theory, we show centre vertices and corner vertices of  $SiO_4$  with silicon nodes and oxygen nodes. If we require a variety of silicate networks, it is easy to change the arrangement of the tetrahedron silicate. Zinc silicate related MON is  $Zn_4O(PDC)_3$  which is also known as IRMOF-14. IRMOF-14 is three dimensional cubic structures with pore size 14.7/20.1  $A^0$  in diameter, see [58]. The MON of zinc silicate of dimention 1 is presented in Figure 2.

**Figure 2:** Zinc silicate network (ZNSL(p)  $\cong K$ ). In particular p=1.

Let  $S \cong ZNOX(p)$  be the metal organic (zinc silicate) network of dimention p in the plane, see Figure 2. The partition of *S* with respect to vertex set V(*S*) and edge set E(*S*). We can easily see that each vertex of degrees and connection numbers sets are {2,3,4} and {2,3,4,5,6,8} respectively. We have V<sub>1</sub> = {  $n \in V(S) | d_n = 2$ }, V<sub>2</sub> = {  $n \in V(S) | d_n = 3$ } and V<sub>3</sub> = {  $n \in V(S) | d_n = 4$ }, where  $|V_1| = 42p + 30$ ,  $|V_2| = 38p + 18$  and  $|V_3| = 2p + 2$ . So,  $|V(S)| = |V_1| + |V_2| + |V_3| = 82p + 50$ . The partition of vertices with respect to connection numbers are V<sub>1</sub> = {  $n \in V(S) | \tau_n = 2$ }, V<sub>2</sub> = {  $n \in V(S) | \tau_n = 3$ }, V<sub>3</sub> = {  $n \in V(S) | \tau_n = 4$ }, V<sub>4</sub> = {  $n \in V(S) | \tau_n = 5$ }, V<sub>5</sub> = {  $n \in V(S) | \tau_n = 6$ }, and V<sub>6</sub> = {  $n \in V(S) | \tau_n = 8$ }, where  $|V_1| = 2p+6$ ,  $|V_2| = 16p+16$ ,  $|V_3| = 48p+16$ ,  $|V_4| = 8p+8$ ,  $|V_5| = 6p+2$  and  $|V_6| = 2p+2$ . So,  $|V(S)| = |V_1| + |V_2| + |V_3| + |V_4| + |V_5| + |V_6| = 82p + 50$ . Now, the partition of vertices with respect to degrees and connection numbers are V<sub>1</sub> =  $V_{1,2} = V_{2,2} = {n \in V(S) | d_n = 2, \tau_n = 2$ }, V<sub>2</sub> =  $V_{2,3} = {n \in V(S) | d_n = 2, \tau_n = 3$ }, V<sub>3</sub> =  $V_{2,4} = {n \in V(S) | d_n = 2, \tau_n = 4$ }, V<sub>4</sub> =  $V_{3,4} = {n \in V(S) | d_n = 3, \tau_n = 5$ }, V<sub>5</sub> = {  $n \in V(S) | d_n = 3, \tau_n = 6$ }, and V<sub>7</sub> =  $V_{4,8} = {n \in V(S) | d_n = 3, \tau_n = 5}$ , V<sub>6</sub> =  $N_{3,6} = {n \in V(S) | d_n = 3, \tau_n = 6}$ , and V<sub>7</sub> =  $V_{4,8} = {n \in V(S) | d_n = 4, \tau_n = 8}$  where  $|V_1| = 8p, |V_2| = 30p + 1$ ,  $|V_3| = 30p + 3, |V_4| = 30p + 3, |V_5| = 14p + 1$  and  $|V_6| = 8p$  and  $|V_7| = 4p$  So,  $|V(S)| = |V_1| + |V_2| + |V_3| + |V_4| + |V_5| + |V_6| + |V_7| = 124p + 8$ . These vertex partitions are presented in Tables 2.6, 2.7 and 2.8.

**Table 2.6:** Partitions of S's vertices with respect to degree.

| $V_d$   | 2      | 3      | 4    |
|---------|--------|--------|------|
| $ V_d $ | 42p+30 | 38p+18 | 2p+2 |

Table 2.7: Partitions of S's vertices with respect to connection number.

| V 	au       | 2    | 3      | 4      | 5    | 6    | 8    |
|-------------|------|--------|--------|------|------|------|
| $ V_{	au} $ | 2p+6 | 16p+16 | 48p+16 | 8p+8 | 6p+2 | 2p+2 |

Table 2.8: Partitions of S's vertices with respect to degree and connection number.

| $V_{d,	au}$               | 2,2 | 2,3   | 2,4   | 3,4   | 3,5   | 3,6 | 4,8 |
|---------------------------|-----|-------|-------|-------|-------|-----|-----|
| $\left V_{d,\tau}\right $ | 8p  | 30p+1 | 30p+3 | 30p+3 | 14p+1 | 8p  | 4p  |

Now, there are four types partitions of edge sets of S with respect to degree as  $|E(S)| = |E_{2,2}^d| + |E_{2,3}^d| + |E_{3,4}^d| = 103p + 61$  and there are seven types partitions of edge sets of S with respect to

connection number of vertices as  $|\mathbf{E}(S)| = |E_{2,3}^c| + |E_{3,3}^c| + |E_{3,4}^c| + |E_{3,5}^c| + |E_{4,4}^c| + |E_{4,5}^c| + |E_{4,6}^c| + |E_{5,8}^c| + |E_{6,6}^c| = 103p + 61$ . These edge partitions are shown in Table 2.9 and 2.10.

|                                  |             | 88          |             |             |
|----------------------------------|-------------|-------------|-------------|-------------|
| $E^d_{d(m),d(n)}$                | $E^d_{2,2}$ | $E^d_{2,3}$ | $E^d_{3,3}$ | $E^d_{3,4}$ |
| $\left E^{d}_{d(m),d(n)}\right $ | 10p+14      | 64p+32      | 21p+7       | 8p+8        |

**Table 2.9**: Partitions of S's edges according to degree.

**Table 2.10**: Partition of S's edges according to connection number.

| $E^c_{\tau(m),\tau(n)}$             | $E_{2,3}^{c}$ | $E_{3,3}^{c}$ | $E_{3,4}^{c}$ | $E_{3,5}^{c}$ | $E^{c}_{4,4}$ | $E_{4,5}^{c}$ | $E^{c}_{4,6}$ | $E^{c}_{5,8}$ | $E^{c}_{6,6}$ |
|-------------------------------------|---------------|---------------|---------------|---------------|---------------|---------------|---------------|---------------|---------------|
| $\left E^{c}_{	au(m),	au(n)} ight $ | 4p+12         | 6p+2          | 12p+4         | 4p+12         | 42p+14        | 12p+4         | 12p+4         | 8p+8          | 3p+1          |

## 3. Main Results for MONs

In this section, we compute the main results for first multiplicative ZCI, second multiplicative ZCI, third multiplicative ZCI fourth multiplicative ZCI and fifth multiplicative ZCI of two different MONs (zinc oxide and zinc silicate).

**Theorem 3.1:** Let  $R \cong ZNOX(p)$  and  $S \cong ZNOX(p)$  be two MONs of dimensions  $p \ge 1$ . Then, first multiplicative ZCI of two MONs R and S are as follows:

(a) 
$$MZC_1(R) = 2.4772608 \times 10^{10} p^5 + 1.49815296 \times 10^{11} p^4 + 3.016359936 \times 10^{11} p^3$$

 $+2.504392704 \times 10^{11} p^{2} + 7.56154368 \times 10^{10} p + 1.769472000 \times 10^{9},$ 

**(b)**  $MZC_1(S) = 4.892236186 \times 10^{12} p^6 + 3.261490421 \times 10^{13} p^5 + 7.881936078 \times 10^{13} p^4$ 

 $+9.132173844 \times 10^{\scriptscriptstyle 13}\,p^{\scriptscriptstyle 3} + 5.381459805 \times 10^{\scriptscriptstyle 13}\,p^{\scriptscriptstyle 2} + 1.522029036 \times 10^{\scriptscriptstyle 13}\,p + 1.630745795 \times 10^{\scriptscriptstyle 12}\,.$ 

**Proof** (a). By principle,

$$MZC_{1}(G) = \prod_{n \in V_{2}^{c}} [\tau_{G}(n)]^{2}$$
$$= \prod_{n \in V_{2}^{c}} [\tau_{R}(n)]^{2} \times \prod_{n \in V_{3}^{c}} [\tau_{R}(n)]^{2} \times \prod_{n \in V_{4}^{c}} [\tau_{R}(n)]^{2} \times \prod_{n \in V_{5}^{c}} [\tau_{R}(n)]^{2} \times \prod_{n \in V_{8}^{c}} [\tau_{R}(n)]^{2}$$

By using Table 2.2

$$= (2p+6)(2)^2 \times (28p+20)(3)^2 \times (30p+10)(4)^2 \times (8p+8)(5)^2 \times (2p+2)(8)^2$$

 $= (2016p^{2} + 7488p + 4320) \times (96000p^{2} + 128000p + 3200) \times (128p + 128)$ 

$$= 2.4772608 \times 10^{10} p^5 + 1.49815296 \times 10^{11} p^4 + 3.016359936 \times 10^{11} p^3 + 2.504392704 \times 10^{11} p^2$$

 $+7.56154368 \times 10^{10} p + 1.769472000 \times 10^{9}$ .

(b). By principle,

$$\begin{split} MZC_1(G) &= \prod_{n \in V(G)} [\tau_G(n)]^2 \\ &= \prod_{n \in V_2^c} [\tau_S(n)]^2 \times \prod_{n \in V_3^c} [\tau_S(n)]^2 \times \prod_{n \in V_4^c} [\tau_S(n)]^2 \times \prod_{n \in V_5^c} [\tau_S(n)]^2 \times \prod_{n \in V_6^c} [\tau_S(n)]^2 \times \prod_{n \in V_6^c} [\tau_S(n)]^2 \\ By \text{ using Table 2.7} \\ &= (2P+6)(2)^2 \times (16p+16)(3)^2 \times (48p+16)(4)^2 \times (8p+8)(5)^2 \times (6p+2)(6)^2 \times (2p+2)(8)^2 \\ &= (1152p^2 + 4608p + 3456) \times (153600p^2 + 204800p + 51200) \times (27648p^2 + 36864p + 9216) \\ &= 4.892236186 \times 10^{12}p^6 + 3.261490421 \times 10^{13}p^5 + 7.881936078 \times 10^{13}p^4 + 9.132173844 \times 10^{13}p^3 \\ &+ 5.381459805 \times 10^{13}p^2 + 1.522029036 \times 10^{13}p + 1.630745795 \times 10^{12} . \end{split}$$

**Theorem 3.2:** Let  $R \cong ZNOX(p)$  and  $S \cong ZNOX(p)$  be two MONs of dimensions  $p \ge 1$ . Then, second multiplicative ZCI of two MONs R and S are as follows:

(a)  $MZC_2(R) = 9.57655233 \times 10^{14} p^8 + 1.33829567 \times 10^{17} p^7 + 9.785365205 \times 10^{17} p^6$ + 2.469533816×10<sup>18</sup> p<sup>5</sup> + 2.48995058×10<sup>18</sup> p<sup>4</sup> + 11.43990477×10<sup>17</sup> p<sup>3</sup> + 2.729399844×10<sup>17</sup> p<sup>2</sup> + 4.004443423×10<sup>16</sup> p + 3.522410054×10<sup>15</sup>,

(b)  $MZC_2(S) = 1.479074071 \times 10^{21} p^{10} + 1.380469133 \times 10^{22} p^9 + 4.979549374 \times 10^{22} p^8 + 9.11547872 \times 10^{22} p^7 + 9.688848174 \times 10^{22} p^6 + 6.931561944 \times 10^{22} p^5 + 2.775140623 \times 10^{22} p^4 + 13.68160423 \times 10^{22} p^2 + 13.7965757 \times 10^{19} p + 6.086724573 \times 10^{18}$ .

**Proof** (a). By principle,

$$MZC_2(G) = \prod_{mn \in E(G)} \left[ \tau_G(m) \times \tau_G(n) \right]$$

$$= \prod_{nn\in E_{2,3}^{c}} [\tau_{R}(m) \times \tau_{R}(n)] \times \prod_{nn\in E_{3,3}^{c}} [\tau_{R}(m) \times \tau_{R}(n)] \times \prod_{nn\in E_{3,5}^{c}} [\tau_{R}(m) \times \tau_{R}(n)] \times \prod_{nn\in E_{3,4}^{c}} [\tau_{R}(m) \times \tau_{R}(n)] \times \prod_{nn\in E_{3,4}^{c}$$

(**b**). By principle,

$$\begin{split} MZC_{2}(G) &= \prod_{mn \in E_{3,3}^{c}} [\tau_{G}(m) \times \tau_{G}(n)] \\ &= \prod_{mn \in E_{3,3}^{c}} [\tau_{S}(m) \times \tau_{S}(n)] \times \prod_{mn \in E_{3,4}^{c}} [\tau_{S}(m) \times \tau_{S}(n)] \times$$

**Theorem 3.3:** Let  $R \cong ZNOX(p)$  and  $S \cong ZNOX(p)$  be two MONs of dimensions  $p \ge 1$ . Then, third multiplicative ZCI of two MONs R and S are as follows:

(a) 
$$MZC_{3}(R) = 8.719958016 \times 10^{12} p^{6} + 5.707608883 \times 10^{11} p^{5} + 7.927234560 \times 10^{9} p^{4}$$
,  
(b)  $MZC_{3}(S) = 1.926317998 \times 10^{15} p^{7} + 5.872683423 \times 10^{14} p^{6} + 6.421059994 \times 10^{13} p^{5}$   
 $+ 2.935341711 \times 10^{12} p^{4} + 4.586471424 \times 10^{10} p^{3}$ .  
**Proof (a).** By principle,  
 $MZC_{3}(G) = \prod_{n \in V(G)} [d_{G}(n) \times \tau_{G}(n)]$   
 $= \prod_{n \in V_{2,2}} [d_{R}(n) \times \tau_{R}(n)] \times \prod_{n \in V_{2,3}} [d_{R}(n) \times \tau_{R}(n)] \times \prod_{n \in V_{2,4}} [d_{R}(n) \times \tau_{R}(n)] \times \prod_{n \in V_{3,4}} [d_{R}(n) \times \tau_{R}(n)]$   
 $\times \prod_{n \in V_{3,5}} [d_{R}(n) \times \tau_{R}(n)] \times \prod_{n \in V_{4,8}} [d_{R}(n) \times \tau_{R}(n)]$   
By using Table 2.3,  
 $= (8p)(2 \times 2) \times (50p+1)(2 \times 3) \times (14p)(2 \times 4) \times (22p+1)(3 \times 4) \times (16p)(3 \times 5) \times (4p)(4 \times 8)$   
 $= (9600p^{2} + 192p) \times (29568p^{2} + 1344p) \times (30720p^{2})$ 

 $= 8.719958016 \times 10^{12} p^6 + 5.707608883 \times 10^{11} p^5 + 7.927234560 \times 10^9 p^4.$ 

(b). By principle,

$$\begin{split} MZC_{3}(G) &= \prod_{n \in V(G)} \left[ d_{G}(n) \times \tau_{G}(n) \right] \\ &= \prod_{n \in V_{2,2}} \left[ d_{S}(n) \times \tau_{S}(n) \right] \times \prod_{n \in V_{2,3}} \left[ d_{S}(n) \times \tau_{S}(n) \right] \times \prod_{n \in V_{2,4}} \left[ d_{S}(n) \times \tau_{S}(n) \right] \times \prod_{n \in V_{3,4}} \left[ d_{S}(n) \times \tau_{S}(n) \right] \\ &\times \prod_{n \in V_{3,5}} \left[ d_{S}(n) \times \tau_{S}(n) \right] \times \prod_{n \in V_{3,6}} \left[ d_{S}(n) \times \tau_{S}(n) \right] \times \prod_{n \in V_{4,8}} \left[ d_{S}(n) \times \tau_{S}(n) \right] \end{split}$$

By using Table 2.8,

 $= (8p)(2 \times 2) \times (30p+1)(2 \times 3) \times (30p+3)(2 \times 4) \times (30p+3)(3 \times 4) \times (14p+1)(3 \times 5) \times (8p)(3 \times 6) \times (4p)(4 \times 8)$ = (5760p<sup>2</sup>+192p) × (86400p<sup>2</sup>+17280p+864) × (30240p<sup>2</sup>+2160p) × (128p)

 $= 1.926317998 \times 10^{15} p^{7} + 5.872683423 \times 10^{14} p^{6} + 6.421059994 \times 10^{13} p^{5} + 2.935341711 \times 10^{12} p^{4} + 4.586471424 \times 10^{10} p^{3}.$ 

**Theorem 3.4:** Let  $R \cong ZNOX(p)$  and  $S \cong ZNOX(p)$  be two MONs of dimensions  $p \ge 1$ . Then, fourth multiplicative ZCI of two MONs R and S are as follows:

(a) 
$$MZC_4(R) = 6.010112154 \times 10^{14} p^8 + 5.208763867 \times 10^{15} p^7 + 16.69475598 \times 10^{15} p^6$$
  
+ 2.533150975 × 10<sup>16</sup>  $p^5$  + 2.062710329 × 10<sup>16</sup>  $p^4$  + 9.611232853 × 10<sup>15</sup>  $p^3$  + 2.577175665 × 10<sup>15</sup>  $p^2$   
+ 3.709945774 × 10<sup>14</sup>  $p$  + 2.225967464 × 10<sup>13</sup>,  
(b)  $MZC_4(S) = 1.298184225 \times 10^{18} p^{10} + 1.21163861 \times 10^{19} p^9 + 4.370553558 \times 10^{19} p^8 +$   
3.915708269 × 10<sup>19</sup>  $p^7$  + 8.503908024 × 10<sup>19</sup>  $p^6$  + 5.6457658 × 10<sup>19</sup>  $p^5$  + 2.383565961 × 10<sup>19</sup>  $p^4$   
+ 5.69847671 × 10<sup>18</sup>  $p^3$  6.309875773 × 10<sup>17</sup>  $p^2$  + 3.561547944 × 10<sup>16</sup>  $p$  + 5.342321915 × 10<sup>15</sup>.  
**Proof (a).** By principle,  
 $MZC_4(G) = \prod_{mn \in E_{3,5}} [\tau_R(m) + \tau_R(n)] \times \prod_{mn \in E_{3,5}} [\tau_R(m) + \tau_R(n)] \times \prod_{mn \in E_{4,5}} [\tau_R(m) + \tau_R(n)]$ 

$$\begin{aligned} \prod_{mn\in E_{4,4}^{c}} |t_{R}(m) + t_{R}(n)| &\propto \prod_{mn\in E_{3,4}^{c}} |t_{R}(m) + t_{R}(n)| \\ &\times \prod_{mn\in E_{4,4}^{c}} [\tau_{R}(m) + \tau_{R}(n)] \\ &= \left| E_{2,3(R)}^{c} \right| (2+3) \times \left| E_{3,3(R)}^{c} \right| (3+3) \times \left| E_{3,5(R)}^{c} \right| (3+5) \times \left| E_{4,5(R)}^{c} \right| (4+5) \times \left| E_{4,4(R)}^{c} \right| (4+4) \times \left| E_{3,4(R)}^{c} \right| (3+4) \times \left| E_{4,4(R)}^{c} \right| (4+4) \times \left| E_{5,8(R)}^{c} \right| (5+8) \\ &\text{By using Table 2.5,} \end{aligned}$$

$$= (4p+12)(5) \times (12p+4)(6) \times (4p+12)(8) \times (12p+4)(9) \times (12p+4)(8) \times (24p+8)(7) \times (9p+3)(8) \times (8p+8)(13)$$
  
= (1440 p<sup>2</sup> + 4800 p + 1440)(3456 p<sup>2</sup> + 11520 p + 3456)(16128 p<sup>2</sup> + 10752 p + 1792)  
(7488 p<sup>2</sup> + 9984 p + 2496)  
= 6.010112154 \times 10^{14} p^8 + 5.208763867 \times 10^{15} p^7 + 16.69475598 \times 10^{15} p^6 + 2.533150975 \times 10^{16} p^5 + 2.062710329 \times 10^{16} p^4 + 9.611232853 \times 10^{15} p^3 + 2.577175665 \times 10^{15} p^2 + 3.709945774 \times 10^{14} p + 2.225967464 \times 10^{13}.

(b). By principle,

$$\begin{split} MZC_4(G) &= \prod_{nm\in E_{3,3}} [\tau_G(m) + \tau_G(n)] \\ &= \prod_{nm\in E_{3,3}} [\tau_S(m) + \tau_S(n)] \times \prod_{nm\in E_{3,3}^c} [\tau_S(m) + \tau_S(n)] \times \prod_{nm\in E_{3,4}^c} [\tau_S(m) + \tau_S(n)] \\ &= \left| E_{2,3(5)}^c (2+3) \times \left| E_{3,3(5)}^c \right| (3+3) \times \left| E_{3,5(5)}^c \right| (3+5) \times \left| E_{4,5(5)}^c \right| (4+5) \times \left| E_{4,4(5)}^c \right| (4+4) \times \left| E_{3,4(5)}^c \right| (3+4) \times \left| E_{4,4(5)}^c \right| (4+4) \times \left| E_{4,6(5)}^c \right| (3+4) \times \left| E_{4,4(5)}^c \right| (4+4) \times \left| E_{4,6(5)}^c \right| (3+4) \times \left| E_{4,4(5)}^c \right| (4+4) \times \left| E_{4,6(5)}^c \right| (3+4) \times \left| E_{4,4(5)}^c \right| (4+4) \times \left| E_{4,6(5)}^c \right| (3+4) \times \left| E_{4,4(5)}^c \right| (4+4) \times \left| E_{4,6(5)}^c \right| (3+4) \times \left| E_{4,4(5)}^c \right| (4+4) \times \left| E_{4,6(5)}^c \right| (3+4) \times \left| E_{4,4(5)}^c \right| (4+4) \times \left| E_{4,6(5)}^c \right| (3+4) \times \left| E_{4,4(5)}^c \right| (4+4) \times \left| E_{4,4(5)}^c \right| (3+4) \times \left| E_{4,4(5)}^c \right| (4+4) \times \left| E_{4,6(5)}^c \right| (3+4) \times \left| E_{4,4(5)}^c \right| (4+4) \times \left| E_{4,4(5)}^c \right| (3+4) \times \left| E_{4,4(5)}^c \right| (4+4) \times \left| E_{4,4(5)}^c \right| (3+4) \times \left| E_{4,4(5)}^c \right| (4+4) \times \left| E_{4,4(5)}^c \right| (3+4) \times \left| E_{4,4(5)}^c \right| (4+4) \times \left| E_{4,4(5)}^c \right| (3+4) \times \left| E_{4,4(5)}^c \right| (4+4) \times \left| E_{4,4(5)}^c \right| (3+4) \times \left| E_{4,4(5)}^c \right| (4+4) \times \left| E_{4,4(5)}^c \right| (3+4) \times \left| E_{4,4(5)}^c \right| (3+4)$$

**Theorem 3.5:** Let  $R \cong ZNOX(p)$  and  $S \cong ZNOX(p)$  be two MONs of dimensions  $p \ge 1$ . Then, fifth multiplicative ZCI of two MONs R and S are as follows:

(a) 
$$MZC_5(R) = 6.35830272 \times 10^{11} p^6 + 4.161798144 \times 10^{10} p^5 + 5.78027520 \times 10^8 p^4$$
,

**(b)** 
$$MZC_5(S) = 7.023034368 \times 10^{13} p^7 + 2.140353331 \times 10^{13} p^6 + 2.341011456 \times 10^{12} p^5$$

 $+1.070176666 \times 10^{11} p^4 + 1.672151040 \times 10^9 p^3$ .

**Proof** (a). By principle,

$$\begin{split} MZC_5(G) &= \prod_{n \in V(G)} \left[ d_G(n) + \tau_G(n) \right] \\ &= \prod_{n \in V_{2,2}} \left[ d_R(n) + \tau_R(n) \right] \times \prod_{n \in V_{2,3}} \left[ d_R(n) + \tau_R(n) \right] \times \prod_{n \in V_{2,4}} \left[ d_R(n) + \tau_R(n) \right] \times \prod_{n \in V_{3,4}} \left[ d_R(n) + \tau_R(n) \right] \\ &\times \prod_{n \in V_{3,5}} \left[ d_R(n) + \tau_R(n) \right] \times \prod_{n \in V_{4,8}} \left[ d_R(n) + \tau_R(n) \right] \\ By \text{ using Table 2.3,} \\ &= (8p)(2+2) \times (50p+1)(2+3) \times (14p)(2+4) \times (22p+1)(3+4) \times (16p)(3+5) \times (4p)(4+8)) \\ &= (8000p^2 + 160p) \times (12936p^2 + 588p) \times (6144p^2) \end{split}$$

 $= 6.35830272 \times 10^{11} p^6 + 4.161798144 \times 10^{10} p^5 + 5.78027520 \times 10^8 p^4.$ 

(b). By principle,

$$\begin{split} MZC_{5}(G) &= \prod_{n \in V(G)} [d_{G}(n) + \tau_{G}(n)] \\ &= \prod_{n \in V_{2,2}} [d_{S}(n) + \tau_{S}(n)] \times \prod_{n \in V_{2,3}} [d_{S}(n) + \tau_{S}(n)] \times \prod_{n \in V_{2,4}} [d_{S}(n) + \tau_{S}(n)] \times \prod_{n \in V_{3,4}} [d_{S}(n) + \tau_{S}(n)] \\ &\times \prod_{n \in V_{3,5}} [d_{S}(n) + \tau_{S}(n)] \times \prod_{n \in V_{3,6}} [d_{S}(n) + \tau_{S}(n)] \times \prod_{n \in V_{4,8}} [d_{S}(n) + \tau_{S}(n)] \\ By using Table 2.8, \\ &= (8p)(2+2) \times (30p+1)(2+3) \times (30p+3)(2+4) \times (30p+3)(3+4) \times (14p+1)(3+5) \times (8p)(3+6) \\ &\times (4p)(4+8) \end{split}$$

 $= (4800 p^{2} + 160 p) \times (37800 p^{2} + 7560 p + 3787) \times (387072 p^{3} + 27648 p^{2})$ 

 $= 7.023034368 \times 10^{13} p^{7} + 2.140353331 \times 10^{13} p^{6} + 2.341011456 \times 10^{12} p^{5} + 1.070176666 \times 10^{11} p^{4} + 1.672151040 \times 10^{9} p^{3}.$ 

### Conclusions

We computed multiplicative Zagreb connection indices such as first multiplicative ZCI, second multiplicative ZCI, third multiplicative ZCI, fourth multiplicative ZCI and fifth multiplicative ZCI of two different MONs which are zinc oxide (R) and zinc silicate (S) networks with respect to the increasing layers  $p \ge 1$ , taking both metal nodes and linkers together.

Now, the problem is still open for product, subdivision, prism and their compliment networks with the help of degree as well as connection number indices.

## **Conflict of Interest**

The authors declare no conflict of interest.

#### References

- [1] Cui Y, Xu H, Yue Y, Gao Z, Yu J. Chen Z, Gao J, Yang Y, Qian G, Chen B. A luminescent mixed-lauthanide metal-organic framework thermometer. J. Am. Chem. Soc. 2012; 134: 3979-3982.
- [2] Wang C, Tian L, Zhu W, Wang S, Wang P, Liang Y, Zhang W, Zhao H, Li G. Dye@bio-MOF-1 composite as a dual emitting platform for explosive molecules. ACS Appl. Mater Interfaces, 2017; 9: 20076-20085.
- [3] Bahrani S, Hashemi SA, Mousavi SM, Azhdari R. Zinc-based metal-organic frameworks as nontoxic and biodegradable platforms for biomedical applications: review study. *Drug metabolism Review*, 2019; 51(3): 356-377.
- [4] Eddaoudi M, Kim J, Rosi N, Vodak D, Wachter J, Okeeffe M, Yaghi OM. Systematic design of pore size and functionality in isoreticular MOFs and their application in methane storage. *Science*, 2002; 295: 469-472.
- [5] Keskin S, Sholl D. Efficient methods for screening of metal organic frame work membranes for gas separations using atomically detailed models. *Langmuir*, 2009; 25(19): 11786-11795.
- [6] Ahmad I, Jhung SH. Composites of metal-organic frameworks: preparation and application in adsorption. *Materials Today*, 2014; 17(3): 136-146.
- [7] Li H, Li L, Lin R.-B, Zhou W, Zhang Z, Xiang S, Chen B. Porous metal-organic frameworks for gas storage and separation: status and challenges. *Elsevier*, 2019; 1(1).
- [8] Thornton AW, Nairn KM, Hill JM, Hill AJ, Hill MR. Metal-organic frameworks impregnated with magnesium-decorated fullerenes for methane and hydrogen storage. J. Am. Chem. Soc. 2009; 131(30): 10662-10669.
- [9] Hwang YK, Hong DY, Chang JS, Jhung SH, Seo YK, Kim J. Amine grafting on coordinatively unsaturated metal centers of MOFs: consequences for catalysis and metal encapsulation. *Angew. Chem. Int. Edit.* 2008; 47(22): 4144-4148.
- [10] Kim M, Cahill JF, Fei H, Prather KA, Cohen SM. Postsynthetic ligand and cation exchange in robust metal–organic frameworks. *J. Am. Chem. Soc.* 2012; 134(43): 18082-18088.
- [11] Yin Z, Zhou YL, Zeng MH, Kurmoo M. The concept of mixed organic ligands in metal–organic frameworks: design, tuning and functions. *Dalton T.* 2015; 44(12): 5258-5275.
- [12] Ding G, Yuan J, Jin F, Zhang Y, Han L, Ling X, Zhao H, Ma W. High performance all-polymer non-fullerence solar cells by employing an efficient polymer-small molecule acceptor alloy strategy. *Nano Energy*, 2017; 36: 356-365.
- [13] Lin R.B, Xiang S, Xing H, Zhou W, Chen B. Exploration of porous metal–organic frameworks for gas separation and purification. *Coordin. Chem. Rev.* 2019; 378: 87-103.
- [14] Mandal B, Chung JS, Kang SG. Exploring the geometric, magnetic and electronic properties of Hofmann MOFs for drug delivery. Physical Chemistry Chemical Physics, 2017; 19(46): 31316–31324.
- [15] Geier SJ, Mason JA, Bloch ED. Selective adsorption of ethylene over ethane and propylene over propane in the metal-organic frameworks M2 (dobdc) (M=Mg, Mn, Fe, Co, Ni, Zn). *Chemical Science*, 2013; 4(5): 2054–2061.

- [16] Murray LJ, Dinca M, Long JR. Hydrogen storage in metal-organic frameworks. *Chemical Society Reviews*, 2009; 38(5); 1294–1314.
- [17] Rosi NL, Eckert J, Eddaoudi M. Hydrogen storage in microporous metalorganic frameworks. *Science*, 2003; 300(5622) 1127–1129.
- [18] Kennedy RD, Krungleviciute V, Clingerman DJ. Carborane-based metalorganic framework with high methane and hydrogen storage capacities. *Chemistry* of Materials, 2013; 25(17): 3539–3543.
- [19] Sarkisov L. Toward rational design of metal-organic frameworks for sensing applications: efficient calculation of adsorption characteristics in zero loading regime. Journal of Physical Chemistry C, 2012; 116(4): 3025–3033.
- [20] Li J.-R, Kuppler RJ, Zhou H.-C. Selective gas adsorption and separation in metalorganic frameworks. *Chemical Society Reviews*, 2009; 38(5): 1477–1504.
- [21] Kim JY, Balderas-Xicohtencatl R, Zhang L. Exploiting diffusion barrier and chemical affinity of metalorganic frameworks for efficient hydrogen isotope separation. *Journal of the American Chemical Society*, 2017; 139(42) 15135–15141.
- [22] Klavzar S, Gutman I. Selected properties of the Schultz molecular topological index. J. Chem. Inf. Comput. Sci. 1996; 36: 1001-1003.
- [23] Rucker G, Rucker C. On topological indices, boiling points and cycloalkanes. J. Chem. Inf. Comp. Sci. 1999; 39: 788-802.
- [24] Gonzalez-Diaz H, Vilar S, Santana L, Uriarte E. Medicinal chemistry and bioinformatics-current trends in drug discovery with network topological indices. *Current Topics in Medicinal Chemistry*, 2007; 7(10): 1015-1029.
- [25] Gutman I, Trinajstić N. Graph theory and molecular orbitals. Total  $\pi$ -electron energy of alternant hydrocarbons. *Chem. Phys. Lett.* 1972; 17(4): 535-538.
- [26] Awais HM, Jamal M, Javaid M. Topological properties of metal-organic frameworks. *Main Group Metal Chemistry*, 2020; 43(1): 67-76.
- [27] Hong G, Gu Z, Javaid M, Awais HM, Siddiqui MK. Degree-based topological invariants of metalorganic networks. *IEEE Access*, 2020; 8: 68288-68300.
- [28] Nadeem MF, Imran M, Siddiqui HMA, Azeem M, Khalil A, Ali Y. Topological aspects of metal-organic structure with the help of underlying networks. *Arabian Journal of Chemistry*, 2021; 14: 103157.
- [29] Haoer RS. Topological indices of metal-organic networks via neighborhood M-polynomial. *Journal of Discrete Mathematical Sciences and Cryptography*, 2021; 24(2): 369-390.
- [30] Kashif A, Aftab S, Javaid M, Awais HM. M-polynomial-based topological indices of metalorganic networks, Main Group Metal Chemistry, 2021; 44: 129-140.
- [31] Min HY, Kam LF, George ZC. Study suggests choice between green energy or economic growth. *Green Energy Environ.* 2017; 2 (8): 218–245.
- [32] Tea KW, Shaopeng Q, Alan FO, Gaurav J, Soo JJ, Vivian TC, Doo KL, Reginald M. Composite nanowires for fast responding and transparent hydrogen sensors. *Am. Chem. Soc. Appl. Matter Interf.* 2017; 9 (45): 39464–39474.

- [33] Wasson, MC, Lyu J, Islamoglu T, Farha OK. Linker competition within a metal-organic framework for topological insights. *Inorg. Chem.* 2019; 58 (2): 1513–1517.
- [34] Tang J.-H, Ali U, Javaid M, Shabbir K. Zagreb connection indices of subdivision and semi-total point operations on graphs. *Journal of Chemistry*, 2020; Article ID 9846913: 14 pages.
- [35] Javaid M, Abbas M, Liu J.-B, The WC, Cao J. Topological properties of four-layered neural networks. *JAISCR*, 2019; 9(2): 111-122.
- [36] Javaid M, Rehman M, Cao J. Topological indices of rhombus type silicate and oxide
- [37] Liu J.-B, Raza Z, Javaid M. Zagreb connection indices for cellular neural networks. *Discrete Dynamics in Nature and Society*, 2020; Article ID 8038304: 8 pages.
- [38] Javaid M, Jung CY. M-polynomial and topological indices of silicate and oxide networks. *Int. J. Pure and Appl. Math.* 2017; 115(1): 129-152.
- [39] Raheem A, Javaid M, The WC, Wang S, Liu J.-B. M-polynomial method for topological indices of 2D-lattice of three-layered single-walled titania nanotubes. *Journal of Information and Optimization Sciences*, 2019; 1-11.
- [40] Zhao D, Chu Y.-M, Siddiqui MK, Ali K, Nasir M, Younas MT, Cancan M. On reverse degree based topological indices of polycyclic metal organic network. *Polycyclic Aromatic compounds*, 2021.
- [41] Dayan F, Javaid M, ur Rehman MA. On leap Gourava indices of some wheel related graphs. *Sci. Inquiry Rev.* 2018; 3(4):
- [42] Dayan F, Javaid M, ur Rehman MA. On leap reduced reciprocal randic and leap reduced second Zagreb indices of some graphs. *Sci Inquiry Rev.* 2019; 3(2):27–35.
- [43] Cao J, Ali U, Javaid M, Huang C. Zagreb connection indices of molecular graphs based on opoerations. *Complexity*, 2020; Article ID 7385682: 15 pages.
- [44] Ali U, Javaid M, and Alanazi AM. Computing analysis of connection-based indices and coindices for product of molecular networks. *Symmetry*, 2020; 12(8): 1320.doi:10.3390/sym 12081320.
- [45] Ali U, Javaid M. Upper bounds of Zagreb connection indices of tensor and strong product on graphs. *Punjab University Journal of Mathematics*, 2020; 52(4): 89-100.
- [46] Ali U, Javaid M. Zagreb connection indices of disjunction and symmetric difference operations on graphs. *Journal of Prime Research in mathematics*, 2020; 16(2): 1-15.
- [47] Javaid M, Ali U, Liu J.-B. Computing first Zagreb connection index and coindex of resultant graphs. *Mathematical Problems in Engineering*, 2021; Article ID 6019517: 19 pages.
- [48] Todeschini R, Consonni V. Handbook of molecular descriptors. *Wiley-VCH, Germany*, 2002.
- [49] Gutman I, Polansky OE. Mathematical concepts in organic chemistry. *Springer-Verlag Berlin, Heidelberg New York, London, Paris, Tokyo,* 1986; DOI: 10.1007/978-3-642-70982-1.
- [50] Gutman I, Ruscic B, Trinajstić N, Wilson CF. Graph theory and molecular XII. orbitals. Acyclic polyenes. J. Chem. Phys. 1975; 62: 3399-3405.

- [51] Furtula B, Gutman I. Aforgotten topological index. J. Math. Chem. 2015; 53(4): 1184-1190.
- [52] Gutman I. Selected properties of the schultz molecular topological index. J. Chem. Inf. Model. 1994; 34(5): 1087-1089.
- [53] Matamala AR, Estrada E. Generalised topological indices: Optimisation methodology and physico-chemical interpretation. *Chem. Phys. Lett.* 2005; 410(4-6): 343\_347.
- [54] Todeschini R, Consonni V. New local vertex invariants and molecular descriptors based on functions of the vertex degrees. MATCH-Communications in Mathematical and in Computer Chemistry, 2010; 64: 359-372.
- [55] Eliasi M, Gutman I, Iranmanesh A. Multiplicative versions of first Zagreb index. MATCH-Communications in Mathematical and in Computer Chemistry, 2012; 68: 217-230.
- [56] Ali A, Trinajstić N. A novel/old modification of the first Zagreb index, Mol. Inform. 2018; 37: 1-7.
- [57] Haoer, RS, Mohammed MA, Selvarasan T, Chidambaram N, Devadoss N. Multiplicative Leap Zagreb Indices of T-thorny Graphs. Eurasian Chemical Communications, 2020; 8: 841-846.

[58] Keskin S, Sholl DS. Screening metal-organic framework materials for membrane-based methane/carbon dioxide seprations. J. Phys. Chem. 2007; 111(38): 14055-14059.