IEEE Access
Multidisciplinary ⋮ Rapid Review ⋮ Open Access Journal

Received April 12, 2021, accepted April 24, 2021, date of publication April 27, 2021, date of current version May 6, 2021.

Digital Object Identifier 10.1109/ACCESS.2021.3076036

Computation of Vertex-Edge Degree Based Topological Descriptors for Metal Trihalides Network

FOUAD A. ABOLABAN[1], ALI AHMAD[2], AND MUHAMMAD AHSAN ASIM[2]
[1]Department of Nuclear Engineering, College of Engineering, King Abdulaziz University, Jeddah 21589, Saudi Arabia
[2]College of Computer Science and Information Technology, Jazan University, Jazan 45142, Saudi Arabia

Corresponding author: Muhammad Ahsan Asim (mr.ahsan.asim@gmail.com)

This project was funded by the Deanship of Scientific Research (DSR) at King Abdulaziz University, Jeddah, under grant no. RG-6-135-40. The authors, therefore, gratefully acknowledge DSR technical and financial support.

ABSTRACT In recent past 2D metal trihalides have evolved as useful gapless semiconductor due to their physical properties like low dimensional magnetism and thermo electric performance. Such highly appreciable physical properties of these material are because enormous natural properties like half-metallicity, polarization, spin-orbit coupling impacts, layered structure and low cost. Layered formation of these materials provides an opportunity for the field of mathematical chemistry for identification of patterns and computation of mathematical properties. This article is dedicated to compute vertex-edge-degree based topological characterization of 2D trihalides. General mathematical expressions of several vertex-edge-degree based topological indices are presented in terms of research outcomes so they can be effectively used in future industrial projects.

INDEX TERMS Degree, topological descriptors, metal trihalides network.

I. INTRODUCTION

Recently, $2D$ graphene materials have gotten impressive consideration inferable from their novel electrical, thermal and mechanical properties [1]–[3]. Animated by such scans for novel $2D$ materials, a few investigation have been done on other two dimensional novel materials with surprising electrical, attractive and topological properties, for example, hexagonal boron nitride, progress metal dichalcogenides, transition metal and heavy main fundamental gathering trihalides with uncommon Dirac half-metallicity, novel topological spintronic properties emerging from enormous spin-orbit coupling of heavy particles and inalienable charge [4]–[11]. Also these $2D$ materials find different applications in various regions for example, optoelectronics, spintronics, room temperature radiation finders, chemical and biological sensors, supercapacitors, etc., [12]–[17] attributable to their wide band holes, stoping force, strange attractive properties emerging from open-shell *d* orbitals and spinorbit coupling all of which add to their novel properties and upgraded usefulness [4]. Dissimilar to the restrictions of $2D$ graphene for example, inadmissible band holes and too enormous a gap in boron nitride [18] the heavier progress metal and bismuth halides with layered structures show wanted band holes, attractive properties and Curie temperatures that are appropriate for a few down to earth applications.

A portion of the ferromagnetic $2D$ materials with huge surface territory are promising contender for treating harmful tumors through magnetically coordinated medication conveyance joined with hyperthermia as close to infrared light has penchant to destroy the tumor cells without causing critical obtrusive reactions. Consequently such procedures are more preferred contrasted with the regular strategies like medical procedure and chemotherapy inferable from their harmful reactions. It has been seen that chromium trihalides CrX_3 are perfect applicants due to their biocompatible nature [9]. Bismuth triiodide (BiI_3) is another less poisonous heavy metal halide which is utilized for room temperature γ-ray discovery on account of its higher Curie temperature and appropriate band hole [19] and these materials too discover possible applications in photonics and photovoltaic sunlight based cells [16], [20]. Recently theoretical examinations have highlighted its featured as a $2D$ material with promising optoelectronic properties [15], [20].

Chemical graph theory manages the investigation of topological properties of atoms/molecules wherein we first

The associate editor coordinating the review of this manuscript and approving it for publication was Donghyun Kim.

proselyte the structure of the molecules into a diagram and then assess its topological descriptors. A few investigations have uncovered structure property relations of molecules and materials, that is physico-chemical properties are personally identified with the fundamental topological characteristic of molecules structures [21], [22]. In this way, scientific relations that give topological descriptors of molecules and $2D$ materials can anticipate their physico-chemical properties, and in this manner such structure-property relations discover various applications in a few area, for example, anticipate toxicology and PC helped tranquilize revelation [23]–[25].

Topological descriptors which are obtained from the basic network of the $2D$ materials can give significant relationships to properties of these materials through quantitative structure activity, property and toxicity relationships (QSAR/QSPR/QSTR) obtained from the topological system of these materials [26]–[28]. For instance, polarizability and magnetic properties of these materials associate with the topological molecular structure descriptors. In the previous decades, a few investigations were coordinated towards the progress of topological descriptors due to their significance [30]–[34]. In any case, the majority of these investigations do exclude loads to bonds and vertices as the basic topology is treated inside basic graph theory that doesn't modify among bonds and heteroatoms.

Almost after 44 years, this methodology was returned to in Ref. [35] wherein a basic formula model is proposed instilling the compound qualities of atoms and bonds in the molecular diagram by associating every vertex and edge with certain weights that are obtained by any atomic or bond property counts along these lines redesigning the chemical diagram theoretical model of the molecule. Therefore, this basic formula-based weighted molecular diagram [35] gives a superior model to break down the characteristics of molecule, as it consolidates the chemical data in regards to the sort of atoms and the idea of the bond alongside the topology of the given molecular structure. In the current investigation as we are dealing $2D$ metal halides, we propose a novel way to deal with characterizing their properties through *ve*-degree topological descriptors.

Zhong and Ediz [36], [37] defined Harmonic index and most of work is done by using classical degree concept. Recently, Chellali *et al.* [38] introduced new degree concepts namely, "*ve*-degree and *ev*-degree". The relation between "classical degree-based" and "*ve*-degree and *ev*-degree" can be seen in [39]–[42] and found that "*ve*-degree Zagreb index" has stronger result and the "classical Zagreb index".

II. *ve*-DEGREE TOPOLOGICAL DESCRIPTORS

Let G be a simple connected graph with vertex sets $V(G)$ and edge sets $E(G)$. The degree of a vertex x_1, denoted by $\xi(x_1)$, is the number of edges that are incident to the x_1. The open neighborhood of x_1 is defined as $N(x_1) = \{x_2 \in V(G) : x_1x_2 \in E(G)\}$ and closed neighborhood $N[x_1] = N(x_1) \cup \{x_1\}$ [38]. The *ve*-degree, denoted by $\xi_{ve}(x_1)$, of any vertex $x_1 \in V$ is the number of different edges that are incident to any vertex from the $N[x_1]$. For details see [37]–[41].

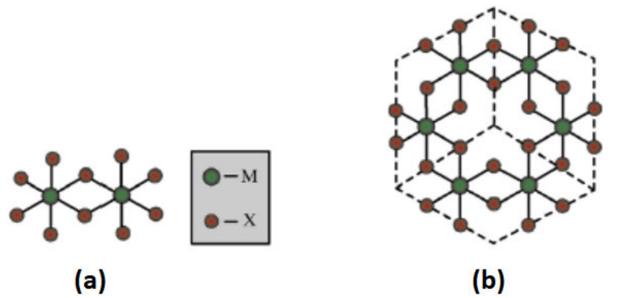

FIGURE 1. The metal trihalides MX_3 (a) Unit cell of MX_3 (b) monolayer of MX_3.

We define general *ve*-degree topological invariant $\mathbf{T}(G)$ as follows:

$$\mathbf{T}(G) = \sum_{x_1x_2 \in E(G)} \psi(\xi_{ve}(x_1), \xi_{ve}(x_2)). \tag{1}$$

- If $\psi(\xi_{ve}(x_1), \xi_{ve}(x_2)) = (\xi_{ve}(x_1) + \xi_{ve}(x_2))^{\lambda}$, then $\mathbf{T}(G)$ represents the first *ve*-degree Zagreb β index ($M^1_{\beta ve}(G)$) and *ve*-degree sum-connectivity index ($\chi_{ve}(G)$) for $\lambda = 1$ and $\lambda = -\frac{1}{2}$, respectively.
- If $\psi(\xi_{ve}(x_1), \xi_{ve}(x_2)) = (\xi_{ve}(x_1) \times \xi_{ve}(x_2))^{\theta}$, then $\mathbf{T}(G)$ represents the second *ve*-degree Zagreb index ($M^2_{ve}(G)$) and *ve*-degree Randic index ($R_{ve}(G)$) for $\theta = 1$ and $\theta = -\frac{1}{2}$, respectively.

Similarly if $\psi(\xi_{ve}(x_1), \xi_{ve}(x_2)) = \left(\frac{\xi_{ve}(x_1)+\xi_{ve}(x_2)-2}{\xi_{ve}(x_1)\times\xi_{ve}(x_2)}\right)^{\frac{1}{2}}$, $\frac{2(\xi_{ve}(x_1)\times\xi_{ve}(x_2))^{\frac{1}{2}}}{\xi_{ve}(x_1)+\xi_{ve}(x_2)}$, $\frac{2}{\xi_{ve}(x_1)+\xi_{ve}(x_2)}$, we obtained *ve*-degree atom-bond connectivity ($ABC_{ve}(G)$), geometric-arithmetic ($GA_{ve}(G)$), harmonic ($H_{ve}(G)$) descriptors, respectively.

III. STRUCTURES OF METAL TRIHALIDES

In this section, we discuss metal trihalides and derive their explanatory general expressions to determine the *ve*-degree topological descriptors. The unit cell of metal trihalides is depicted in Figure 1(a) where every M atom bonded to six X atoms to shape an octahedral coordination and the monolayers of trihalide structures are appeared in Figure 1(b).

Stacking such monolayers on head of one another structures the mass material and different stacking polytypes, for example, rhombohedral and monoclinic likewise exist. We discuss the paralellogram, hexagonal and triangular stacking of metal trihalides [43], [44] as shown in Figures 2–4.

IV. MAIN RESULTS

In this section, we determined the first *ve*-degree Zagreb β index, second *ve*-degree Zagreb β index, *ve*-degree atom-bond connectivity (ABC_{ve}) index, *ve*-degree geometric-arithmetic (GA_{ve}) index, *ve*-degree Randic index, *ve*-degree sum-connectivity (χ_{ve}) index and *ve*-degree harmonic (H_{ve}) for metal trihalides. We give a general result for each metal trihalides, which are used to obtained any *ve*-degree topological descriptors. Vetrík [45] introduced a new method to

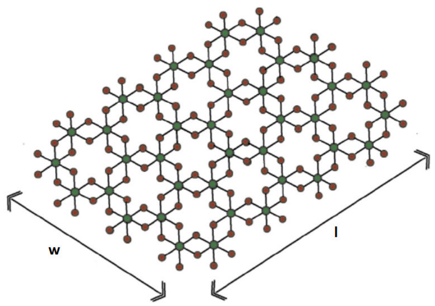

FIGURE 2. **The paralellogram shaped metal trihalides PMX_3.**

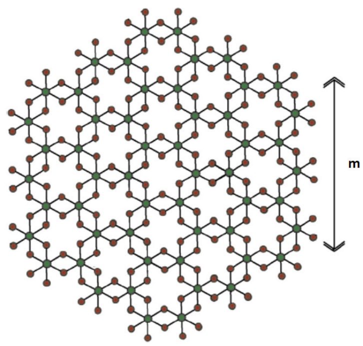

FIGURE 3. **The hexagonal shaped metal trihalides HMX_3.**

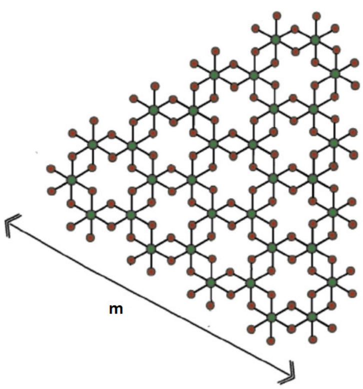

FIGURE 4. **The triangular shaped metal trihalides TMX_3.**

calculate the topological indices and also in [46], we follow the same technique in this paper.

A. PARALELLOGRAM SHAPED METAL TRIHALIDES

We presents a formula, which can be used to obtain any *ve*-degree topological descriptors for paralellogram shaped metal trihalides PMX_3.

Lemma 1: Let PMX_3 be a paralellogram shaped metal trihalides. Then

$$\begin{aligned}\mathbf{T}(PMX_3) &= 12lw\psi(12,12)+4\left(\psi(6,10)+2\psi(10,12)\right)(l+w)\\ &\quad +4\left(\psi(6,10)+2\psi(10,12)-3\psi(12,12)\right).\end{aligned}$$

Proof: The graph PMX_3 contains $8lw+10l+10w+2$ vertices and $12lw+12l+12w$ edges. The each vertex of PMX_3 has *ve*-degree 6, 10 or 12, can be partitioned according to their degrees and *ve*-degrees. Let

$$\mathbb{V}^j_{ve_i} = \{x_1 \in V(PMX_3) : d(x_1) = j, \xi(x_1) = i\}.$$

It means that the set $\mathbb{V}^j_{ve_i}$ contains the vertices of degree j with *ve*-degree i. The set of vertices with respect to their degrees and *ve*-degrees are as follows:

$$\begin{aligned}\mathbb{V}^1_{ve_6} &= \{x_1 \in \mathbb{V}(PMX_3) : d(x_1) = 1, \xi(x_1) = 6\}\\ \mathbb{V}^2_{ve_{12}} &= \{x_1 \in \mathbb{V}(PMX_3) : d(x_1) = 2, \xi(x_1) = 12\}\\ \mathbb{V}^6_{ve_{10}} &= \{x_1 \in \mathbb{V}(PMX_3) : d(x_1) = 6, \xi(x_1) = 10\}\\ \mathbb{V}^6_{ve_{12}} &= \{x_1 \in \mathbb{V}(PMX_3) : d(x_1) = 6, \xi(x_1) = 12\}\end{aligned}$$

Since, $|\mathbb{V}^1_{ve_6}| = 4l+4w+4$, $|\mathbb{V}^2_{ve_{12}}| = 6lw+4l+4w-2$, $|\mathbb{V}^6_{ve_{10}}| = 2l+2w+2$ and $|\mathbb{V}^6_{ve_{12}}| = 12lw-2$. Let us partitioned the edges of PMX_3 according to its degrees and *ve*-degrees. Let

$$\begin{aligned}\Xi^{1,6}_{ve_{6,10}} &= \{x_1x_2 \in \mathbb{E}(PMX_3) : d(x_1) = 1, d(x_2) = 6,\\ &\qquad \times \xi(x_1) = 6, \xi(x_2) = 10\}\\ \Xi^{2,6}_{ve_{10,12}} &= \{x_1x_2 \in \mathbb{E}(PMX_3) : d(x_1) = 2, d(x_2) = 6,\\ &\qquad \times \xi(x_1) = 10, \xi(x_2) = 12\}\\ \Xi^{2,6}_{ve_{12,12}} &= \{x_1x_2 \in \mathbb{E}(PMX_3) : d(x_1) = 2, d(x_2) = 6,\\ &\qquad \times \xi(x_1) = 12, \xi(x_2) = 12\}\end{aligned}$$

Note that $\mathbb{E}(PMX_3) = \Xi^{1,6}_{ve_{6,10}} \cup \Xi^{2,6}_{ve_{10,12}} \cup \Xi^{2,6}_{ve_{12,12}}$ and $|\Xi^{1,6}_{ve_{6,10}}| = 4l+4w+4$, $|\Xi^{2,6}_{ve_{10,12}}| = 8l+8w+8$, $|\Xi^{2,6}_{ve_{12,12}}| = 12lw-12$. Hence,

$$\begin{aligned}\mathbf{T}(PMX_3) &= \sum_{x_1x_2\in\mathbb{E}(PMX_3)} \psi(\xi(x_1),\xi(x_2))\\ &= \sum_{x_1x_2\in\Xi^{1,6}_{ve_{6,10}}} \psi(6,10) + \sum_{x_1x_2\in\Xi^{2,6}_{ve_{10,12}}} \psi(10,12)\\ &\quad + \sum_{x_1x_2\in\Xi^{2,6}_{ve_{12,12}}} \psi(12,12)\\ &= (4l+4w+4)\psi(6,10)+(8l+8w+8)\psi(10,12)\\ &\quad +(12lw-12)\psi(12,12).\end{aligned}$$

After simplification, we get

$$\begin{aligned}&\mathbf{T}(PMX_3)\\ &\quad = 12lw\psi(12,12)+4\left(\psi(6,10)+2\psi(10,12)\right)(l+w)\\ &\qquad +4\left(\psi(6,10)+2\psi(10,12)-3\psi(12,12)\right).\end{aligned}$$

Theorem 1: Let PMX_3 be a paralellogram shaped metal trihalides. Then the first *ve*-degree Zagreb β index:

$$M^1_{\beta ve}(PMX_3) = 288\,lw + 240\,l + 240\,w - 48$$

the second *ve*-degree Zagreb index:

$$M^2_{ve}(PMX_3) = 1728\,lw + 1200\,l + 1200\,w - 528$$

the *ve*-degree Randic index:

$$\begin{aligned}R_{ve}(PMX_3) &= lw + 4\left(\frac{\sqrt{15}+\sqrt{30}}{30}\right)(l+w)\\ &\quad + \frac{2\sqrt{15}+2\sqrt{30}-15}{15}\end{aligned}$$

the *ve*-degree atom-bond connectivity index:

$$ABC_{ve}(PMX_3) = \sqrt{22}\,lw + 4\left(\frac{\sqrt{210}+10\sqrt{6}}{30}\right)(l+w) + \frac{2\sqrt{210}+20\sqrt{6}-15\sqrt{22}}{15}$$

the *ve*-degree geometric-arithmetic index:

$$GA_{ve}(PMX_3) = 12\,lw + 4\left(\frac{\sqrt{15}}{4}+\frac{4\sqrt{30}}{11}\right)(l+w) + \sqrt{15}+\frac{16}{11}\sqrt{30}-12$$

the *ve*-degree harmonic index:

$$H_{ve}(PMX_3) = lw + \frac{27}{22}l + \frac{27}{22}w + \frac{5}{22}$$

the *ve*-degree sum-connectivity index:

$$\chi_{ve}(PMX_3) = lw\sqrt{6} + 4\left(\frac{1}{4}+\frac{\sqrt{22}}{11}\right)(l+w) + 1 + \frac{4\sqrt{22}}{11} - \sqrt{6}.$$

Proof: For $M^1_{\beta ve}(PMX_3)$ which is the first *ve*-degree Zagreb β index of PMX_3, we have $\psi(\xi_{ve}(x_1), \xi_{ve}(x_2)) = \xi_{ve}(x_1) + \xi_{ve}(x_2)$, therefore $\psi(12, 12) = 24$, $\psi(6, 10) = 16$ and $\psi(10, 12) = 22$. Thus by Lemma 1,

$$\begin{aligned} M^1_{\beta ve}(PMX_3) &= 12lw(24) + 4\,(16+44)\,(l+w) + 4\,(16+44-72) \\ &= 288\,lw + 240\,l + 240\,w - 48. \end{aligned}$$

For $M^2_{ve}(PMX_3)$ which is the second *ve*-degree Zagreb index of PMX_3, we have $\psi(\xi_{ve}(x_1), \xi_{ve}(x_2)) = \xi_{ve}(x_1) \times \xi_{ve}(x_2)$, therefore $\psi(12, 12) = 144$, $\psi(6, 10) = 60$ and $\psi(10, 12) = 120$. Thus by Lemma 1,

$$\begin{aligned} M^2_{ve}(PMX_3) &= 12lw(144) + 4\,(60+240)\,(l+w) + 4\,(60+240-432) \\ &= 1728\,lw + 1200\,l + 1200\,w - 528. \end{aligned}$$

For $R_{ve}(PMX_3)$ which is the *ve*-degree Randic index of PMX_3, we have $\psi(\xi_{ve}(x_1), \xi_{ve}(x_2)) = (\xi_{ve}(x_1) \times \xi_{ve}(x_2))^{-\frac{1}{2}}$, therefore $\psi(12, 12) = \frac{1}{12}$, $\psi(6, 10) = \frac{1}{\sqrt{60}}$ and $\psi(10, 12) = \frac{1}{\sqrt{120}}$. Thus by Lemma 1,

$$\begin{aligned} R_{ve}(PMX_3) &= 12lw(\frac{1}{12}) + 4\left(\frac{1}{\sqrt{60}}+\frac{2}{\sqrt{120}}\right)(l+w) + 4\left(\frac{1}{\sqrt{60}}+\frac{2}{\sqrt{120}}-\frac{3}{12}\right) \\ &= lw + 4\left(\frac{\sqrt{15}+\sqrt{30}}{30}\right)(l+w) + \frac{2\sqrt{15}+2\sqrt{30}-15}{15}. \end{aligned}$$

For $ABC_{ve}(PMX_3)$ which is the *ve*-degree atom-bond connectivity index of PMX_3, we have $\psi(\xi_{ve}(x_1), \xi_{ve}(x_2)) = \left(\frac{\xi_{ve}(x_1)+\xi_{ve}(x_2)-2}{\xi_{ve}(x_1)\times\xi_{ve}(x_2)}\right)^{\frac{1}{2}}$, therefore $\psi(12, 12) = \sqrt{\frac{22}{144}}$, $\psi(6, 10) = \sqrt{\frac{14}{60}}$ and $\psi(10, 12) = \sqrt{\frac{20}{120}}$. Thus by Lemma 1,

$$\begin{aligned} ABC_{ve}(PMX_3) &= 12lw\sqrt{\frac{22}{144}} + 4\left(\sqrt{\frac{14}{60}}+2\sqrt{\frac{20}{120}}\right)(l+w) + 4\left(\sqrt{\frac{14}{60}}+2\sqrt{\frac{20}{120}}-3\sqrt{\frac{22}{144}}\right) \\ &= \sqrt{22}\,lw + 4\left(\frac{\sqrt{210}+10\sqrt{6}}{30}\right)(l+w) + \frac{2\sqrt{210}+20\sqrt{6}-15\sqrt{22}}{15}. \end{aligned}$$

For $GA_{ve}(PMX_3)$ which is the *ve*-degree geometric-arithmetic index of PMX_3, we have $\psi(\xi_{ve}(x_1), \xi_{ve}(x_2)) = \frac{2(\xi_{ve}(x_1)\times\xi_{ve}(x_2))^{\frac{1}{2}}}{\xi_{ve}(x_1)+\xi_{ve}(x_2)}$, therefore $\psi(12, 12) = 1$, $\psi(6, 10) = \frac{2\sqrt{60}}{16}$ and $\psi(10, 12) = \frac{2\sqrt{120}}{22}$. Thus by Lemma 1,

$$\begin{aligned} GA_{ve}(PMX_3) &= 12lw + 4\left(\frac{2\sqrt{60}}{16}+2\frac{2\sqrt{120}}{22}\right)(l+w) + 4\left(\frac{2\sqrt{60}}{16}+\frac{4\sqrt{120}}{22}-3\right) \\ &= 12\,lw + 4\left(\frac{\sqrt{15}}{4}+\frac{4\sqrt{30}}{11}\right)(l+w) + \sqrt{15}+\frac{16}{11}\sqrt{30}-12. \end{aligned}$$

For $H_{ve}(PMX_3)$ which is the *ve*-degree harmonic index of PMX_3, we have $\psi(\xi_{ve}(x_1), \xi_{ve}(x_2)) = \frac{2}{\xi_{ve}(x_1)+\xi_{ve}(x_2)}$, therefore $\psi(12, 12) = \frac{1}{12}$, $\psi(6, 10) = \frac{1}{8}$ and $\psi(10, 12) = \frac{1}{11}$. Thus by Lemma 1,

$$\begin{aligned} H_{ve}(PMX_3) &= 12lw\frac{1}{12} + 4\left(\frac{1}{8}+\frac{2}{11}\right)(l+w) + 4\left(\frac{1}{8}+\frac{2}{11}-\frac{3}{12}\right) \\ &= lw + \frac{27}{22}l + \frac{27}{22}w + \frac{5}{22}. \end{aligned}$$

For $\chi_{ve}(PMX_3)$ which is the *ve*-degree sum-connectivity index of PMX_3, we have $\psi(\xi_{ve}(x_1), \xi_{ve}(x_2)) = (\xi_{ve}(x_1)+\xi_{ve}(x_2))^{-\frac{1}{2}}$, therefore $\psi(12, 12) = \frac{1}{\sqrt{24}}$, $\psi(6, 10) = \frac{1}{\sqrt{16}}$ and $\psi(10, 12) = \frac{1}{\sqrt{22}}$. Thus by Lemma 1,

$$\begin{aligned} \chi_{ve}(PMX_3) &= 12lw\frac{1}{\sqrt{24}} + 4\left(\frac{1}{\sqrt{16}}+\frac{2}{\sqrt{22}}\right)(l+w) + 4\left(\frac{1}{\sqrt{16}}+\frac{2}{\sqrt{22}}-\frac{3}{\sqrt{24}}\right) \\ &= lw\sqrt{6} + 4\left(\frac{1}{4}+\frac{\sqrt{22}}{11}\right)(l+w) + 1 + \frac{4\sqrt{22}}{11} - \sqrt{6}. \end{aligned}$$

B. HEXAGONAL SHAPED METAL TRIHALIDES

We presents a formula, which can be used to obtain any *ve*-degree topological descriptors for hexagonal shaped metal trihalides HMX_3.

Lemma 2: Let HMX_3 be a hexagonal shaped metal trihalides. Then

$$\mathbf{T}(HMX_3) = 36m^2\psi(12,12) + 12m\left(\psi(6,10) - 3\psi(12,12) + 2\psi(10,12)\right).$$

Proof: The graph HMX_3 contains $24m^2 + 6m$ vertices and $36m^2$ edges. The each vertex of HMX_3 has *ve*-degree 6, 10 or 12, can be partitioned according to their degrees and *ve*-degrees. Let

$$\mathbb{V}^j_{ve_i} = \{x_1 \in V(HMX_3) : d(x_1) = j, \xi(x_1) = i\}.$$

It means that the set $\mathbb{V}^j_{ve_i}$ contains the vertices of degree j with *ve*-degree i. The set of vertices with respect to their degrees and *ve*-degrees are as follows:

$$\begin{aligned}
\mathbb{V}^1_{ve_6} &= \{x_1 \in \mathbb{V}(HMX_3) : d(x_1) = 1, \xi(x_1) = 6\}\\
\mathbb{V}^2_{ve_{12}} &= \{x_1 \in \mathbb{V}(HMX_3) : d(x_1) = 2, \xi(x_1) = 12\}\\
\mathbb{V}^6_{ve_{10}} &= \{x_1 \in \mathbb{V}(HMX_3) : d(x_1) = 6, \xi(x_1) = 10\}\\
\mathbb{V}^6_{ve_{12}} &= \{x_1 \in \mathbb{V}(HMX_3) : d(x_1) = 6, \xi(x_1) = 12\}
\end{aligned}$$

Since, $|\mathbb{V}^1_{ve_6}| = 12m$, $|\mathbb{V}^2_{ve_{12}}| = 18m^2 - 6m$, $|\mathbb{V}^6_{ve_{10}}| = 6m$ and $|\mathbb{V}^6_{ve_{12}}| = 6m^2 - 6m$. Let us partitioned the edges of HMX_3 according to its degrees and *ve*-degrees. Let

$$\begin{aligned}
\Xi^{1,6}_{ve_{6,10}} &= \{x_1x_2 \in \mathbb{E}(HMX_3) : d(x_1) = 1, d(x_2) = 6,\\
&\quad \times \xi(x_1) = 6, \xi(x_2) = 10\}\\
\Xi^{2,6}_{ve_{10,12}} &= \{x_1x_2 \in \mathbb{E}(HMX_3) : d(x_1) = 2, d(x_2) = 6,\\
&\quad \times \xi(x_1) = 10, \xi(x_2) = 12\}\\
\Xi^{2,6}_{ve_{12,12}} &= \{x_1x_2 \in \mathbb{E}(HMX_3) : d(x_1) = 2, d(x_2) = 12,\\
&\quad \times \xi(x_1) = 12, \xi(x_2) = 12\}
\end{aligned}$$

Note that $\mathbb{E}(HMX_3) = \Xi^{1,6}_{ve_{6,10}} \cup \Xi^{2,6}_{ve_{10,12}} \cup \Xi^{2,6}_{ve_{12,12}}$ and $|\Xi^{1,6}_{ve_{6,10}}| = 12m$, $|\Xi^{2,6}_{ve_{10,12}}| = 24m$, $|\Xi^{2,6}_{ve_{12,12}}| = 36m^2 - 36m$. Hence,

$$\begin{aligned}
\mathbf{T}(HMX_3) &= \sum_{x_1x_2\in\mathbb{E}(HMX_3)} \psi(\xi(x_1), \xi(x_2))\\
&= \sum_{x_1x_2\in\Xi^{1,6}_{ve_{6,10}}} \psi(6,10) + \sum_{x_1x_2\in\Xi^{2,6}_{ve_{10,12}}} \psi(10,12)\\
&\quad + \sum_{x_1x_2\in\Xi^{2,6}_{ve_{12,12}}} \psi(12,12)\\
&= (12m)\psi(6,10) + (24m)\psi(10,12)\\
&\quad + (36m^2 - 36m)\psi(12,12).
\end{aligned}$$

After simplification, we get

$$\mathbf{T}(HMX_3) = 36m^2\psi(12,12) + 12m(\psi(6,10) - 3\psi(12,12) + 2\psi(10,12)).$$

Theorem 2: Let HMX_3 be a hexagonal shaped metal trihalides. Then the first *ve*-degree Zagreb β index:

$$M^1_{\beta ve}(HMX_3) = 864\,m^2 - 144\,m$$

the second *ve*-degree Zagreb index:

$$M^2_{ve}(HMX_3) = 5184\,m^2 - 1584\,m$$

the *ve*-degree Randic index:

$$R_{ve}(HMX_3) = 3\,m^2 + 12\,m\left(\frac{\sqrt{15}+\sqrt{30}}{30} - \frac{1}{4}\right)$$

the *ve*-degree atom-bond connectivity index:

$$ABC_{ve}(HMX_3) = 3\sqrt{22}\,m^2 + 12\,m\left(\frac{\sqrt{210}+10\sqrt{6}}{30} - \frac{\sqrt{22}}{4}\right)$$

the *ve*-degree geometric-arithmetic index:

$$GA_{ve}(HMX_3) = 36\,m^2 + 12\,m\left(\frac{\sqrt{15}}{4} + \frac{4\sqrt{30}}{11} - 3\right)$$

the *ve*-degree harmonic index:

$$H_{ve}(HMX_3) = 3\,m^2 + \frac{15}{22}\,m$$

the *ve*-degree sum-connectivity index:

$$\chi_{ve}(HMX_3) = 3\sqrt{6}\,m^2 + 12\,m\left(\frac{1-\sqrt{6}}{4} + \frac{\sqrt{22}}{11}\right).$$

Proof: For $M^1_{\beta ve}(HMX_3)$ which is the first *ve*-degree Zagreb β index of HMX_3, we have $\psi(\xi_{ve}(x_1), \xi_{ve}(x_2)) = \xi_{ve}(x_1) + \xi_{ve}(x_2)$, therefore $\psi(12,12) = 24$, $\psi(6,10) = 16$ and $\psi(10,12) = 22$. Thus by Lemma 1,

$$\begin{aligned}
M^1_{\beta ve}(HMX_3) &= 36m^2(24) + 12m\,(16 - 3(24) + 2(22))\\
&= 864\,m^2 - 144\,m.
\end{aligned}$$

For $M^2_{ve}(HMX_3)$ which is the second *ve*-degree Zagreb index of HMX_3, we have $\psi(\xi_{ve}(x_1), \xi_{ve}(x_2)) = \xi_{ve}(x_1) \times \xi_{ve}(x_2)$, therefore $\psi(12,12) = 144$, $\psi(6,10) = 60$ and $\psi(10,12) = 120$. Thus by Lemma 1,

$$\begin{aligned}
M^2_{ve}(HMX_3) &= 36m^2(144) + 12m\,(60 - 3(144) + 2(120))\\
&= 5184\,m^2 - 1584\,m.
\end{aligned}$$

For $R_{ve}(HMX_3)$ which is the *ve*-degree Randic index of HMX_3, we have $\psi(\xi_{ve}(x_1), \xi_{ve}(x_2)) = (\xi_{ve}(x_1) \times \xi_{ve}(x_2))^{-\frac{1}{2}}$, therefore $\psi(12,12) = \frac{1}{12}$, $\psi(6,10) = \frac{1}{\sqrt{60}}$ and $\psi(10,12) = \frac{1}{\sqrt{120}}$. Thus by Lemma 1,

$$\begin{aligned}
R_{ve}(HMX_3) &= 36m^2\frac{1}{12} + 12m\left(\frac{1}{\sqrt{60}} - 3\frac{1}{12} + 2\frac{1}{\sqrt{120}}\right)\\
&= 3\,m^2 + 12\,m\left(\frac{\sqrt{15}+\sqrt{30}}{30} - \frac{1}{4}\right).
\end{aligned}$$

For $ABC_{ve}(HMX_3)$ which is the *ve*-degree atom-bond connectivity index of HMX_3, we have $\psi(\xi_{ve}(x_1), \xi_{ve}(x_2)) = \left(\frac{\xi_{ve}(x_1)+\xi_{ve}(x_2)-2}{\xi_{ve}(x_1)\times\xi_{ve}(x_2)}\right)^{\frac{1}{2}}$, therefore $\psi(12,12) = \sqrt{\frac{22}{144}}$,

$\psi(6,10) = \sqrt{\frac{14}{60}}$ and $\psi(10,12) = \sqrt{\frac{20}{120}}$. Thus by Lemma 1,

$$\begin{aligned} &ABC_{ve}(HMX_3) \\ &= 36m^2\sqrt{\frac{22}{144}} + 12m\left(\sqrt{\frac{14}{60}} - 3\sqrt{\frac{22}{144}} + 2\sqrt{\frac{20}{120}}\right) \\ &= 3\sqrt{22}\,m^2 + 12\,m\left(\frac{\sqrt{210}+10\sqrt{6}}{30} - \frac{\sqrt{22}}{4}\right). \end{aligned}$$

For $GA_{ve}(HMX_3)$ which is the ve-degree geometric-arithmetic index of HMX_3, we have $\psi(\xi_{ve}(x_1), \xi_{ve}(x_2)) = \frac{2(\xi_{ve}(x_1)\times\xi_{ve}(x_2))^{\frac{1}{2}}}{\xi_{ve}(x_1)+\xi_{ve}(x_2)}$, therefore $\psi(12,12) = 1$, $\psi(6,10) = \frac{2\sqrt{60}}{16}$ and $\psi(10,12) = \frac{2\sqrt{120}}{22}$. Thus by Lemma 1,

$$\begin{aligned} GA_{ve}(HMX_3) &= 36m^2 + 12m\left(\frac{2\sqrt{60}}{16} - 3 + 2\frac{2\sqrt{120}}{22}\right) \\ &= 36\,m^2 + 12\,m\left(\frac{\sqrt{15}}{4} + \frac{4\sqrt{30}}{11} - 3\right). \end{aligned}$$

For $H_{ve}(HMX_3)$ which is the ve-degree harmonic index of HMX_3, we have $\psi(\xi_{ve}(x_1), \xi_{ve}(x_2)) = \frac{2}{\xi_{ve}(x_1)+\xi_{ve}(x_2)}$, therefore $\psi(12,12) = \frac{1}{12}$, $\psi(6,10) = \frac{1}{8}$ and $\psi(10,12) = \frac{1}{11}$. Thus by Lemma 1,

$$\begin{aligned} H_{ve}(HMX_3) &= 36m^2\frac{1}{12} + 12m\left(\frac{1}{8} - 3\frac{1}{12} + 2\frac{1}{11}\right) \\ &= 3\,m^2 + \frac{15}{22}\,m. \end{aligned}$$

For $\chi_{ve}(HMX_3)$ which is the ve-degree sum-connectivity index of HMX_3, we have $\psi(\xi_{ve}(x_1), \xi_{ve}(x_2)) = (\xi_{ve}(x_1)+\xi_{ve}(x_2))^{-\frac{1}{2}}$, therefore $\psi(12,12) = \frac{1}{\sqrt{24}}$, $\psi(6,10) = \frac{1}{\sqrt{16}}$ and $\psi(10,12) = \frac{1}{\sqrt{22}}$. Thus by Lemma 1,

$$\begin{aligned} \chi_{ve}(HMX_3) &= 36m^2\frac{1}{\sqrt{24}} + 12m\left(\frac{1}{\sqrt{16}} - 3\frac{1}{\sqrt{24}} + 2\frac{1}{\sqrt{22}}\right) \\ &= 3\sqrt{6}\,m^2 + 12\,m\left(\frac{1-\sqrt{6}}{4} + \frac{\sqrt{22}}{11}\right). \end{aligned}$$

V. TRIANGULAR SHAPED METAL TRIHALIDES

We presents a formula, which can be used to obtain any ve-degree topological descriptors for triangular shaped metal trihalides TMX_3.

Lemma 3: Let TMX_3 be a triangular shaped metal trihalides. Then

$$\begin{aligned} &\mathbf{T}(TMX_3) \\ &= 6m^2\psi(12,12) + 6m\left(\psi(6,10) + 2\psi(10,12) + \psi(12,12)\right) \\ &\quad + 6\left(\psi(6,10) + 2\psi(10,12) - 2\psi(12,12)\right). \end{aligned}$$

Proof: The graph TMX_3 contains $4m^2+19m+7$ vertices and $6m^2+24m+6$ edges. The each vertex of TMX_3 has ve-degree 6, 10 or 12, can be partitioned according to their degrees and ve-degrees. Let

$$\mathbb{V}^j_{ve_i} = \{x_1 \in V(TMX_3) : d(x_1) = j, \xi(x_1) = i\}.$$

It means that the set $\mathbb{V}^j_{ve_i}$ contains the vertices of degree j with ve-degree i. The set of vertices with respect to their degrees and ve-degrees are as follows:

$$\begin{aligned} \mathbb{V}^1_{ve_6} &= \{x_1 \in \mathbb{V}(TMX_3) : d(x_1) = 1, \xi(x_1) = 6\} \\ \mathbb{V}^2_{ve_{12}} &= \{x_1 \in \mathbb{V}(TMX_3) : d(x_1) = 2, \xi(x_1) = 12\} \\ \mathbb{V}^6_{ve_{10}} &= \{x_1 \in \mathbb{V}(TMX_3) : d(x_1) = 6, \xi(x_1) = 10\} \\ \mathbb{V}^6_{ve_{12}} &= \{x_1 \in \mathbb{V}(TMX_3) : d(x_1) = 6, \xi(x_1) = 12\} \end{aligned}$$

Since, $|\mathbb{V}^1_{ve_6}| = 6m+6$, $|\mathbb{V}^2_{ve_{12}}| = 3m^2+9m$, $|\mathbb{V}^6_{ve_{10}}| = 3m+3$ and $|\mathbb{V}^6_{ve_{12}}| = m^2+m-2$. Let us partitioned the edges of TMX_3 according to its degrees and ve-degrees. Let

$$\begin{aligned} \Xi^{1,6}_{ve_{6,10}} &= \{x_1x_2 \in \mathbb{E}(TMX_3) : d(x_1) = 1, d(x_2) = 6, \\ &\quad \times \xi(x_1) = 6, \xi(x_2) = 10\} \\ \Xi^{2,6}_{ve_{10,12}} &= \{x_1x_2 \in \mathbb{E}(TMX_3) : d(x_1) = 2, d(x_2) = 6, \\ &\quad \times \xi(x_1) = 10, \xi(x_2) = 12\} \\ \Xi^{2,6}_{ve_{12,12}} &= \{x_1x_2 \in \mathbb{E}(TMX_3) : d(x_1) = 2, d(x_2) = 12, \\ &\quad \times \xi(x_1) = 12, \xi(x_2) = 12\} \end{aligned}$$

Note that $\mathbb{E}(TMX_3) = \Xi^{1,6}_{ve_{6,10}} \cup \Xi^{2,6}_{ve_{10,12}} \cup \Xi^{2,6}_{ve_{12,12}}$ and $|\Xi^{1,6}_{ve_{6,10}}| = 6m+6$, $|\Xi^{2,6}_{ve_{10,12}}| = 12m+12$, $|\Xi^{2,6}_{ve_{12,12}}| = 6m^2+6m-12$. Hence,

$$\begin{aligned} \mathbf{T}(TMX_3) &= \sum_{x_1x_2\in\mathbb{E}(TMX_3)} \psi(\xi(x_1), \xi(x_2)) \\ &= \sum_{x_1x_2\in\Xi^{1,6}_{ve_{6,10}}} \psi(6,10) + \sum_{x_1x_2\in\Xi^{2,6}_{ve_{10,12}}} \psi(10,12) \\ &\quad + \sum_{x_1x_2\in\Xi^{2,6}_{ve_{12,12}}} \psi(12,12) \\ &= (6m+6)\psi(6,10) + (12m+12)\psi(10,12) \\ &\quad + (6m^2+6m-12)\psi(12,12). \end{aligned}$$

After simplification, we get

$$\begin{aligned} &\mathbf{T}(TMX_3) \\ &= 6m^2\psi(12,12) + 6m(\psi(6,10) + 2\psi(10,12) + \psi(12,12)) \\ &\quad + 6(\psi(6,10) + 2\psi(10,12) - 2\psi(12,12)). \end{aligned}$$

Theorem 3: Let TMX_3 be a triangular shaped metal trihalides. Then the first ve-degree Zagreb β index:

$$M^1_{\beta ve}(TMX_3) = 144\,m^2 + 504\,m + 72$$

the second ve-degree Zagreb index:

$$M^2_{ve}(TMX_3) = 864\,m^2 + 2664\,m + 72$$

the ve-degree Randic index:

$$\begin{aligned} R_{ve}(TMX_3) &= \frac{1}{2}\,m^2 + 6\,m\left(\frac{\sqrt{15}+\sqrt{30}}{30} + \frac{1}{12}\right) \\ &\quad + \frac{\sqrt{15}+\sqrt{30}-5}{5} \end{aligned}$$

the ve-degree atom-bond connectivity index:

$$ABC_{ve}(TMX_3)=\frac{\sqrt{22}}{2}m^2+6m\left(\frac{\sqrt{210}+10\sqrt{6}}{30}+\frac{\sqrt{22}}{12}\right)+\frac{\sqrt{210}}{5}+2\sqrt{6}-\sqrt{22}$$

the ve-degree geometric-arithmetic index:

$$GA_{ve}(TMX_3)=6m^2+6m\left(\frac{\sqrt{15}}{4}+\frac{4\sqrt{30}}{11}+1\right)+\frac{3\sqrt{15}}{2}+\frac{24\sqrt{30}}{11}-12$$

the ve-degree harmonic index:

$$H_{ve}(TMX_3)=\frac{1}{2}m^2+\frac{103}{44}m+\frac{37}{44}$$

the ve-degree sum-connectivity index:

$$\chi_{ve}(TMX_3)=\frac{\sqrt{6}}{2}m^2+6m\left(\frac{1}{4}+\frac{\sqrt{22}}{11}+\frac{\sqrt{6}}{12}\right)+\frac{3}{2}+\frac{6\sqrt{22}}{11}-\sqrt{6}.$$

Proof: For $M^1_{\beta ve}(TMX_3)$ which is the first ve-degree Zagreb β index of TMX_3, we have $\psi(\xi_{ve}(x_1),\xi_{ve}(x_2))=\xi_{ve}(x_1)+\xi_{ve}(x_2)$, therefore $\psi(12,12)=24$, $\psi(6,10)=16$ and $\psi(10,12)=22$. Thus by Lemma 1,

$$\begin{aligned}M^1_{\beta ve}(HMX_3)&=6m^2(24)+6m(16+2(22)+24)+6(16+2(22)-2(24))\\&=144m^2+504m+72.\end{aligned}$$

For $M^2_{ve}(TMX_3)$ which is the second ve-degree Zagreb index of TMX_3, we have $\psi(\xi_{ve}(x_1),\xi_{ve}(x_2))=\xi_{ve}(x_1)\times\xi_{ve}(x_2)$, therefore $\psi(12,12)=144$, $\psi(6,10)=60$ and $\psi(10,12)=120$. Thus by Lemma 1,

$$\begin{aligned}M^2_{ve}(TMX_3)&=6m^2(144)+6m(60+2(120)+144)\\&\quad+6(60+2(120)-2(144))\\&=864m^2+2664m+72.\end{aligned}$$

For $R_{ve}(TMX_3)$ which is the ve-degree Randic index of TMX_3, we have $\psi(\xi_{ve}(x_1),\xi_{ve}(x_2))=(\xi_{ve}(x_1)\times\xi_{ve}(x_2))^{-\frac{1}{2}}$, therefore $\psi(12,12)=\frac{1}{12}$, $\psi(6,10)=\frac{1}{\sqrt{60}}$ and $\psi(10,12)=\frac{1}{\sqrt{120}}$. Thus by Lemma 1,

$$\begin{aligned}R_{ve}(TMX_3)&=6m^2\frac{1}{12}+6m\left(\frac{1}{\sqrt{60}}+\frac{2}{\sqrt{120}}+\frac{1}{12}\right)\\&\quad+6\left(\frac{1}{\sqrt{60}}+\frac{2}{\sqrt{120}}-\frac{2}{12}\right)\\&=\frac{1}{2}m^2+6m\left(\frac{\sqrt{15}+\sqrt{30}}{30}+\frac{1}{12}\right)\\&\quad+\frac{\sqrt{15}+\sqrt{30}-5}{5}.\end{aligned}$$

TABLE 1. Numerical representation of ve-degree results for PMX_3.

$[m,n]$	$M^1_{\beta ve}$	M^2_{ve}	ABC_{ve}	R_{ve}	GA_{ve}	H_{ve}	χ_{ve}
[2, 2]	2064.0	11184.0	40.062	9.2335	95.199	9.1364	20.876
[3, 3]	3984.0	22224.0	73.910	16.727	178.88	16.591	38.535
[4, 4]	6480.0	36720.0	117.14	26.221	286.56	26.045	61.092
[5, 5]	9552.0	54672.0	169.75	37.713	418.24	37.500	88.550
[6, 6]	13200.0	76080.0	231.74	51.207	573.92	50.955	120.90
[7, 7]	17424.0	100940.0	303.11	66.700	753.60	66.409	158.16
[8, 8]	22224.0	129260.0	383.87	84.194	957.27	83.864	200.32
[9, 9]	27600.0	161040.0	473.99	103.69	1185.0	103.32	247.37
[10, 10]	33552.0	196270.0	573.51	125.18	1436.6	124.77	299.32

For $ABC_{ve}(TMX_3)$ which is the ve-degree atom-bond connectivity index of TMX_3, we have $\psi(\xi_{ve}(x_1),\xi_{ve}(x_2))=\left(\frac{\xi_{ve}(x_1)+\xi_{ve}(x_2)-2}{\xi_{ve}(x_1)\times\xi_{ve}(x_2)}\right)^{\frac{1}{2}}$, therefore $\psi(12,12)=\sqrt{\frac{22}{144}}$, $\psi(6,10)=\sqrt{\frac{14}{60}}$ and $\psi(10,12)=\sqrt{\frac{20}{120}}$. Thus by Lemma 1,

$$\begin{aligned}&ABC_{ve}(TMX_3)\\&=6m^2\sqrt{\frac{22}{144}}+6m\left(\sqrt{\frac{14}{60}}+2\sqrt{\frac{20}{120}}+\sqrt{\frac{22}{144}}\right)\\&\quad+6\left(\sqrt{\frac{14}{60}}+2\sqrt{\frac{20}{120}}-2\sqrt{\frac{22}{144}}\right)\\&=\frac{\sqrt{22}}{2}m^2+6m\left(\frac{\sqrt{210}+10\sqrt{6}}{30}+\frac{\sqrt{22}}{12}\right)\\&\quad+\frac{\sqrt{210}}{5}+2\sqrt{6}-\sqrt{22}.\end{aligned}$$

For $GA_{ve}(TMX_3)$ which is the ve-degree geometric-arithmetic index of TMX_3, we have $\psi(\xi_{ve}(x_1),\xi_{ve}(x_2))=\frac{2(\xi_{ve}(x_1)\times\xi_{ve}(x_2))^{\frac{1}{2}}}{\xi_{ve}(x_1)+\xi_{ve}(x_2)}$, therefore $\psi(12,12)=1$, $\psi(6,10)=\frac{2\sqrt{60}}{16}$ and $\psi(10,12)=\frac{2\sqrt{120}}{22}$. Thus by Lemma 1,

$$\begin{aligned}GA_{ve}(TMX_3)&=6m^2+6m\left(\frac{2\sqrt{60}}{16}+2\frac{2\sqrt{120}}{22}+1\right)\\&\quad+6\left(\frac{2\sqrt{60}}{16}+2\frac{2\sqrt{120}}{22}-2\right)\\&=6m^2+6m\left(\frac{\sqrt{15}}{4}+\frac{4\sqrt{30}}{11}+1\right)\\&\quad+\frac{3\sqrt{15}}{2}+\frac{24\sqrt{30}}{11}-12.\end{aligned}$$

For $H_{ve}(TMX_3)$ which is the ve-degree harmonic index of TMX_3, we have $\psi(\xi_{ve}(x_1),\xi_{ve}(x_2))=\frac{2}{\xi_{ve}(x_1)+\xi_{ve}(x_2)}$, therefore $\psi(12,12)=\frac{1}{12}$, $\psi(6,10)=\frac{1}{8}$ and $\psi(10,12)=\frac{1}{11}$. Thus by Lemma 1,

$$\begin{aligned}H_{ve}(TMX_3)&=6m^2\frac{1}{12}+6m\left(\frac{1}{8}+2\frac{1}{11}+\frac{1}{12}\right)\\&\quad+6\left(\frac{1}{8}+2\frac{1}{11}-2\frac{1}{12}\right)\\&=\frac{1}{2}m^2+\frac{103}{44}m+\frac{37}{44}.\end{aligned}$$

TABLE 2. Numerical representation of *ve*-degree results for HMX_3.

m	$M^1_{\beta ve}$	M^2_{ve}	ABC_{ve}	R_{ve}	GA_{ve}	H_{ve}	χ_{ve}
2.	3168	17568	59.331	13.480	143.04	13.364	30.931
3	7344	41904	131.21	29.221	322.56	29.045	68.441
4	13248	76608	231.23	50.960	574.08	50.727	120.65
5	20880	121680	359.39	78.700	897.60	78.409	187.55
6	30240	177120	515.71	112.44	1293.1	112.09	269.16
7	41328	242930	700.15	152.18	1760.6	151.77	365.46
8	54144	319100	912.74	197.92	2300.2	197.45	476.46
9	68688	405650	1153.5	249.66	2911.7	249.14	602.14
10	84960	502560	1422.4	307.40	3595.2	306.82	742.53

TABLE 3. Numerical representation of *ve*-degree results for TMX_3.

m	$M^1_{\beta ve}$	M^2_{ve}	ABC_{ve}	R_{ve}	GA_{ve}	H_{ve}	χ_{ve}
2	1656	8856	32.7726	7.61013	77.2793	7.52273	17.0742
3	2880	15840	54.6411	12.4802	131.039	12.3636	28.4811
4	4392	24552	81.2001	18.3502	196.799	18.2045	42.3374
5	6192	34992	112.450	25.2203	274.559	25.0455	58.6434
6	8280	47160	148.389	33.0903	364.318	32.8864	77.3987
7	10656	61056	189.019	41.9604	466.078	41.7273	98.6035
8	13320	76680	234.341	51.8304	579.838	51.5682	122.258
9	16272	94032	284.351	62.7005	705.598	62.4091	148.362
10	19512	113112	339.053	74.5705	843.358	74.2500	176.914

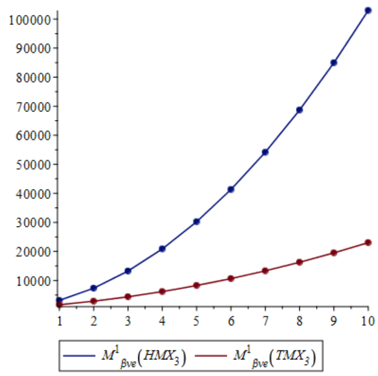

FIGURE 5. The first *ve*-degree Zagreb α index for HMX_3 and TMX_3.

For $\chi_{ve}(TMX_3)$ which is the *ve*-degree sum-connectivity index of TMX_3, we have $\psi(\xi_{ve}(x_1), \xi_{ve}(x_2)) = (\xi_{ve}(x_1) + \xi_{ve}(x_2))^{-\frac{1}{2}}$, therefore $\psi(12, 12) = \frac{1}{\sqrt{24}}$, $\psi(6, 10) = \frac{1}{\sqrt{16}}$ and $\psi(10, 12) = \frac{1}{\sqrt{22}}$. Thus by Lemma 1,

$$\begin{aligned}\chi_{ve}(TMX_3) &= 6m^2\frac{1}{\sqrt{24}} + 6m\left(\frac{1}{\sqrt{16}} + \frac{2}{\sqrt{22}} + \frac{1}{\sqrt{24}}\right) \\ &\quad + 6\left(\frac{1}{\sqrt{16}} + \frac{2}{\sqrt{22}} - \frac{2}{\sqrt{24}}\right) \\ &= \frac{\sqrt{6}}{2}\,m^2 + 6\,m\left(\frac{1}{4} + \frac{\sqrt{22}}{11} + \frac{\sqrt{6}}{12}\right) \\ &\quad + \frac{3}{2} + \frac{6\sqrt{22}}{11} - \sqrt{6}.\end{aligned}$$

VI. NUMERICAL RESULTS AND DISCUSSION OF METAL TRIHALIDES

In this section we present numerical results related to the *ve*-degree topological descriptors for metal trihalides.

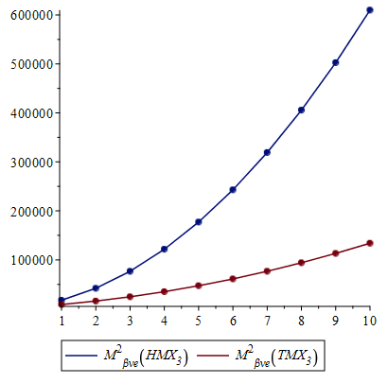

FIGURE 6. The second *ve*-degree Zagreb index for HMX_3 and TMX_3.

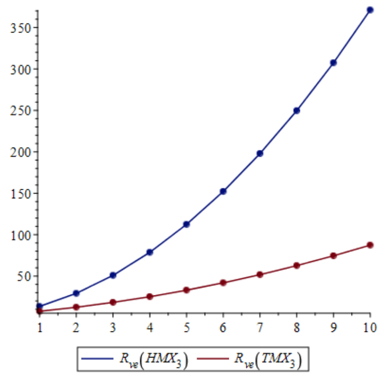

FIGURE 7. The *ve*-degree Randic index for HMX_3 and TMX_3.

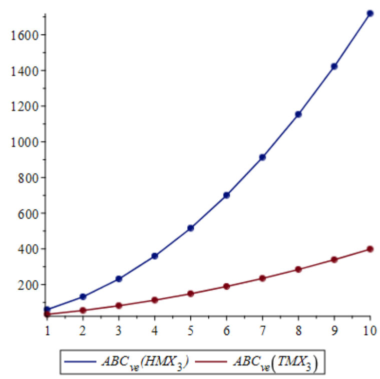

FIGURE 8. The *ve*-degree atom-bond connectivity index for HMX_3 and TMX_3.

We have used different values of l, w and m to compute numerical tables for the *ve*-degree indices such as the first *ve*-degree Zagreb β index, the second *ve*-degree Zagreb index, *ve*-degree Randic index, *ve*-degree atom-bond connectivity (ABC_{ve}) index, *ve*-degree geometric-arithmetic (GA_{ve}) index, *ve*-degree harmonic (H_{ve}) index and *ve*-degree sum-connectivity (χ_{ve}) for the metal trihalides, (see Tables 1 2, 3). Moreover, we have drawn the graphical representation based on the above numerical computation in Figures 5–11 for

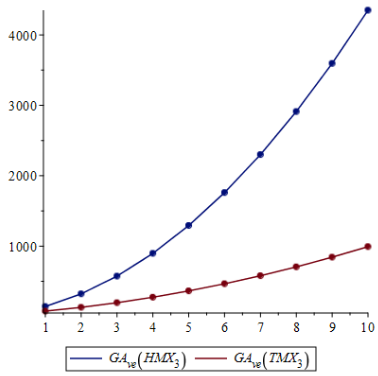

FIGURE 9. The *ve*-degree geometric-arithmetic index for HMX_3 and TMX_3.

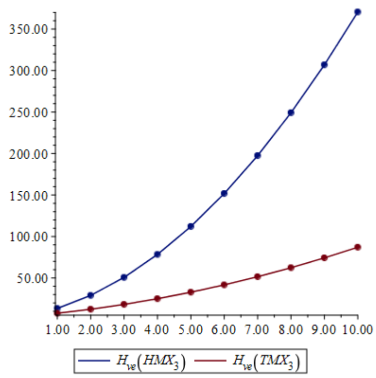

FIGURE 10. The *ve*-degree harmonic index for HMX_3 and TMX_3.

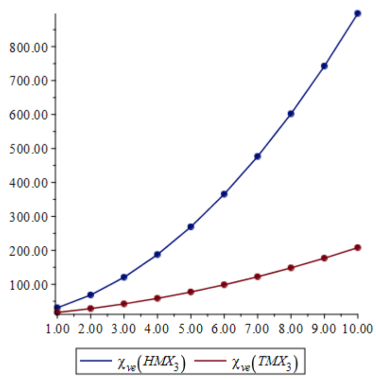

FIGURE 11. The *ve*-degree sum-connectivity index for HMX_3 and TMX_3.

HMX_3 & TMX_3 to study the behavior of above computed topological descriptors.

VII. CONCLUSION

The study of graphs and networks through topological descriptors is important to understand their underlying topologies. Such investigations have a wide range of applications in cheminformatics, bioinformatics and biomedicine fields, where various graph invariants based assessments are used to deal with several challenging schemes. In the analysis of the quantitative structure property relationships (QSPRs) and the quantitative structure-activity relationships (QSARs), graph invariants are important tools to approximate and predicate the properties of the biological and chemical compounds. More preciously in this paper, we have computed results *ve*-degree indices such as the first *ve*-degree Zagreb β index, the second *ve*-degree Zagreb index, *ve*-degree Randic index, *ve*-degree atom-bond connectivity (ABC_{ve}) index, *ve*-degree geometric-arithmetic (GA_{ve}) index, *ve*-degree harmonic (H_{ve}) index and *ve*-degree sum-connectivity (χ_{ve}) for themetal trihalides. Also the graphical comparison between the *ve*-degree indices for hexagonal and triangular shaped metal trihalides are shown in Figures 5–11.

ACKNOWLEDGMENT

This project was funded by the Deanship of Scientific Research (DSR) at King Abdulaziz University, Jeddah, under grant no. RG-6-135-40. The authors are gratefully acknowledge DSR technical and financial support.

REFERENCES

[1] P. Avouris, "Graphene: Electronic and photonic properties and devices," *Nano Lett.*, vol. 10, no. 11, pp. 4285–4294, Nov. 2010.
[2] A. Ahmad, "On the degree based topological indices of benzene ring embedded in P-type-surface in 2D network," *Hacettepe J. Math. Statist.*, vol. 47, no. 1, pp. 9–18, 2018.
[3] G. Cao, "Atomistic studies of mechanical properties of graphene," *Polymer*, vol. 6, no. 9, pp. 2404–2432, 2014.
[4] M. Arockiaraj, S. R. J. Kavitha, S. Mushtaq, and K. Balasubramanian, "Relativistic topological molecular descriptors of metal trihalides," *J. Mol. Struct.*, vol. 1217, Oct. 2020, Art. no. 128368.
[5] P. Liu, F. Lu, M. Wu, X. Luo, Y. Cheng, X.-W. Wang, W. Wang, W.-H. Wang, H. Liu, and K. Cho, "Electronic structures and band alignments of monolayer metal trihalide semiconductors MX_3," *J. Mater. Chem. C*, vol. 5, no. 35, pp. 9066–9071, 2017.
[6] P. Miro, M. Audiffred, and T. Heine, "An atlas of two-dimensional materials," *Chem. Soc. Rev.*, vol. 43, no. 18, pp. 6537–6554, 2014.
[7] J. He, S. Ma, P. Lyu, and P. Nachtigall, "Unusual Dirac half-metallicity with intrinsic ferromagnetism in vanadium trihalide monolayers," *J. Mater. Chem. C*, vol. 4, no. 13, pp. 2518–2526, 2016.
[8] C. Huang, J. Zhou, H. Wu, K. Deng, P. Jena, and E. Kan, "Quantum anomalous Hall effect in ferromagnetic transition metal halides," *Phys. Rev. B, Condens. Matter*, vol. 95, no. 4, 2017, Art. no. 045113.
[9] J. Liu, Q. Sun, Y. Kawazoe, and P. Jena, "Exfoliating biocompatible ferromagnetic Cr-trihalide monolayers," *Phys. Chem. Chem. Phys.*, vol. 18, no. 13, pp. 8777–8784, 2016.
[10] Z. Raza, "Leap Zagreb connection numbers for some networks models," *Indonesian J. Chem.*, vol. 20, no. 6, pp. 1407–1413, 2020.
[11] M. K. Siddiqui, M. Imran, and A. Ahmad, "On Zagreb indices, Zagreb polynomials of some nanostar dendrimers," *Appl. Math. Comput.*, vol. 280, pp. 132–139, Apr. 2016.
[12] M. Xu, T. Liang, M. Shi, and H. Chen, "Graphene-like two-dimensional materials," *Chem. Rev.*, vol. 113, no. 5, pp. 3766–3798, 2013.
[13] Q. H. Wang, K. Kalantar-Zadeh, A. Kis, J. N. Coleman, and M. S. Strano, "Electronics and optoelectronics of two-dimensional transition metal dichalcogenides," *Nature Nanotechnol.*, vol. 7, no. 11, pp. 699–712, Nov. 2012.
[14] A. Ahmad, K. Elahi, R. Hasni, and M. F. Nadeem, "Computing the degree based topological indices of line graph of benzene ring embedded in P-type-surface in 2D network," *J. Inf. Optim. Sci.*, vol. 40, no. 7, pp. 1511–1528, Oct. 2019.
[15] W.-B. Zhang, L.-J. Xiang, and H.-B. Li, "Theoretical perspective of energy harvesting properties of atomically thin BiI_3," *J. Mater. Chem. A*, vol. 4, no. 48, pp. 19086–19094, 2016.
[16] U. H. Hamdeh, R. D. Nelson, B. J. Ryan, U. Bhattacharjee, J. W. Petrich, and M. G. Panthani, "Solution-processed BiI_3 thin films for photovoltaic applications: Improved carrier collection via solvent annealing," *Chem. Mater.*, vol. 28, no. 18, pp. 6567–6574, 2016.

[17] M. Imran, A. Q. Baig, and H. Ali, "On molecular topological properties of hex-derived networks," *J. Chemometrics*, vol. 30, no. 3, pp. 121–129, Feb. 2016.
[18] Q. Tang, Z. Zhou, and Z. Chen, "Molecular charge transfer: A simple and effective route to engineer the band structures of BN nanosheets and nanoribbons," *J. Phys. Chem. C*, vol. 115, no. 38, pp. 18531–18537, Sep. 2011.
[19] M. Matsumoto, K. Hitomi, T. Shoji, and Y. Hiratate, "Bismuth tri-iodide crystal for nuclear radiation detectors," *IEEE Trans. Nucl. Sci.*, vol. 49, no. 5, pp. 2517–2520, Oct. 2002.
[20] F. Ma, M. Zhou, Y. Jiao, G. Gao, Y. Gu, A. Bilic, Z. Chen, and A. Du, "Single layer bismuth iodide: Computational exploration of structural, electrical, mechanical and optical properties," *Sci. Rep.*, vol. 5, no. 1, P. 17558, Dec. 2015.
[21] P. Khadikar, S. Karmarkar, V. Agrawal, J. Singh, A. Shrivastava, I. Lukovits, and M. Diudea, "Szeged index-applications for drug modeling," *Lett. Drug Des. Discovery*, vol. 2, no. 8, pp. 606–624, Dec. 2005.
[22] R. Todeschini, V. Consonni, *Molecular Descriptors for Chemoinformatics*. Weinheim, Germany: Wiley-VCH, 2009.
[23] K. Balasubramanian, "Mathematical and computational techniques for drug discovery: Promises and developments," *Current Topics Medicinal Chem.*, vol. 18, no. 32, pp. 2774–2799, Mar. 2019.
[24] K. Balasubramanian and S. P. Gupta, "Quantum molecular dynamics, topological, group theoretical and graph theoretical studies of protein-protein interactions," *Current Topics Medicinal Chem.*, vol. 19, no. 6, pp. 426–443, May 2019.
[25] S. C. Basak, B. D. Gute, G. D. Grunwald, D. W. Opitz, and K. Balasubramanian, "Use of statistical and neural net methods in predicting toxicity of chemicals: A hierarchical QSAR approach, predictive toxicology of chemicals: Experiences and impacts of artificial intelligence tools," AAAI Tech. Rep. SS-99-01, 1999, pp. 108–111. [Online]. Available: https://www.aaai.org/Papers/Symposia/Spring/1999/SS-99-01/SS99-01-025.pdf
[26] S. C. Basak, K. Balasubramanian, B. D. Gute, D. Mills, A. Gorczynska, and S. Roszak, "Prediction of cellular toxicity of halocarbons from computed chemodescriptors: A hierarchical QSAR approach," *J. Chem. Inf. Comput. Sci.*, vol. 43, no. 4, pp. 1103–1109, Jul. 2003.
[27] S. C. Basak, D. Mills, and M. M. Mumtaz, "A quantitative structure–activity relationship (QSAR) study of dermal absorption using theoretical molecular descriptors," *SAR QSAR Environ. Res.*, vol. 18, nos. 1–2, pp. 45–55, 2007.
[28] M. Arockiaraj, J. Clement, D. Paul, and K. Balasubramanian, "Quantitative structural descriptors of sodalite materials," *J. Mol. Struct.*, vol. 1223, Jan. 2021, Art. no. 128766, doi: 10.1016/j.molstruc.2020.128766.
[29] M. Arockiaraj, J. Clement, D. Paul, and K. Balasubramanian, "Relativistic distance-based topological descriptors of linde type a zeolites and their doped structures with very heavy elements," *Mol. Phys.*, vol. 119, no. 3, Feb. 2021, Art. no. e1798529, doi: 10.1080/00268976.2020.1798529.
[30] M. Arockiaraj, J. Clement, and K. Balasubramanian, "Analytical expressions for topological properties of polycyclic benzenoid networks," *J. Chemometrics*, vol. 30, no. 11, pp. 682–697, Nov. 2016.
[31] M. Arockiaraj, S. Klavžar, J. Clement, S. Mushtaq, and K. Balasubramanian, "Edge distance-based topological indices of strength-weighted graphs and their application to coronoid systems, carbon nanocones and SiO_2 nanostructures," *Mol. Informat.*, vol. 38, nos. 11–12, Nov. 2019, Art. no. 1900039, doi: 10.1002/minf.201900039.
[32] A. N. A. Koam, A. Ahmad, and A. Haider, "On eccentric topological indices based on edges of zero divisor graphs," *Symmetry*, vol. 11, no. 7, p. 907, Jul. 2019.
[33] H. Wiener, "Structural determination of paraffin boiling points," *J. Amer. Chem. Soc.*, vol. 69, no. 1, pp. 17–20, Jan. 1947.
[34] M. Randić, "On history of the Randić index and emerging hostility toward chemical graph theory," *Match Commun. Math. Comput. Chem.*, vol. 59, no. 1, pp. 5–24, 2008.
[35] J. C. Dobrowolski, "The structural formula version of graph theory," *Match Commun. Math. Comput. Chem.*, vol. 81, pp. 527–555, 2019.
[36] L. Zhong, "The harmonic index for graphs," *Appl. Math. Lett.*, vol. 25, no. 3, pp. 561–566, Mar. 2012.
[37] S. Ediz, "A new tool for QSPR researches: *Ev*-degree Randic index," *Celal Bayar Univ. J. Sci.*, vol. 13, no. 3, pp. 615–618, 2017.
[38] M. Chellali, T. W. Haynes, S. T. Hedetniemi, and T. M. Lewis, "On *ve*-degrees and *ev*-degrees in graphs," *Discrete Math.*, vol. 340, no. 2, pp. 31–38, 2017.
[39] B. Horoldagva, K. C. Das, and T. A. Selenge, "On *ve*-degree and *ev*-degree of graphs," *Discrete Optim.*, vol. 31, pp. 1–7, Feb. 2019.
[40] S. Ediz, "On *ve*-degree molecular topological properties of silicate and oxygen networks," *Int. J. Comput. Sci. Math.*, vol. 9, no. 1, pp. 1–12, 2018.
[41] B. Sahin and S. Ediz, "On *ev*-degree and *ve*-degree topological indices," *Iran. J. Math. Chem.*, vol. 9, no. 4, pp. 263–277, 2018.
[42] J. Zhang, M. K. Siddiqui, A. Rauf, and M. Ishtiaq, "On *ve*-degree and ev-degree based topological properties of single walled titanium dioxide nanotube," *J. Cluster Sci.*, pp. 1–12, Jul. 2020. [Online]. Available: https://link.springer.com/article/10.1007/s10876-020-01842-3, doi: 10.1007/s10876-020-01842-3.
[43] B. Huang, G. Clark, E. Navarro-Moratalla, D. R. Klein, R. Cheng, K. L. Seyler, D. Zhong, E. Schmidgall, M. A. McGuire, D. H. Cobden, W. Yao, D. Xiao, P. Jarillo-Herrero, and X. Xu, "Layer-dependent ferromagnetism in a van der Waals crystal down to the monolayer limit," *Nature*, vol. 546, no. 7657, pp. 270–273, Jun. 2017.
[44] M. McGuire, "Crystal and magnetic structures in layered, transition metal dihalides and trihalides," *Crystals*, vol. 7, no. 5, p. 121, Apr. 2017.
[45] T. Vetrík, "Polynomials of degree-based indices for hexagonal nanotubes," *UPB Sci. Bull., Ser. B*, vol. 81, no. 1, pp. 109–120, 2019.
[46] A. Ahmad, "Topological properties of sodium chloride," *UPB Sci. Bull., Ser. B*, vol. 82, no. 1, pp. 35–46, 2020.

FOUAD A. ABOLABAN received the Ph.D. degree from the Department of Medical Physics, Faculty of Engineering and Physics Sciences, University of Surrey, U.K., in 2012. He is currently working as an Associate Professor with the Department of Nuclear Engineering, King Abdulaziz University, Jeddah. He also runs more than eight grant projects from the Deanship of Scientific Research, King Abdulaziz University. He holds two American patents: U.S. Patent Office: patent No 17/018,193: Ac255 Production. (Accepted)
U.S. Patent Office: patent No 17/012,820: New Nanoparticle shape design. (Submitted). He has published more than 20 articles in peer-reviewed scientific journals and in proceedings of international conferences covering both general medical physics and radiation therapy physics. His main research interests include medical physics and radiation therapy using nanoparticles.

ALI AHMAD received the M.Sc. degree in mathematics from the University of the Punjab, Lahore, Pakistan, in 2000, the M.Phil. degree in mathematics from Bahauddin Zakariya University, Multan, Pakistan in 2005, and the Ph.D. degree in mathematics from the Abdus Salam School of Mathematical Sciences, GC University, Lahore, in 2010. He is currently an Assistant Professor with the College of Computer Science and Information Technology, Jazan University, Saudi Arabia. His research interests include graph labeling, metric dimension, minimal doubly resolving sets, distances in graphs, and topological indices of graphs.

MUHAMMAD AHSAN ASIM received the master's degree from the Blekinge Institute of Technology (BTH), Sweden, and the Ph.D. degree in mathematical sciences from Universiti Malaysia Terengganu (UMT), Malaysia, in 2018. He is currently working as a Lecturer with the Department of Information Technology and Security, Jazan University, Saudi Arabia. He is also doing research and teaching responsibilities in interdisciplinary filed of graph theory and graph algorithms and experimental mathematics.