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# Computation of degree based topological aspects of 2D Kagome lattice $M_3C_{12}X_{12}$

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**Abstract**

To connect the biological activity of quantitative structure - activity (QSAR) and quantitative structure - property (QSPR) interactions, topological indices are employed in structural underpinnings with their physical attributes, such as strain energy, chromatic aberration, boiling point, melting point, stability, etc. Such projections can be completed quickly and easily, degree - based topological indices are in the middle of the many types of descriptors in this research. In this study, we calculate the 2$D$ structures of $M_3C_{12}X_{12}$ lattice. Additionally, we compute the general Randic index, first and second Zagreb indices, atom - bond connectivity, geometric arithmetic index multiple geometric - arithmetic index and multiple atom - bond connectivity. We also give the exact formulas for the 5th iteration of the GA index and 4th iteration of the ABC index for these chemical graphs.

***Subject Classification (2020):*** *05C92.*

***Keywords:*** *$M_3C_{12}X_{12}$ lattice, Chemical graph, QSAR, QSPR, Topological descriptors.*

## 1. Introduction

Since graphene has been discovered, (2D) organic-covalent frameworks and 2$D$ materials have sparked a lot of interest [1]. Similar to graphene, a great deal of other 2$D$ materials have been investigated conceptually or efficiently generated experimentally for their potential uses in nanodevices and nanotechnology. [2, 3] These materials include

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2*D* boron nitride nanomesh [4], metal carbide particles [5], graphene oxide [6], silicene [7], porous graphene [8] and $MoS_2$ [9]. To address the significant need for materials for the next nanotechnology [5, 10] there is an immediate need for additional 2*D* materials and the examination of their distinct characteristics. In addition, significant advancements have been achieved in the composition of different types of MOF and the exploration of their possible uses across many industries [11-13]. Every graph in the article will be a finite, simple, linked molecular graph. Consider the graph $\Omega$, which has an edge set of $E(\Omega)$ and a vertex set of $V(\Omega)$. Atoms are associated with the vertices of $\Omega$, while chemical bonds between atoms are related to the edges. Iff $x$ and $y$ are the end vertices of a shared edge $z \in E(\Omega)$, which we express as $z = xy$, then they are referred to as neighboring vertices. $N_x$ describes the set of vertices adjacent to a vertex $x$, that is, $N_x = \{y \in V(\Omega) \mid xy \in E(\Omega)\}$.$\lambda_x$, which denotes the number of vertices incident to $x$, is used to express the degree of a vertex $x \in V(\Omega)$. Let $S_x$ be the total of all vertex $x$'s surrounding vertices' degrees. Suppose $\varepsilon_{(l,m)}$ represent he set containing the $l$ degrees of all edges and $m$ at their end vertices. Since graph theory was crucial to the evaluation of (QSPR) and (QSAR) investigations, it has grown to be an important and necessary component of predictive pharmacology and drug development. Thus, the study of quantitative structure - activity, quantitative structure toxicity relationships, quantitative structure - property (QSAR/QSTR/QSPR) has shown to be a useful field for estimating the physical and chemical characteristics, biological in nature and pharmacological activities of substances and supplies. This is because multiple characteristics of molecules are dependent on their structures. Numerous fields, including toxicology, chemical analysis, pharmaceutical dynamics and pharmacokinetics, have made extensive use of these investigations [14]. Because topological descriptors are simple to construct and can be evaluated quickly, they have proven to be extremely important. Numerous numerical descriptors related to graphs are useful in a variety of contexts. Consequently, the task of identifying topological descriptors has emerged as an intriguing and desirable area of study. The degree - based approach stands out among the others and is useful in describing the fundamental characteristics of chemical compounds. It considers attributes such as molecular weight, population density, melting and boiling temperatures and so on. Among the useful varieties of graph - related descriptors are those that are accumulating-distance, counting - related and degree - based. Table 1, shows the degree-based topological descriptor mathematical equations that we covered in this essay.

**Table 1**

**Topological descriptors on degree - based.**

| **Topological descriptors** | **Mathematical from** |
|---|---|
| General R̂andic index Li and I. Gutman [14] | $R_\alpha(\Omega)=\sum_{lm\in E(\Omega)}(\lambda_l\lambda_m)^\alpha$ |
| First Źagreb (Ḡutman and Ṫrinajstic, 1972) | $M_1(\Omega)=\sum_{lm\in E(\Omega)}(\lambda_l+\lambda_m)$ |
| Second Źagreb (Ḡutman and Ṫrinajstic, 1972) | $M_2(\Omega)=\sum_{lm\in E(\Omega)}(\lambda_l\lambda_m)$ |
| Sum - connectivity index (Źhou, N. Ṫrinajstic, 2010) | $SCI(\Omega)=\sum_{lm\in E(\Omega)}\frac{1}{\sqrt{\lambda_l+\lambda_m}}$ |
| Atom - bond connectivity index (Estrada et al, 1998) | $ABC(\Omega)=\sqrt{\frac{\lambda_l+\lambda_m-2}{\lambda_l\lambda_m}}$ |
| Geometric - arithmetic (Vukicevic and Furtula, 2009) | $GA(\Omega)=\sum_{lm\in E(\Omega)}\frac{2\sqrt{\lambda_l+\lambda_m}}{\lambda_l+\lambda_m}$ |
| Multiple atom - bond connectivity index | $ABC_\mu(\Omega)=\sum_{lm\in E(\Omega)}\sqrt{\frac{\mu_l+\mu_m-2}{\mu_l\mu_m}}$ |
| Fourth version of atom - bond connectivity index (Ghorbani and Hosseinzadeh, 2010) | $ABC_4(\Omega)=\sum_{lm\in E(\Omega)}\sqrt{\frac{\mathbb{S}_l+\mathbb{S}_m-2}{\mathbb{S}_l\mathbb{S}_m}}$ |
| Multiple geometric - arithmetic index | $GA_\mu(\Omega)=\sum_{lm\in E(\Omega)}\frac{2\sqrt{\mu_l\mu_m}}{\mu_l+\mu_m}$ |
| Fifth version of geometric - arithmetic index (Graovac et al., 2011) | $GA_5(\Omega)=\sum_{lm\in E(\Omega)}\frac{2\sqrt{\mathbb{S}_l\mathbb{S}_m}}{\mathbb{S}_l+\mathbb{S}_m}$ |

We directed the curious reader to (Aslam et al. [15], Bashir et al. [16], Gao et al. [17] and Gao et al. [18], Gao et al. [19], Iqbal, Ishaq, and Aamir

[20], Iqbal et al. [21], Iqbal et al. [22], Yang et al. [23], Zheng et al. [25], Zhao et al. [24], Zhou et al. [26]) and other researchers [27-31] for the comprehensive negotiations of topological descriptors.

## 2. Topological aspects of 2D $M_3C_{12}X_{12}$ lattice

Materials with potential benefits in quantum computing and spintronics are known as topological insulators. To address the needs of multifunctional applications in spintronic devices, Wang et al. [34] presented a 2D structure of the $M_3C_{12}X_{12}$ lattice, where metal atoms, carbon and organic linkers are employed. This structure might function as a topological insulator and be easily constructed. Figure 1 displays the molecular graph of the $M_3C_{12}X_{12}$ lattice. Keep in mind that a kagome lattice makes up each unit cell of the $M_3C_{12}X_{12}$ lattice. The molecular diagram of the $M_3C_{12}X_{12}$ lattice, consists of m unit cells per row and n unit cells per column., is identified by the notation Ω(m,n). The Ω(m,n) molecular graph is portrayed in Figure 1. The calculation finds that $\Omega(m,n)$ has $29mn-(n-1)-n(m-1) = 27mn+m+n$ vertices and $36mn$ edges [32-34].

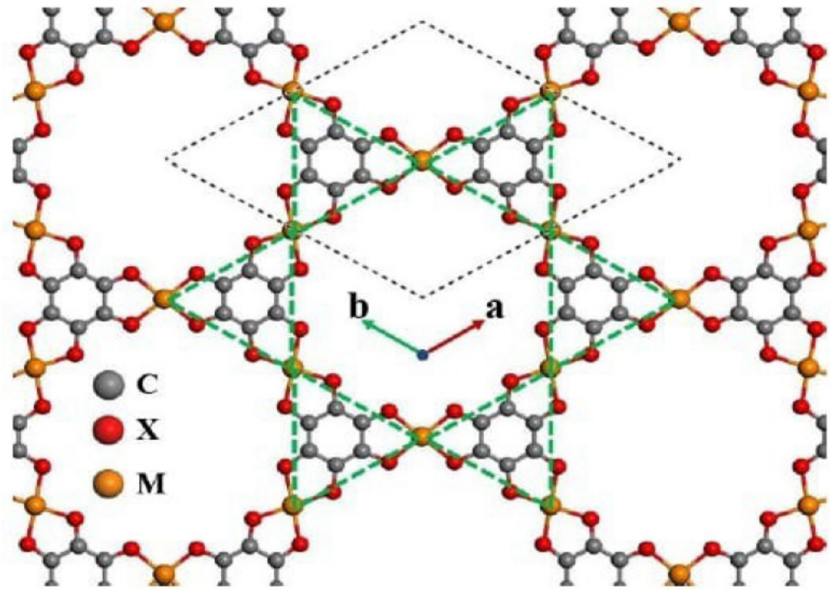


**Figure 1**

**Molecular Graph of $M_3C_{12}X_{12}$ lattice.**

**Table 2**

**Partitioning of set of edges of Ω(m,n) is specified to the degree of the graph's vertices.**

| $(\lambda_l, \lambda_m)$ where $lm \in E(\Omega(m,n))$ | Number of edges |
|---|---|
| (2, 2) | $(4m + 4n)$ |
| (2, 3) | $(12\ mn)$ |
| (2, 4) | $(12mn - 4m - 4n)$ |
| (3, 3) | $(12mn)$ |

**Theorem 1:** *The Randic connectivity index of graph* Ω(m,n) *is:*

$$R_{-\frac{1}{2}}(\Omega(m,n)) = \left(4+2\sqrt{6}+3\sqrt{2}\right)mn + \left(2-\sqrt{2}\right)(m+n).$$

$$R_{\frac{1}{2}}(\Omega(m,n)) = \left(36+12\sqrt{6}+24\sqrt{2}\right)mn + 8\left(1-\sqrt{2}\right)(m+n).$$

$$R_1(\Omega(m,n)) = 276mn - 16(m+n).$$

$$R_{-1}(\Omega(m,n)) = \frac{29}{6}mn + \frac{1}{2}(m+n).$$

***Proof:*** By utilizing Table 1 and the mathematical equation for the Randic connectivity index, the index's values can be summed as follows:

**Randic Index** for $\alpha = 1$

$$R_1(\Omega(m,n)) = \sum_{lm\in E(\Omega)} \lambda_l\lambda_m = \sum_{lm\in E_{(2,2)}(\Omega(m,n))} \lambda_l\lambda_m + \sum_{lm\in E_{(2,3)}(\Omega(m,n))} \lambda_l\lambda_m + \sum_{lm\in E_{(2,4)}(\Omega(m,n))} \lambda_l\lambda_m + \sum_{lm\in E_{(3,3)}(\Omega(m,n))} \lambda_l\lambda_m$$

$$R_1(\Omega(m,n)) = (4m+4n)(4) + (12mn)(6) + (12mn-4m-4n)(8) + (12mn)(9)$$

$$R_1(\Omega(m,n)) = 276mn - 16(m+n).$$

***Proof.*** **Randic Index** for $\alpha = {}^1\!/_2$

$$R_{\frac{1}{2}}(\Omega(m,n)) = \sum_{lm\in E_{(2,2)}(\Omega(m,n))} \sqrt{\lambda_l\lambda_m} + \sum_{lm\in E_{(2,3)}(\Omega(m,n))} \sqrt{\lambda_l\lambda_m} + \sum_{lm\in E_{(2,4)}(\Omega(m,n))} \sqrt{\lambda_l\lambda_m} + \sum_{lm\in E_{(3,3)}(\Omega(m,n))} \sqrt{\lambda_l\lambda_m}$$

$$R_{\frac{1}{2}}(\Omega(m,n)) = \left(4m+4n\right)\sqrt{4} + \left(12mn\right)\sqrt{6} + \left(12mn-4m-4n\right)2\sqrt{2} + \left(12mn\right)\sqrt{9}$$

$$R_{\frac{1}{2}}(\Omega(m,n)) = \left(36+12\sqrt{6}+24\sqrt{2}\right)mn + 8\left(1-\sqrt{2}\right)\left(m+n\right).$$

$$R_{\frac{1}{2}}(\Omega(m,n)) \simeq 99.33500241035242mn - 3.31370849898476\left(m+n\right).$$

***Proof:*** **Randic Index** for $\alpha = -1/2$

$$R_{-1/2}(\Omega(m,n)) = \sum_{lm\in E_{(2,2)}(\Omega(m,n))} 1/\sqrt{\lambda_l\lambda_m} + \sum_{lm\in E_{(2,3)}(\Omega(m,n))} 1/\sqrt{\lambda_l\lambda_m} + \sum_{lm\in E_{(2,4)}(\Omega(m,n))} 1/\sqrt{\lambda_l\lambda_m} + \sum_{lm\in E_{(3,3)}(\Omega(m,n))} 1/\sqrt{\lambda_l\lambda_m}$$

$$R_{-\frac{1}{2}}(\Omega(m,n)) = \left(4m+4n\right)(\frac{1}{2}) + \left(12mn\right)(\frac{1}{\sqrt{6}}) + \left(12mn-4m-4n\right)(\frac{1}{2\sqrt{2}}) + \left(12mn\right)(\frac{1}{3})$$

$$R_{-\frac{1}{2}}(\Omega(m,n)) = \left(4+2\sqrt{6}+3\sqrt{2}\right)mn + \left(2-\sqrt{2}\right)\left(m+n\right).$$

$$R_{-\frac{1}{2}}(\Omega(m,n)) \simeq 10.24264068711929mn + 0.585786437626905\left(m+n\right).$$

**Randic Index** for $\alpha = -1$

$$R_{-1}(\Omega(m,n)) = \sum_{lm\in E_{(2,2)}(\Omega(m,n))} 1/\lambda_l\lambda_m + \sum_{lm\in E_{(2,3)}(\Omega(m,n))} 1/\lambda_l\lambda_m + \sum_{lm\in E_{(2,4)}(\Omega(m,n))} 1/\lambda_l\lambda_m + \sum_{lm\in E_{(3,3)}(\Omega(m,n))} 1/\lambda_l\lambda_m$$

$$R_{-1}(\Omega(m,n)) = \left(4m+4n\right)(\frac{1}{4}) + \left(12mn\right)(\frac{1}{6}) + \left(12mn-4m-4n\right)(\frac{1}{8}) + \left(12mn\right)(\frac{1}{9})$$

$$R_{-1}(\Omega(m,n)) = \frac{29}{6}mn + \frac{1}{2}\left(m+n\right).$$

**Theorem 2:** *The first Zagreb index of a graph* $\Omega$(m,n) *is*

$$M_1(\Omega(m,n)) = 204mn - 8m - 8n.$$

***Proof:*** By utilizing Table 1 and the mathematical equation for first Zagreb index, the index's values can be summed as follows:

$$M_1(\Omega(m,n)) = \sum_{lm\in E(\Omega)} \left(\lambda_l+\lambda_m\right) = \sum_{lm\in E_{(2,2)}(\Omega(m,n))} \left(\lambda_l+\lambda_m\right) + \sum_{lm\in E_{(2,3)}(\Omega(m,n))} \left(\lambda_l+\lambda_m\right) + \sum_{lm\in E_{(2,4)}(\Omega(m,n))} \left(\lambda_l+\lambda_m\right) + \sum_{lm\in E_{(3,3)}(\Omega(m,n))} \left(\lambda_l+\lambda_m\right)$$

$M_1(\Omega(m,n)) = (4m + 4n)(4) + (12mn))(5) + (12mn - 4m - 4n)(6) + (12mn)(6) = 204mn - 8m - 8n.$

**Theorem 3**: *The second Zagreb index of a graph* $\Omega(m,n)$ *is*

$$M_2(\Omega(m,n)) = 276mn - 16m - 16n$$

***Proof:*** By utilizing Table 1 and the mathematical equation for second Zagreb index, the index's values can be summed as follows:

$$M_2(\Omega(m,n)) = \sum_{lm\in E_{(2,2)}(\Omega(m,n))} \lambda_l\lambda_m + \sum_{lm\in E_{(2,3)}(\Omega(m,n))} \lambda_l\lambda_m + \sum_{lm\in E_{(2,4)}(\Omega(m,n))} \lambda_l\lambda_m + \sum_{lm\in E_{(3,3)}(\Omega(m,n))} \lambda_l\lambda_m$$

$M_2(\Omega(m,n)) = (4m + 4n)(4) + (12mn))(6) + (12mn - 4m - 4n)(8) + (12mn)(9) = 276mn - 16m - 16n.$

**Theorem 4:** *The sum connectivity index of a graph* $\Omega(m,n)$ *is:*

$$SCI(\Omega(m,n)) = \left(2.4\sqrt{5} + 4\sqrt{6}\right)mn + \left(1 - \frac{2\sqrt{6}}{3}\right)\left(m+n\right).$$

***Proof:*** By utilizing Table 1 and the mathematical equation for sum connectivity index, the index's values can be summed as follows:

$$SCI(\Omega(m,n)) = \sum_{lm\in E_{(2,2)}(\Omega(m,n))} \frac{1}{\sqrt{\lambda_l + \lambda_m}} + \sum_{lm\in E_{(2,3)}(\Omega(m,n))} \frac{1}{\sqrt{\lambda_l + \lambda_m}} + \sum_{lm\in E_{(2,4)}(\Omega(m,n))} \frac{1}{\sqrt{\lambda_l + \lambda_m}} + \sum_{lm\in E_{(3,3)}(\Omega(m,n))} \frac{1}{\sqrt{\lambda_l + \lambda_m}}$$

$$SCI(\Omega(m,n)) = \left(4m+4n\right)\left(\frac{1}{\sqrt{4}}\right) + \left(12mn\right)\left(\frac{1}{\sqrt{5}}\right) + \left(12mn - 4m - 4n\right)\left(\frac{1}{\sqrt{6}}\right) + \left(12mn\right)\left(\frac{1}{\sqrt{6}}\right)$$

$$= \left(2.4\sqrt{5} + 4\sqrt{6}\right)mn + \left(1 - \frac{2\sqrt{6}}{3}\right)\left(m+n\right).$$

$$SCI(\Omega(m,n)) \simeq 15.16452211713221mn - 0.6329931618554521\left(m+n\right).$$

**Theorem 5:** *The atom bond connectivity of a graph* $\Omega(m,n)$ *is*

$$ABC(\Omega(m,n)) = 4\left(3\sqrt{2} + 2\right)mn.$$

$$ABC(\Omega(m,n)) \approx 24.97056274847714mn.$$

***Proof:*** By utilizing Table 1 and along with the mathematical expression for the atom-bond connectivity index, the index's values can be summed as follows:

$$ABC(\Omega(m,n)) = \sum_{lm\in E_{(2,2)}(\Omega(m,n))} \sqrt{\frac{\lambda_l+\lambda_m-2}{\lambda_l\lambda_m}} + \sum_{lm\in E_{(2,3)}(\Omega(m,n))} \sqrt{\frac{\lambda_l+\lambda_m-2}{\lambda_l\lambda_m}}$$
$$+ \sum_{lm\in E_{(2,4)}(\Omega(m,n))} \sqrt{\frac{\lambda_l+\lambda_m-2}{\lambda_l\lambda_m}} + \sum_{lm\in E_{(3,3)}(\Omega(m,n))} \sqrt{\frac{\lambda_l+\lambda_m-2}{\lambda_l\lambda_m}}$$
$$ABC(\Omega(m,n)) = \left(4m+4n\right)\left(\frac{1}{\sqrt{2}}\right) + \left(12mn\right)\left(\frac{1}{\sqrt{2}}\right)$$
$$+\left(12mn-4m-4n\right)\left(\frac{1}{\sqrt{2}}\right) + \left(12mn\right)\left(\frac{2}{3}\right)$$
$$ABC(\Omega(m,n)) = 4\left(3\sqrt{2}+2\right)mn.$$
$$ABC(\Omega(m,n)) \approx 24.97056274847714mn.$$

**Theorem 6**: *The Geometric - arithmetic index of a graph* $\Omega(m,n)$ *is*

$$GA(\Omega(m,n)) = 4\left(1.2\sqrt{6}+2\sqrt{2}+3\right)mn + 4\left(1-\frac{2\sqrt{2}}{3}\right)\left(m+n\right).$$
$$GA(\Omega(m,n)) \approx 35.07125926434402mn + 0.2287638336717465\left(m+n\right).$$

***Proof:*** By utilizing Table 1 and the mathematical equation of geometric-arithmetic index, the values of this index can be computed as follows:

$$GA(\Omega(m,n)) = \sum_{lm\in E_{(2,2)}(\Omega(m,n))} \frac{2\sqrt{\lambda_l\lambda_m}}{\lambda_l+\lambda_m} + \sum_{lm\in E_{(2,3)}(\Omega(m,n))} \frac{2\sqrt{\lambda_l\lambda_m}}{\lambda_l+\lambda_m}$$
$$+ \sum_{lm\in E_{(2,4)}(\Omega(m,n))} \frac{2\sqrt{\lambda_l\lambda_m}}{\lambda_l+\lambda_m} + \sum_{lm\in E_{(3,3)}(\Omega(m,n))} \frac{2\sqrt{\lambda_l\lambda_m}}{\lambda_l+\lambda_m}$$
$$GA(\Omega(m,n)) = \left(4m+4n\right)(1) + \left(12mn\right)\left(\frac{2\sqrt{6}}{5}\right)$$
$$+\left(12mn-4m-4n\right)\left(\frac{2\sqrt{2}}{3}\right) + \left(12mn\right)(1)$$
$$GA(\Omega(m,n)) = 4\left(1.2\sqrt{6}+2\sqrt{2}+3\right)mn + 4\left(1-\frac{2\sqrt{2}}{3}\right)\left(m+n\right).$$

**Table 3**

**The graph Ω(*m, n*)'s edge partition is determined by adding the neighbor vertices of each edge's end vertices.**

| $(S_l, S_m)$ in which $lm \in E(\Omega(m,n))$ | Number of edges |
|---|---|
| (4, 5) | $8m + 8n - 8$ |
| (5, 8) | $32mn - 24m - 24n + 24$ |
| (7, 8) | $16mn - 8m - 8n + 8$ |
| (8, 8) | $24mn - 12m - 12n + 12$ |

**Theorem 7:** *The fourth version of atom bond connectivity index of the graph* Ω(m,n) *is:*

$$ABC_4(\Omega(m,n)) = \frac{8143}{228}mn - \frac{3845}{222}\left(m+n-1\right).$$

***Proof:*** By utilizing Table 2 and along with the mathematical expression of fourth version of atom bond connectivity index, the index's values can be summed as follows:

Fourth version of Atom Bond Connectivity

$$ABC_4(\Omega(m,n)) = \sum_{lm \in E_{(2,2)}(\Omega(m,n))} \sqrt{\frac{\mathbb{S}_l + \mathbb{S}_m - 2}{\mathbb{S}_l \mathbb{S}_m}} + \sum_{lm \in E_{(2,3)}(\Omega(m,n))} \sqrt{\frac{\mathbb{S}_l + \mathbb{S}_m - 2}{\mathbb{S}_l \mathbb{S}_m}} + \sum_{lm \in E_{(2,4)}(\Omega(m,n))} \sqrt{\frac{\mathbb{S}_l + \mathbb{S}_m - 2}{\mathbb{S}_l \mathbb{S}_m}} + \sum_{lm \in E_{(3,3)}(\Omega(m,n))} \sqrt{\frac{\mathbb{S}_l + \mathbb{S}_m - 2}{\mathbb{S}_l \mathbb{S}_m}}$$

$$ABC_4(\Omega(m,n)) = \frac{8143}{228}mn - \frac{3845}{222}m - \frac{3845}{222}n + \frac{3845}{222}.$$

**Theorem 8:** *The fifth version of geometric arithmetic index of the graph* Ω(m,n) *is:*

$$GA_5(\Omega(m,n)) = \frac{10594}{149}mn - \frac{3963}{112}m - \frac{3963}{112}n + \frac{3963}{112}.$$

***Proof:*** By utilizing Table 2 and along with the mathematical expression of fifth version of geometric arithmetic index, the index's values can be summed as follows:

Fifth version of geometric - arithmetic index

$$GA_5(\Omega(m,n)) = \sum_{lm\in E(\Omega)} \frac{2\sqrt{\mathbb{S}_l\mathbb{S}_m}}{\mathbb{S}_l+\mathbb{S}_m} = \sum_{lm\in E_{(2,2)}(\Omega(m,n))} \frac{2\sqrt{\mathbb{S}_l\mathbb{S}_m}}{\mathbb{S}_l+\mathbb{S}_m} + \sum_{lm\in E_{(2,3)}(\Omega(m,n))} \frac{2\sqrt{\mathbb{S}_l\mathbb{S}_m}}{\mathbb{S}_l+\mathbb{S}_m}$$
$$+ \sum_{lm\in E_{(2,4)}(\Omega(m,n))} \frac{2\sqrt{\mathbb{S}_l\mathbb{S}_m}}{\mathbb{S}_l+\mathbb{S}_m} + \sum_{lm\in E_{(3,3)}(\Omega(m,n))} \frac{2\sqrt{\mathbb{S}_l\mathbb{S}_m}}{\mathbb{S}_l+\mathbb{S}_m}$$
$$GA_5(\Omega(m,n)) = \frac{10594}{149}mn - \frac{3963}{112}m - \frac{3963}{112}n + \frac{3963}{112}.$$

**Table 4**

**The graph (m, n)'s edge partition is determined by multiplying the neighbor vertices of each edge's end vertices.**

| **($\mu_l, \mu_m$) in which $st\in E(\Omega(m,n))$** | **Number of edges** |
|---|---|
| (4, 6) | $8m + 8n - 8$ |
| (6, 18) | $16mn - 8m - 8n + 8$ |
| (18, 18) | $24mn - 12m - 12n + 12$ |
| (12, 16) | $24mn - 20m - 20n + 20$ |
| (12, 18) | $8mn - 4m - 4n + 4$ |

**Theorem 9:** *The multiple atom bond connectivity index of graph* Ω(m,n) *is:*

$$ABC_\mu(\Omega(m,n)) = \frac{4300}{161}mn - \frac{2184}{187}\left(m+n-1\right).$$

***Proof:*** By utilizing Table 3 and the mathematical equation of multiple atom bond connectivity index, the index's values can be summed as follows:

**Multiple atom - bond connectivity**

$$ABC_\mu(\Omega(m,n)) = \sum_{lm\in E_{(2,2)}(\Omega(m,n))} \sqrt{\frac{\mu_l+\mu_m-2}{\mu_l\mu_m}} + \sum_{lm\in E_{(2,3)}(\Omega(m,n))} \sqrt{\frac{\mu_l+\mu_m-2}{\mu_l\mu_m}} +$$
$$\sum_{lm\in E_{(2,4)}(\Omega(m,n))} \sqrt{\frac{\mu_l+\mu_m-2}{\mu_l\mu_m}} + \sum_{lm\in E_{(3,3)}(\Omega(m,n))} \sqrt{\frac{\mu_l+\mu_m-2}{\mu_l\mu_m}}$$
$$ABC_\mu(\Omega(m,n)) = \frac{4300}{161}mn - \frac{2184}{187}m - \frac{2184}{187}n + \frac{2184}{187}.$$

**Theorem 10:** *The multiple geometric arithmetic index of a graph* Ω(m,n) *is:*

$$GA_\mu(\Omega(m,n)) = \frac{7431}{107}mn - \frac{19699}{566}m - \frac{19699}{566}n + \frac{19699}{566}.$$

***Proof:*** By utilizing Table 3 and the mathematical equation of multiple geometric arithmetic index, the values of this index can be computed as:

**Multiple geometric - arithmetic index**

$$GA_{\mu}(\Omega(m,n)) = \sum_{lm\in E_{(2,2)}(\Omega(m,n))} \frac{2\sqrt{\mu_l\mu_m}}{\mu_l+\mu_m} + \sum_{lm\in E_{(2,3)}(\Omega(m,n))} \frac{2\sqrt{\mu_l\mu_m}}{\mu_l+\mu_m} + \sum_{lm\in E_{(2,4)}(\Omega(m,n))} \frac{2\sqrt{\mu_l\mu_m}}{\mu_l+\mu_m} + \sum_{lm\in E_{(3,3)}(\Omega(m,n))} \frac{2\sqrt{\mu_l\mu_m}}{\mu_l+\mu_m}$$

$$GA_{\mu}(\Omega(m,n)) = \frac{7431}{107}mn - \frac{19699}{566}m - \frac{19699}{566}n + \frac{19699}{566}.$$

## Comparison of Results

In this part, numerical and graphical comparisons of the topological indices of two - dimensional organometallic complexes will be made. This comparison helps us understand the real link between the many physical and chemical characteristics of a given MOF. The graphical description of this kind of comparison helps scientists and researchers examine the structural behavior of the chemical component. It is easy to determine the isotropic behavior and interdependence of the given chemical compounds by quantitatively comparing the results of different topological indices. In addition, the different chamical and physical characteristics of the chemical molecule or metal - organic framework are depicted graphically in the topological index data. The comparison between randic index is shown in the table below. For comparison between Randic indices, Zagreb indices, Atom Bond Connectivity indices and Geometric - arithmetic indices of $M_3C_{12}X_{12}$, see Figures 2 and 3 and Tables 4-8.

**Table 5**

**Comparison between Randic index of $M_3C_{12}X_{12}$.**

| (g,h) | $R_{-1}$ | $R_{-1/2}$ | $R_1$ | $R_{1/2}$ |
|---|---|---|---|---|
| (1,1) | 35/6 | 229/16 | 244 | 278/3 |
| (2,2) | 163/6 | 623/9 | 1284 | 2384/5 |
| (3,3) | 407/6 | 1767/10 | 3428 | 6291/5 |
| (4,4) | 767/6 | 1347/4 | 6676 | 2437 |
| (5,5) | 1243/6 | 10987/20 | 11028 | 44144/11 |
| (6,6) | 1835/6 | 15476/19 | 16484 | 11973/2 |
| (7,7) | 2543/6 | 16984/15 | 23044 | 25072/3 |

*Contd...*

| | | | | |
|---|---|---|---|---|
| (8,8) | 3367/6 | 10518/7 | 30708 | 22251/2 |
| (9,9) | 4307/6 | 21180/11 | 39476 | 157200/11 |
| (10,10) | 5363/6 | 21608/9 | 49348 | 71415/4 |

Comparison between the first and second Zagreb indices and Sum connectivity index.

**Table 6**

**Comparison between SCI $M_1$ $M_2$ of $M_3C_{12}X_{12}$.**

| (g,h) | SCI | $M_1$ | $M_2$ |
|---|---|---|---|
| (1,1) | 159/10 | 188 | 244 |
| (2,2) | 3199/41 | 972 | 1284 |
| (3,3) | 1004/5 | 2572 | 3428 |
| (4,4) | 1537/4 | 4988 | 6676 |
| (5,5) | 10682/17 | 8220 | 11028 |
| (6,6) | 8398/9 | 12268 | 16484 |
| (7,7) | 24672/19 | 17132 | 23044 |
| (8,8) | 8623/5 | 22812 | 30708 |
| (9,9) | 6634/3 | 29308 | 39476 |
| (10,10) | 30346/11 | 36620 | 49348 |

In a similar way we will compare the results of fourth version of atom bond connectivity index $ABC_4$, Atom bond connectivity index (ABC) and multiple atom bond connectivity index $ABC_m$ of metal - organic framework of $M_3C_{12}X_{12}$.

**Table 7**

**Comparison between ABC $ABC_4$ and $ABC_m$ of $M_3C_{12}X_{12}$.**

| (g,h) | ABC | $ABC_4$ | $ABC_m$ |
|---|---|---|---|
| (1,1) | 849/34 | 92/5 | 526/35 |
| (2,2) | 874/7 | 909/10 | 359/5 |
| (3,3) | 2597/8 | 1409/6 | 7825/43 |
| (4,4) | 2497/4 | 2251/5 | 2419/7 |
| (5,5) | 5119/5 | 737 | 9564/17 |
| (6,6) | 7616/5 | 9857/9 | 42484/51 |
| (7,7) | 4245/2 | 12199/8 | 8098/7 |

*Contd...*

| | | | |
|---|---|---|---|
| (8,8) | 8465/3 | 46597/23 | 12273/8 |
| (9,9) | 54311/15 | 44174/17 | 9824/5 |
| (10,10) | 13559/3 | 38909/12 | 24489/10 |

In a similar manner we will compare the results of fifth version of geometric arithmetic index $GA_5$, geometric arithmetic index (GA) and multiple geometric arithmetic index $GA_m$ of $M_3C_{12}X_{12}$.

**Table 8**

**Comparison between GA $GA_5$ $GA_m$ of $M_3C_{12}X_{12}$.**

| (g,h) | GA | $GA_5$ | $GA_m$ |
|---|---|---|---|
| (1,1) | 604/17 | 250/7 | 104/3 |
| (2,2) | 707/4 | 713/4 | 1387/8 |
| (3,3) | 2291/5 | 463 | 451 |
| (4,4) | 880 | 11569/13 | 7808/9 |
| (5,5) | 36051/25 | 23345/16 | 1423 |
| (6,6) | 17155/8 | 10852/5 | 27525/13 |
| (7,7) | 2987 | 51407/17 | 44258/15 |
| (8,8) | 47639/12 | 12059/3 | 11768/3 |
| (9,9) | 45838/9 | 41261/8 | 15101/3 |
| (10,10) | 31783/5 | 25751/4 | 31418/5 |

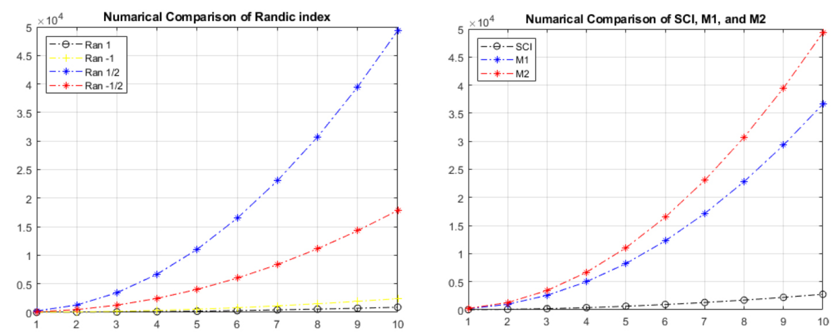


**Figure 2**

**Comparison between Randic indices (left) and SCI, Zagreb $M_1$ and $M_2$ (right) of $M_3C_{12}X_{12}$.**

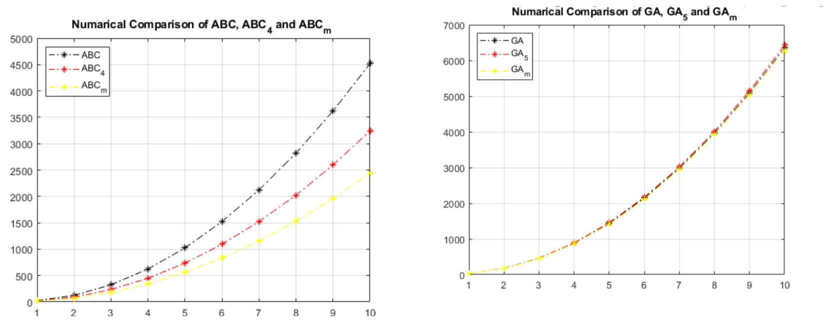


**Figure 3**

**Comparison between Atom Bond Connectivity indices (left) and Geometric - arithmetic indices (right) of $M_3C_{12}X_{12}$.**

## Conclusion

In this study, the Randic index, the first and second Zagreb indexes, the SCI, the ABC index, the $ABC_4$ and $ABC_m$ indices and the GA index, the $GA_5$ and $GA_m$ indexes of a graph of two - dimensional organometallic monolayers $M_3C_{12}X_{12}$ have all been calculated. Up to "l" and "m" cycles, researchers extended two-dimensional organometallic monolayers. In the aforementioned tables, the researcher also expanded the results by providing a correlation for the numerous adaptations of the estimated TIs by mathematical features.

The significance of indices is demonstrated by the correlation of the various indices through tables and diagrams, which demonstrates that these indices' impacts are critically related to one another. The search for indices and polynomials of metal - organic frameworks is still ongoing.

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