

Analysis of degree-based topological indices through M-polynomial of metal trihalides

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Abstract

The progression of 2D novel, metal trihalides MX_3 , has been learned Dirac half-metallicity topological spintronic possessions because of their interest that are inherited magnetic processes reflected by 2D metal trihalide. Recently a new approach has been introduced to calculate the degree-based topological indices of chemical compounds, called the M-polynomial. It gives nice and good results of the topological indices of the corresponding chemical compounds. Then one can use these results to correlate the chemical compounds with their chemical properties and bioactivities. The main interest in this article

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is the computations and comparisons of the general form of M-polynomial of two types of metal trihalides. Then, the general form of obtained M-polynomials is used to determine the degree-based topological indices of these metal trihalides. In the end, graphical comparisons of the M-polynomial and the topological indices of the metal trihalides are described. Mainly, a comparison among the degree-based indices of metal trihalides is performed with the help of 2D-chart plots and numerical tables.

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1. Introduction

In theoretical biology and chemistry, atomic descriptors are used to represent fundamental characteristics of atoms, capturing their intriguing chemical and physical properties. Such descriptors are known as topological indices, specifically referred to as degree-based topological indices (DBTIs) [1,2], which are determined by the degree of the molecular graph. These indices can be employed to model and highlight certain properties of chemical compounds.

In this paper, a simple graph $\Psi = \Psi(V, E)$ is considered, where $V(\Psi)$ is the set of vertices and $E(\Psi)$ is the set of edges, and the graph Ψ has no loops, directed, or multiple edges. The degree of a vertex $v \in V(\Psi)$, represented as $d_\Psi(v)$, is the number of vertices connected to v by edges. In chemistry, the concept of vertex degree is closely related to valence. The first and second Zagreb indices, $M_1(\Psi)$ and $M_2(\Psi)$, [3] are defined as

$$M_1(\Psi) = \sum_{v \in V(\Psi)} d_v^2, M_2(\Psi) = \sum_{vw \in E(\Psi)} d_v d_w.$$

Nikolic et al. introduced second Modified Zagreb index ${}^a M_2(\Psi)$ in [4]

$${}^a M_2(\Psi) = \sum_{vw \in E(\Psi)} \frac{1}{d_v d_w}$$

The symmetric division deg index (SDD) and the inverse sum indeg index (ISI) have been introduced as follows.

$$SDD(\Psi) = \sum_{vw \in E(\Psi)} \left(\frac{d_v}{d_w} + \frac{d_w}{d_v} \right) = \sum_{vw \in E(\Psi)} \frac{d_v^2 + d_w^2}{d_v d_w}$$

$$ISI(\Psi) = \sum_{vw \in E(\Psi)} \frac{1}{\frac{1}{d_w} + \frac{1}{d_v}} = \sum_{vw \in E(\Psi)} \frac{d_v d_w}{d_v + d_w}$$

The harmonic index is formulated as:

$$H(\Psi) = \sum_{vw \in E(\Psi)} \frac{2}{d_v + d_w}$$

The augmented Zagreb index (AZI) is formulated as:

$$AZI(\Psi) = \sum_{vw \in E(\Psi)} \left(\frac{d_v d_w}{d_v + d_w - 2} \right)^3$$

The Randic index was generalized as

$$R_\alpha(\Psi) = \sum_{vw \in E(\Psi)} (d_v d_w)^\alpha \quad \alpha \neq 0$$

The M-polynomial for a simple graph Ψ is defined as follows:

$$M(\Psi, r, s) = \sum_{\delta \leq i \leq j \leq \Delta} m_{(i,j)}(\Psi) r^i s^j, \quad (1.1)$$

where $\delta = \min\{d_a | a \in V(\Psi)\}$, $\Delta = \max\{d_a | a \in V(\Psi)\}$ and $m_{(i,j)}(\Psi)$ is the number of edges $ab \in E(\Psi)$ such that $(d_a, d_b) = (i, j)$.

If the M -polynomial of a graph Ψ is represented by the function $K(r, s)$, then using the following operations: $D_r = r \frac{\partial(K(r,s))}{\partial r}$, $D_s = s \frac{\partial(K(r,s))}{\partial s}$, $S_r = \int_0^r \frac{K(r,s)}{r}$, $S_s = \int_0^s \frac{K(r,s)}{s}$, $J(K(r,s)) = K(r,s)$, and $Q_\beta(K(r,s)) = r^\beta K(r,s)$, Deutsch and Klavžar [6] derived various DBTIs from the M -polynomial, as shown in Table 1.

Table 1
Extraction of descriptors from the M-polynomial.

Indices	Extraction from $M(\mathcal{K}; r, s)$
M_1	$(D_r + D_s)(M(\Psi; r, s)) _{r=s=1}$
M_2	$(D_r D_s)(M(\Psi; r, s)) _{r=s=1}$
$^a M_2$	$(S_r S_s)(M(\Psi; r, s)) _{r=s=1}$
SDD	$(D_r S_s + S_r D_s)(M(\Psi; r, s)) _{r=s=1}$
H	$2S_r J(M(\Psi; r, s)) _{r=1}$
ISI	$S_r J D_r D_s (M(\Psi; r, s)) _{r=1}$
AZI	$S_r^3 Q_{-2} J D_r^3 D_s^3 (M(\Psi; r, s)) _{r=1}$
R_α	$(D_r^\alpha D_s^\alpha)(M(\Psi; r, s)) _{r=s=1}$

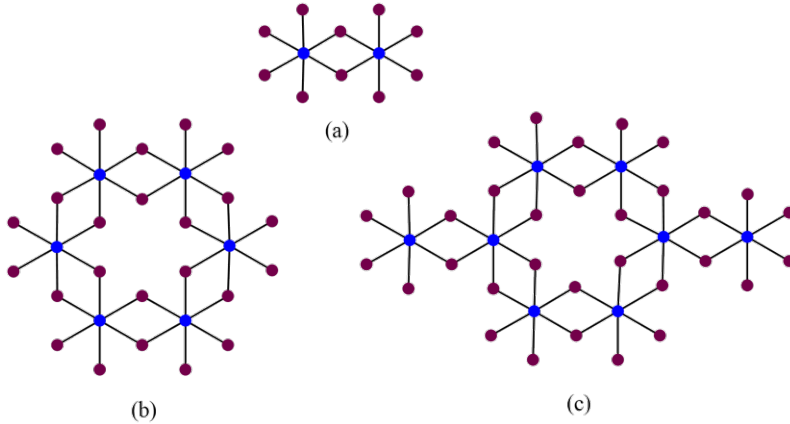


Figure 1
Unit cell of MX₃ (a) Type 1 monolayer (b) Type 2 monolayer (c)

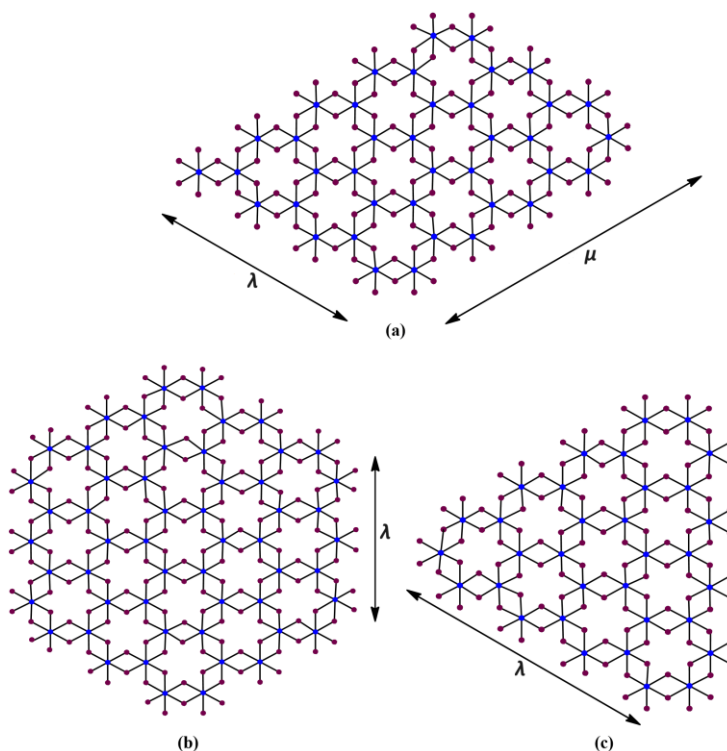


Figure 2
Metal trihalides of type 1 Parallelogram (a) Hexagonal (b) Triangular (c)

In the literature, there are a lot of papers about the computations of different type of topological indices for various structures, see [8, 12]. The M-polynomial of a given structure has been calculated recently. For example, in [10] for two infinite classes of nanostar dendrimers, for polyhex nanotubes in [9]. Recently, M-polynomial for some nano and crystal structures have been outlined in [11, 5]. The M-polynomial plays a vital role to obtain the closed-form formulas for some indices, see [7] and [28, 29, 30].

1.1 Metal trihalides and its uses

Metal trihalides are a group of chemical compounds characterized by a metal atom bonded to three halogen atoms, generally represented by the formula MX_3 , where M is the metal and X is the halogen (fluorine, chlorine, bromine, or iodine) [13, 14, 15, 16, 17, 18, 19, 20, 21, 22]. These compounds exhibit a wide range of chemical properties depending on the metal and halogen involved. The bonding in metal trihalides can vary from ionic to covalent, with some compounds like aluminum trichloride $AlCl_3$ displaying covalent characteristics, while others, such as scandium trifluoride ScF_3 , are more ionic. Metal trihalides

also differ in physical states; many are solid at room temperature, though some may sublime or decompose when heated. Additionally, these compounds often have distinctive colors, influenced by the electronic structure of the metal and the specific halogen present. For instance, iron(III) chloride $FeCl_3$ is known for its dark brown or yellowish hue.

Transition metals such as iron, chromium, and titanium form trihalides that are particularly significant due to their magnetic, catalytic, and electronic properties. Iron(III) chloride $FeCl_3$ is widely used in industrial applications, including water treatment and as a catalyst in organic synthesis. Chromium(III) chloride $CrCl_3$ finds use in the dyeing of fabrics and serves as a precursor to other chromium compounds, while titanium(III) chloride $TiCl_3$ is a key catalyst in polymerization reactions and in producing titanium metal. Lanthanides and actinides also form trihalides, which are often highly ionic, especially with fluorine. These compounds exhibit notable magnetic and optical properties, making them useful in various high-tech applications. For example, lanthanum(III) fluoride LaF_3 is used in optical lenses and coatings, and uranium(III) chloride UCl_3 plays a role in nuclear chemistry.

Main group elements like aluminum also form trihalides, which can display a range of bonding and structural characteristics. Aluminum trichloride $AlCl_3$, a white or yellow solid, is extensively used in the chemical industry as a Lewis acid catalyst in reactions such as the Friedel-Crafts alkylation. It is known for forming a covalent dimer Al_2Cl_6 in the gas phase. Another example is boron trifluoride BF_3 , a colorless gas utilized as a catalyst in organic chemistry and as a precursor to various boron compounds.

The chemical reactivity of metal trihalides varies widely, influenced by the specific metal and halogen. These compounds can hydrolyze in water, forming metal hydroxides and halogen acids, or react with bases, reducing agents, or other metal halides. Typically, the metal in a trihalide is in the +3 oxidation state, though this can vary based on the metal's coordination environment. The coordination geometry of metal trihalides can also differ, with common structures including trigonal planar and octahedral arrangements, depending on factors such as the metal's size and the halogen's electronegativity.

Metal trihalides are used in various applications across industries, including catalysis, electronics, and nuclear chemistry. Many, such as aluminum and titanium trihalides, serve as catalysts in organic synthesis and industrial processes. Iron(III) chloride is employed in the etching and processing of electronic components, while lanthanide and actinide trihalides are important in nuclear fuel processing and other specialized applications. Understanding the diverse properties and behaviors of metal trihalides is crucial in fields ranging from materials science to industrial chemistry, given their broad range of chemical behaviors and industrial uses.

2. Main Results and Discussions

In this section, we examine the stacking of MX_3 in parallelogram, hexagon, and triangle configurations, as illustrated in Fig. 1(a) – 1(c). The number of vertices in a graph is represented by $|V(\Psi)|$, while $|E(\Psi)|$ represents the number of edges. Transition MX_3 are a newly introduced 2D binary compound [23, 24, 25]. The Fig. (a) represents the unit cell of MX_3 and Fig. 1(b) and Fig. 1(c) shown the monolayers of two kinds of trihalide.

Let $\Psi_{p1}(\lambda, \mu)$, $\Psi_{h1}(\lambda)$, and $\Psi_{t1}(\lambda)$ a type 1 parallelogram, hexagonal and triangle shaped trihalide. The their edges can be partition according to the degrees as:

type 1 MX_3	$m_{(1,6)}$	$m_{(2,6)}$
$\Psi_{p1}(\lambda, \mu)$	$12\lambda + 4\mu + 4$	$12\lambda\mu + 8\lambda + 8\mu - 4$
$\Psi_{h1}(\lambda)$	12λ	$36\lambda^2 - 12\lambda$
$\Psi_{t1}(\lambda)$	$6\lambda + 6$	$6\lambda^2 + 18\lambda$

Theorem 2.1: *The M-polynomials of MX_3 of type 1 as given as:*

- (1) $M_{p1}(r, s) = (4\lambda + 4\mu + 4)rs^2 + (12\lambda\mu + 8\lambda + 8\mu - 4)r^2s^6$.
- (2) $M_{h1}(r, s) = 12\lambda rs^2 + (36\lambda^2 - 12\lambda)r^2s^6$
- (3) $M_{t1}(r, s) = (6\lambda + 6)rs^2 + (6\lambda^2 + 18\lambda)r^2s^6$

Proof. We will prove the first part in detail. The number of vertices and edges of type 1 parallelogram $\Psi_{p1}(\lambda, \mu)$ can be noted as $|V(\Psi_{p1}(\lambda, \mu))| = 10\lambda + 10\mu + 8\lambda\mu + 2$, $|E(\Psi_{p1}(\lambda, \mu))| = 12\lambda + 12\mu + 12\lambda\mu$ respectively. From the graph as shown in Fig. 2(a) of type 1 parallelogram shaped $\Psi_{p1}(\lambda, \mu)$, one can see that the partition of edge set as:

$$E_{(1,6)} = \{e = ab \in E : d_a = 1, d_b = 6\}, E_{(2,6)} = \{e = ab \in E : d_a = 2, d_b = 6\}$$

Therefore, by using 2 the associated M-polynomial for $\Psi_{p1}(\lambda, \mu)$ is

$$\begin{aligned}
 M_{p1}(r, s) &= \sum_{i \leq j} E_{(i,j)}(\Psi_{p1}(\lambda, \mu)) r^i s^j \\
 &= \sum_{1 \leq 6} E_{(1,6)} r s^6 + \sum_{2 \leq 6} E_{(2,6)} r^2 s^6 \\
 &= \sum_{uv \in E_{(1,6)}} r s^6 + \sum_{uv \in E_{(2,6)}} r^2 s^6 \\
 &= m_{(1,6)} r s^6 + m_{(2,6)} r^2 s^6 \\
 &= (4\lambda + 4\mu + 4) r s^6 + (12\lambda\mu + 8\lambda + 8\mu - 4) r^2 s^6.
 \end{aligned}$$

Similarly, we can proof the other parts of the theorem.

Now, we study second type of MX_3 [26, 27] with parallelogram, hexagonal and triangular stacking, Fig. 3(a)-3(c). show the second type of MX_3 metal trihalodes.

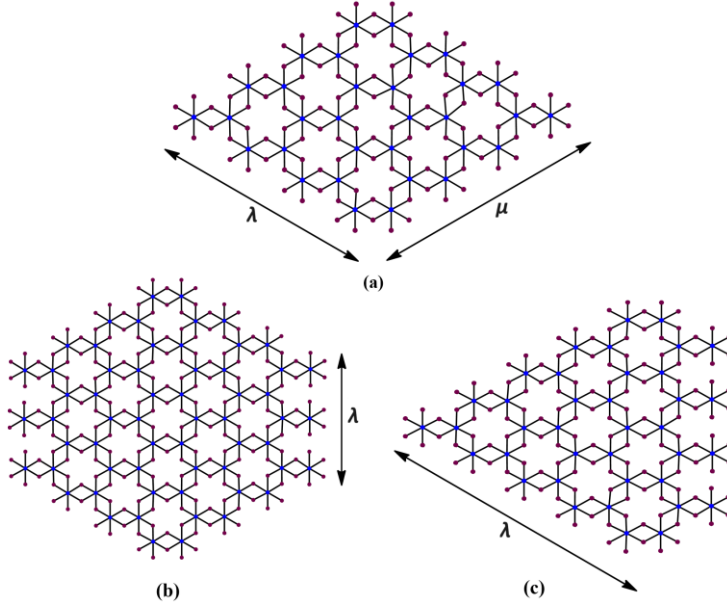


Figure 3
Metal trihalides of type 2 parallelogram (a) hexagonal (b) triangular (c)

Let $\Psi_{p2}(\lambda, \mu)$, $\Psi_{h2}(\lambda)$, and $\Psi_{t2}(\lambda)$ a type 2 parallelogram, hexagonal and triangle shaped trihalide. The their edges can be partition according to the degrees as:

type 2 MX_3	$m_{(1,6)}$	$m_{(2,6)}$
$\Psi_{p2}(\lambda, \mu)$	$4\lambda + 4\mu + 8$	$12\lambda\mu + 8\lambda + 8\mu + 4$
$\Psi_{h2}(\lambda)$	16λ	$36\lambda^2 - 4\lambda$
$\Psi_{t2}(\lambda)$	$8\lambda + 8$	$6\lambda^2 + 22\lambda + 4$

Theorem 2.2: 2The M -polynomials of MX_3 of type 1 as given as:

- (1) $M_{p2}(r, s) = 4(\lambda + \mu + 2)rs^2 + 4(3\lambda\mu + 2\lambda + 2\mu + 1)r^2s^6$
- (2) $M_{h2}(r, s) = 16\lambda rs^2 + (36\lambda^2 - 4\lambda)r^2s^6$
- (3) $M_{t2}(r, s) = (8\lambda + 8)rs^2 + (6\lambda^2 + 22\lambda + 4)r^2s^6$

Proof: We will provide a detailed proof of the first part. By comparing the two types of parallelogram shapes of MX_3 , it is evident that $|V(\Psi)|$ increases by 10 and $|E(\Psi)|$ by 12. Therefore, we have $|V(\Psi_{p2}(\lambda, \mu))| = 10\lambda + 10\mu + 8\lambda\mu + 12$ and $|E(\Psi_{p2}(\lambda, \mu))| = 12\lambda + 12\mu + 12\lambda\mu + 12$ respectively. From the graph as shown in Fig. 3(a) of type 2 parallelogram shaped $\Psi_{p2}(\lambda, \mu)$, one can see that the partition of edge set as:

$$E_{(1,6)} = \{e = ab \in E: d_a = 1, d_b = 6\}, E_{(2,6)} = \{e = ab \in E: d_a = 2, d_b = 6\}$$

Therefore, we can examine that $m_{(1,6)} = |E_{(1,6)}| = 4\lambda + 4\mu + 8$, and $m_{(2,6)} = |E_{(2,6)}| = 12\lambda\mu + 8\lambda + 8\mu + 4$. Thus, the associated M-polynomial for $\Psi_{p2}(\lambda, \mu)$ is

$$\begin{aligned} M_{p2}(r, s) &= \sum_{i \leq j} E_{(i,j)}(\Psi_{p2}(\lambda, \mu)) r^i s^j \\ &= \sum_{1 \leq 6} E_{(1,6)}(\Psi_{p2}(\lambda, \mu)) r s^6 + \sum_{2 \leq 6} E_{(2,6)}(\Psi_{p2}(\lambda, \mu)) r^2 s^6 \\ &= \sum_{uv \in E_{(1,6)}} r s^6 + \sum_{uv \in E_{(2,6)}} r^2 s^6 \\ &= m_{(1,6)} r s^6 + m_{(2,6)} r^2 s^6 \\ &= (4\lambda + 4\mu + 8) r s^6 + (12\lambda\mu + 8\lambda + 8\mu + 4) r^2 s^6. \end{aligned}$$

other parts can be obtained in a similar method.

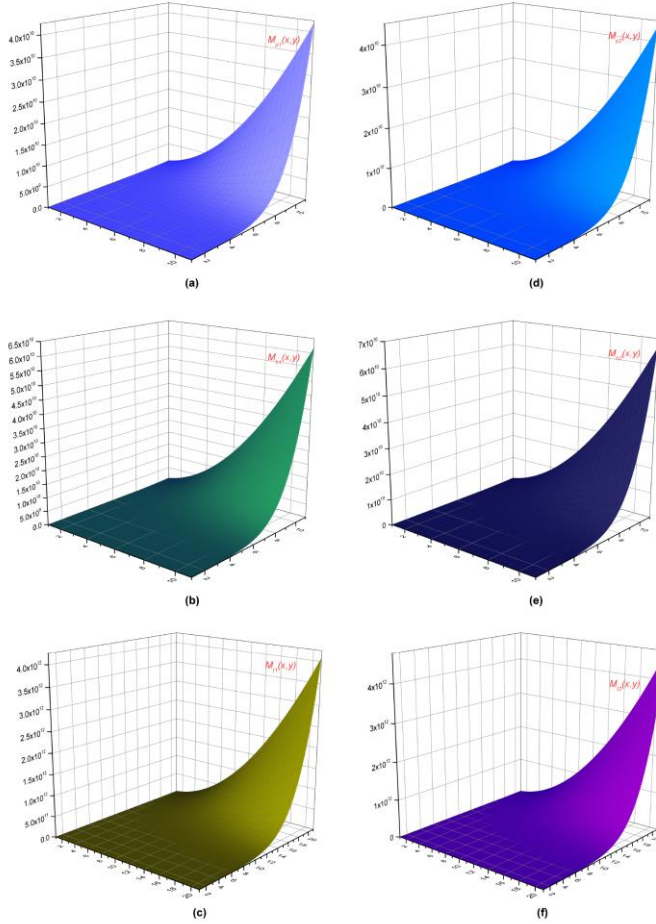


Figure 4
M-polynomial for type 1 and 2 MX_3 .

The graphical profiles of M-polynomials of two type of MX_3 are given in Fig. 4 for fixed values of $\lambda = 3$ and $\mu = 4$.

2.1 DBTIs related with type I shape

Theorem 2.3: *Let $\Psi_{p1}(\lambda, \mu)$ be a MX_3 with a type I parallelogram shaped. Then*

- (1) $M_1(\Psi_{p1}(\lambda, \mu)) = 96\lambda\mu + 92(\lambda + \mu) - 4$
- (2) $M_2(\Psi_{p1}(\lambda, \mu)) = 144\lambda\mu + 120\lambda + 120\mu - 24$
- (3) ${}^aM_2(\Psi_{p1}(\lambda, \mu)) = \frac{1}{3}[3\lambda\mu + 4(\lambda + \mu) + 1]$
- (4) $SDD(\Psi_{p1}(\lambda, \mu)) = \frac{2}{3}[60\lambda\mu + 77(\lambda + \mu) + 17]$
- (5) $ISI(\Psi_{p1}(\lambda, \mu)) = \frac{6}{7}[21\lambda\mu + 18(\lambda + \mu) - 3]$
- (6) $R_\alpha(\Psi_{p1}(\lambda, \mu)) = 12^{\alpha+1}(\lambda\mu) + [6^\alpha(4) + 12^\alpha(8)](\lambda + \mu) + 6^\alpha(4) - 12^\alpha(4)$
- (7) $RR_\alpha(\Psi_{p1}(\lambda, \mu)) = \frac{\lambda\mu}{12^{\alpha-1}} + (\frac{4}{6^\alpha} + \frac{8}{12^\alpha})(\lambda + \mu) + \frac{4}{6^\alpha} - \frac{4}{12^\alpha}$
- (8) $H(\Psi_{p1}(\lambda, \mu)) = \frac{1}{7}[21\lambda\mu + 22(\lambda + \mu) + 1]$
- (9) $AZI(\Psi_{p1}(\lambda, \mu)) = \frac{32}{125}[375\lambda\mu + 277(\lambda + \mu) - 98]$.

Proof: From Theorem 2.1, we have the M-polynomial as:

$$M_{p1}(r, s) = (4\lambda + 4\mu + 4)rs^2 + (12\lambda\mu + 8\lambda + 8\mu - 4)r^2s^6. \text{ So,}$$

$$\begin{aligned} D_r(M_{p1}(r, s)) &= 4(\lambda + \mu + 1)rs^6 + 8(3\lambda\mu + 2(\lambda + \mu) - 1)r^2s^6 \\ D_s((M_{p1}(r, s)) &= 24(\lambda + \mu + 1)rs^6 + 24(3\lambda\mu + 2(\lambda + \mu) - 1)r^2s^6 \\ D_r D_s(M_{p1}(r, s)) &= 24(\lambda + \mu + 1)rs^6 + 48(3\lambda\mu + 2(\lambda + \mu) - 1)r^2s^6 \\ D_r^\alpha(M_{p1}(r, s)) &= 4(\lambda + \mu + 1)rs^6 + 2^\alpha(4)(3\lambda\mu + 2(\lambda + \mu) - 1)r^2s^6 \\ D_s^\alpha(M_{p1}(r, s)) &= 6^\alpha(4)(\lambda + \mu + 1)rs^6 + 6^\alpha(4)(3\lambda\mu + 2(\lambda + \mu) - 1)r^2s^6 \end{aligned}$$

$$\begin{aligned} D_r^\alpha D_s^\alpha(M_{p1}(r, s)) &= 6^\alpha(4)(\lambda + \mu + 1)rs^6 + 12^\alpha(4)(3\lambda\mu + 2(\lambda + \mu) - 1)r^2s^6 \\ J(M_{p1}(r, s)) &= 4(\lambda + \mu + 1)r^7 + 4(3\lambda\mu + 2(\lambda + \mu) - 1)r^8. \end{aligned}$$

$$\text{Now } Q_\beta = r^\beta(M_{p1}(r, s))$$

$$Q_{-2} = r^{-2}(M_{p1}(r, s) = 4(\lambda + \mu + 1)r^{-1}s^6 + 4(3\lambda\mu + 2(\lambda + \mu) - 1)s^6$$

$$S_r = \int \frac{(M_{p1}(r, s))}{r} dr = 4(\lambda + \mu + 1)rs^6 + 2(3\lambda\mu + 2(\lambda + \mu) - 1)r^2s^6$$

$$S_s = \int \frac{(M_{p1}(r, s))ds}{s} = \frac{2}{3}(\lambda + \mu + 1)rs^6 + \frac{2}{3}(3\lambda\mu + 2(\lambda + \mu) - 1)r^2s^6$$

$$S_r S_s = \frac{2}{3}(\lambda + \mu + 1)rs^6 + \frac{1}{3}(3\lambda\mu + 2(\lambda + \mu) - 1)r^2s^6$$

$$S_r^\alpha = 4(\lambda + \mu + 1)rs^6 + \frac{4(3\lambda\mu + 2(\lambda + \mu) - 1)}{2^\alpha}r^2s^6$$

$$\begin{aligned}
S_s^\alpha &= \frac{4(\lambda+\mu+1)}{6^\alpha} r s^6 + \frac{4(3\lambda\mu+2(\lambda+\mu)-1)}{6^\alpha} r^2 s^6 \\
S_r^\alpha S_s^\alpha &= \frac{4(\lambda+\mu+1)}{6^\alpha} r s^6 + \frac{4(3\lambda\mu+2(\lambda+\mu)-1)}{12^\alpha} r^2 s^6 \\
D_r S_s &= \frac{2}{3} (\lambda + \mu + 1) r s^6 + \frac{4}{3} (3\lambda\mu + 2(\lambda + \mu) - 1) r^2 s^6 \\
D_s S_r &= 24(\lambda + \mu + 1) r s^6 + 12(3\lambda\mu + 2(\lambda + \mu) - 1) r^2 s^6 \\
S_r J((M_{p1}(r, s))) &= \frac{4}{7} (\lambda + \mu + 1) r^7 + \frac{1}{2} (3\lambda\mu + 2\lambda + 2\mu - 1) r^8 \\
J D_r^3 D_s^3 &= 864(\lambda + \mu + 1) r^7 + 6912(3\lambda\mu + 2(\lambda + \mu) - 1) r^8 \\
Q_{-2} J D_r^3 D_s^3 &= 864(\lambda + \mu + 1) r^5 + 6912(3\lambda\mu + 2(\lambda + \mu) - 1) r^6 \\
S_r^3 Q_{-2} J D_r^3 D_s^3 &= \frac{864}{125} (\lambda + \mu + 1) r^7 + 32(3\lambda\mu + 2(\lambda + \mu) - 1) r^8. \\
J D_r D_s &= 24(\lambda + \mu + 1) r^7 + 48(3\lambda\mu + 2(\lambda + \mu) - 1) r^8.
\end{aligned}$$

Now we are ready to give some indices by using Tab. 1.

- (1) $M_1(\Psi_{p1}(\lambda, \mu)) = 96\lambda\mu + 92(\lambda + \mu) - 4$
- (2) $M_2(\Psi_{p1}(\lambda, \mu)) = 144\lambda\mu + 120(\lambda + \mu) - 24$
- (3) ${}^a M_2(\Psi_{p1}(\lambda, \mu)) = \frac{1}{3} [3\lambda\mu + 4(\lambda + \mu) + 1]$
- (4) $SDD(\Psi_{p1}(\lambda, \mu)) = \frac{2}{3} [60\lambda\mu + 77(\lambda + \mu) + 17]$
- (5) $ISI(\Psi_{p1}(\lambda, \mu)) = \frac{6}{7} [21\lambda\mu + 18(\lambda + \mu) - 3]$
- (6) $R_\alpha(\Psi_{p1}(\lambda, \mu)) = 12^{\alpha+1}(\lambda\mu) + [6^\alpha(4) + 12^\alpha(8)](\lambda + \mu) + 6^\alpha(4) - 12^\alpha(4)$
- (7) $RR_\alpha(\Psi_{p1}(\lambda, \mu)) = \frac{\lambda\mu}{12^{\alpha-1}} + (\frac{4}{6^\alpha} + \frac{8}{12^\alpha})(\lambda + \mu) + \frac{4}{6^\alpha} - \frac{4}{12^\alpha}$
- (8) $H(\Psi_{p1}(\lambda, \mu)) = \frac{1}{7} [21\lambda\mu + 22(\lambda + \mu) + 1]$
- (9) $AZI(\Psi_{p1}(\lambda, \mu)) = \frac{32}{125} [375\lambda\mu + 277\lambda + 277\mu - 98].$

The followings two theorems can be obtained similarly, so we omit their proofs.

Theorem 2.4: *Let $\Psi_{h1}(\lambda)$ be a MX_3 with a type 1 hexagonal shaped. Then*

- (1) $M_1(\Psi_{h1}(\lambda)) = 288\lambda^2 - 12\lambda$
- (2) $M_2(\Psi_{h1}(\lambda)) = 432\lambda^2 - 72\lambda$
- (3) ${}^a M_2(\Psi_{h1}(\lambda)) = 3\lambda^2 + \lambda$
- (4) $SDD(\Psi_{h1}(\lambda)) = 120\lambda^2 + 34\lambda$
- (5) $ISI(\Psi_{h1}(\lambda)) = 54\lambda^2 - \frac{54}{7}\lambda$
- (6) $R_\alpha(\Psi_{h1}(\lambda)) = 12^{\alpha+1}(3\lambda^2 - \lambda) + 6^{\alpha+1}(2\lambda)$
- (7) $RR_\alpha(\Psi_{h1}(\lambda)) = \frac{2\lambda}{6^{\alpha-1}} + \frac{3\lambda^2 - \lambda}{12^{\alpha-1}}$

- (8) $H(\Psi_{h1}(\lambda)) = 9\lambda^2 + \frac{3}{7}\lambda$
 (9) $AZI(\Psi_{h1}(\lambda)) = 288\lambda^2 - \frac{9408}{125}\lambda.$

Theorem 2.5: *5Let $\Psi_{h1}(\lambda)$ be a MX_3 with a type 1 triangle shaped. Then*

- (1) $M_1(\Psi_{t1}(\lambda)) = 48\lambda^2 + 186\lambda + 42$
 (2) $M_2(\Psi_{t1}(\lambda)) = 72\lambda^2 + 252\lambda + 36$
 (3) $^aM_2(\Psi_{t1}(\lambda)) = \frac{1}{2}\lambda^2 + \frac{5}{2}\lambda + 1$
 (4) $SDD(\Psi_{t1}(\lambda)) = 20\lambda^2 + 97\lambda + 37$
 (5) $ISI(\Psi_{t1}(\lambda)) = 9\lambda^2 + \frac{225}{7}\lambda + \frac{36}{7}$
 (6) $R_\alpha(\Psi_{t1}(\lambda)) = 6^{\alpha+1}(\lambda + 1) + 12^\alpha(6\lambda^2 + 18\lambda)$
 (7) $RR_\alpha(\Psi_{t1}(\lambda)) = \frac{\lambda+1}{6^{\alpha-1}} + \frac{6\lambda^2+18\lambda}{12^\alpha}$
 (8) $H(\Psi_{t1}(\lambda)) = \frac{3}{2}\lambda^2 + \frac{87}{14}\lambda + \frac{12}{7}$
 (9) $AZI(\Psi_{t1}(\lambda)) = 48\lambda^2 + \frac{19296}{125}\lambda + \frac{1296}{125}.$

2.2 DBTIs related with type 2 shape

Theorem 2.6: *6Let $\Psi_{p2}(\lambda, \mu)$ be a MX_3 with a type 2 parallelogram shaped. Then*

- (1) $M_1(\Psi_{p2}(\lambda, \mu)) = 96\lambda\mu + 92(\lambda + \mu) + 88$
 (2) $M_2(\Psi_{p2}(\lambda, \mu)) = 144\lambda\mu + 120(\lambda + \mu) + 96$
 (3) $^aM_2(\Psi_{p2}(\lambda, \mu)) = \frac{1}{3}[3\lambda\mu + 4(\lambda + \mu) + 5]$
 (4) $SDD(\Psi_{p2}(\lambda, \mu)) = \frac{2}{3}[60\lambda\mu + 77(\lambda + \mu) + 94]$
 (5) $ISI(\Psi_{p2}(\lambda, \mu)) = \frac{6}{7}[21\lambda\mu + 18(\lambda + \mu) + 15]$
 (6) $R_\alpha(\Psi_{p2}(\lambda, \mu)) = 6^\alpha(4)(\lambda + \mu + 2) + 12^\alpha(4)(3\lambda\mu + 2\lambda + 2\mu + 1)$
 (7) $RR_\alpha(\Psi_{p2}(\lambda, \mu)) = \frac{4\lambda+4\mu+8}{6^\alpha} + \frac{12\lambda\mu+8\lambda+8\mu+4}{12^\alpha}$
 (8) $H(\Psi_{p2}(\lambda, \mu)) = \frac{1}{7}[21\lambda\mu + 22(\lambda + \mu) + 23]$
 (9) $AZI(\Psi_{p2}(\lambda, \mu)) = \frac{32}{125}[375\lambda\mu + 277(\lambda + \mu) + 179].$

Proof: From Theorem 2.2, we have

$M_{p2}(r, s) = (4\lambda + 4\mu + 8)rs^2 + (12\lambda\mu + 8\lambda + 8\mu + 4)r^2s^6.$ So, we have the following:

$$\begin{aligned} D_r(M_{p2}(r, s)) &= (4\lambda + 4\mu + 8)rs^6 + 8(3\lambda\mu + 2\lambda + 2\mu + 1)r^2s^6 \\ D_s(M_{p2}(r, s)) &= 24(\lambda + \mu + 2)rs^6 + 24(3\lambda\mu + 2(\lambda + \mu) + 1)r^2s^6 \\ D_r D_s(M_{p2}(r, s)) &= 24(\lambda + \mu + 2)rs^6 + 48(3\lambda\mu + 2(\lambda + \mu) + 1)r^2s^6 \\ D_r^\alpha(M_{p2}(r, s)) &= (4\lambda + 4\mu + 8)rs^6 + 2^\alpha(4)(3\lambda\mu + 2\lambda + 2\mu + 1)r^2s^6 \end{aligned}$$

$$\begin{aligned}
D_s^\alpha(M_{p_2}(r, s)) &= 6^\alpha(4)(\lambda + \mu + 2)rs^6 + 6^\alpha(4)(3\lambda\mu + 2(\lambda + \mu) + 1)r^2s^6 \\
D_r^\alpha D_s^\alpha(M_{p_2}(r, s)) &= 6^\alpha(4)(\lambda + \mu + 2)rs^6 + 12^\alpha(4)(3\lambda\mu + 2(\lambda + \mu) + 1)r^2s^6 \\
J(M_{p_2}(r, s)) &= (4\lambda + 4\mu + 8)r^7 + 4(3\lambda\mu + 2(\lambda + \mu) + 1)r^8
\end{aligned}$$

$$\text{Now } Q_\beta = r^\beta M_{p_2}(r, s)$$

$$Q_{-2} = r^{-2}M_{p_2}(r, s) = 4(\lambda + \mu + 2)r^{-1}s^6 + 4(3\lambda\mu + 2(\lambda + \mu) + 1)s^6.$$

$$S_r = \int \frac{M_{p_2}(r, s)}{r} dr = 4(\lambda + \mu + 2)rs^6 + 2(3\lambda\mu + 2(\lambda + \mu) + 1)r^2s^6$$

$$S_s = \int \frac{M_{p_2}(r, s)ds}{s} = \frac{2}{3}(\lambda + \mu + 2)rs^6 + \frac{2}{3}(3\lambda\mu + 2(\lambda + \mu) + 1)r^2s^6$$

$$S_r S_s = \frac{2}{3}(\lambda + \mu + 2)rs^6 + \frac{4}{3}(3\lambda\mu + 2(\lambda + \mu) + 1)r^2s^6$$

$$S_r^\alpha = 4(\lambda + \mu + 2)rs^6 + \frac{4(3\lambda\mu + 2(\lambda + \mu) + 1)}{2^\alpha}r^2s^6$$

$$S_s^\alpha = \frac{4(\lambda + \mu + 2)}{6^\alpha}rs^6 + \frac{4(3\lambda\mu + 2(\lambda + \mu) + 1)}{6^\alpha}r^2s^6$$

$$S_r^\alpha S_s^\alpha = \frac{4(\lambda + \mu + 2)}{6^\alpha}rs^6 + \frac{4(3\lambda\mu + 2(\lambda + \mu) + 1)}{12^\alpha}r^2s^6$$

$$D_r S_s = \frac{2}{3}(\lambda + \mu + 2)rs^6 + \frac{4}{3}(3\lambda\mu + 2(\lambda + \mu) + 1)r^2s^6$$

$$D_s S_r = 24(\lambda + \mu + 2)rs^6 + 12(3\lambda\mu + 2(\lambda + \mu) + 1)r^2s^6$$

$$S_r J(M_{p_2}(r, s)) = \frac{4}{7}(\lambda + \mu + 2)r^7 + \frac{1}{2}(3\lambda\mu + 2(\lambda + \mu) + 1)r^8$$

$$J D_r^3 D_s^3 = 864(\lambda + \mu + 2)r^7 + 6912(3\lambda\mu + 2(\lambda + \mu) + 1)r^8$$

$$Q_{-2} J D_r^3 D_s^3 = 864(\lambda + \mu + 2)r^5 + 6912(3\lambda\mu + 2(\lambda + \mu) + 1)r^6$$

$$S_r^3 Q_{-2} J D_r^3 D_s^3 = \frac{864}{125}(\lambda + \mu + 2)r^7 + 32(3\lambda\mu + 2(\lambda + \mu) + 1)r^8$$

$$J D_r D_s = 24(\lambda + \mu + 2)r^7 + 48(3\lambda\mu + 2(\lambda + \mu) + 1)r^8.$$

Now we are ready to given the general formula for some indices by using Table 1.

- (1) $M_1(\Psi_{p_2}(\lambda, \mu)) = 96\lambda\mu + 92(\lambda + \mu) + 88$
- (2) $M_2(\Psi_{p_2}(\lambda, \mu)) = 144\lambda\mu + 120\lambda + 120\mu + 96$
- (3) ${}^a M_2(\Psi_{p_2}(\lambda, \mu)) = \frac{1}{3}[3\lambda\mu + 4(\lambda + \mu) + 5]$
- (4) $SDD(\Psi_{p_2}(\lambda, \mu)) = \frac{2}{3}[60\lambda\mu + 77(\lambda + \mu) + 94]$
- (5) $ISI(\Psi_{p_2}(\lambda, \mu)) = \frac{6}{7}[21\lambda\mu + 18(\lambda + \mu) + 15]$
- (6) $R_\alpha(\Psi_{p_2}(\lambda, \mu)) = 6^\alpha(4\lambda + 4\mu + 8) + 12^\alpha(12\lambda\mu + 8\lambda + 8\mu + 4)$
- (7) $RR_\alpha(\Psi_{p_2}(\lambda, \mu)) = \frac{4\lambda + 4\mu + 8}{6^\alpha} + \frac{12\lambda\mu + 8\lambda + 8\mu + 4}{12^\alpha}$
- (8) $H(\Psi_{p_2}(\lambda, \mu)) = \frac{1}{7}[21\lambda\mu + 22(\lambda + \mu) + 23]$
- (9) $AZI(\Psi_{p_2}(\lambda, \mu)) = \frac{32}{125}[375\lambda\mu + 277\lambda + 277\mu + 179].$

Similarly, we can obtained the following theorems.

Theorem 2.7: *Let $\Psi_{h2}(\lambda)$ be a MX_3 with a type 2 hexagonal shaped. Then*

- (1) $M_1(\Psi_{h2}(\lambda)) = 288\lambda^2 + 80\lambda$
- (2) $M_2(\Psi_{h2}(\lambda)) = 432\lambda^2 + 48\lambda$
- (3) $^aM_2(\Psi_{h2}(\lambda)) = 3\lambda^2 + \frac{7}{3}\lambda$
- (4) $SDD(\Psi_{h2}(\lambda)) = 120\lambda^2 + \frac{256}{3}\lambda$
- (5) $ISI(\Psi_{h2}(\lambda)) = 54\lambda^2 + \frac{54}{7}\lambda$
- (6) $R_\alpha(\Psi_{h2}(\lambda)) = 12^{\alpha+1}(36\lambda^2 - 4\lambda) + 6^{\alpha+1}(16\lambda)$
- (7) $RR_\alpha(\Psi_{h2}(\lambda)) = \frac{16\lambda}{6^\alpha} + \frac{36\lambda^2 - 4\lambda}{12^\alpha}$
- (8) $H(\Psi_{h2}(\lambda)) = 9\lambda^2 + \frac{25}{7}\lambda$
- (9) $AZI(\Psi_{h2}(\lambda)) = 288\lambda^2 - \frac{544}{125}\lambda.$

Theorem 2.8: *Let $\Psi_{t2}(\lambda)$ be a MX_3 with a type 2 triangle shaped. Then*

- (1) $M_1(\Psi_{t2}(\lambda)) = 48\lambda^2 + 232\lambda + 88$
- (2) $M_2(\Psi_{t2}(\lambda)) = 72\lambda^2 + 312\lambda + 96$
- (3) $^aM_2(\Psi_{t2}(\lambda)) = \frac{1}{2}\lambda^2 + \frac{19}{6}\lambda + \frac{5}{3}$
- (4) $SDD(\Psi_{t2}(\lambda)) = 20\lambda^2 + \frac{368}{3}\lambda + \frac{188}{3}$
- (5) $ISIG_{t2}(\lambda) = 9\lambda^2 + \frac{279}{7}\lambda + \frac{90}{7}$
- (6) $R_\alpha(\Psi_{t2}(\lambda)) = 6^\alpha(8\lambda + 8) + 12^\alpha(6\lambda^2 + 22\lambda + 4)$
- (7) $RR_\alpha(\Psi_{t2}(\lambda)) = \frac{8\lambda+8}{6^\alpha} + \frac{6\lambda^2+22\lambda+4}{12^\alpha}$
- (8) $H(\Psi_{t2}(\lambda)) = \frac{3}{2}\lambda^2 + \frac{109}{14}\lambda + \frac{23}{7}$
- (9) $AZI(\Psi_{t2}(\lambda)) = 48\lambda^2 + \frac{23728}{125}\lambda + \frac{5728}{125}.$

3. Numerical and graphical comparison

In this section, we will give numerical and graphical comparison of the these computed indices through M -polynomial with respect to two kind of MX_3 . Origin pro is used to construct a comparison of these indices related to the aforementioned MX_3 into 2D charts plots as shown in Fig. 5. The numerical comparison is given in Tables (2- 7). The final outcome of these charts and tables is that the second Zagreb index is always greater than other indices.

Table 2
Numerical Comparison of indices for type 1 parallelogram

(m, n)	M_1	M_2	$^aM_2$	SDD	ISI	H	AZI
(4,4)	2268	3240	27	1062	408.86	73.29	2078.2
(4,5)	2744	3936	32.33	1273	496.29	88.43	2533.1
(4,6)	3220	4632	37.67	1485	583.71	103.57	2988
(4,7)	3696	5328	43	1696	671.14	118.71	3442.9
(4,8)	4172	6024	48.33	1907	758.57	133.86	3897.9
(4,9)	4648	6720	53.67	2119	846	149	4352.8
(4,10)	5124	7416	59	2330	933.43	164.14	4807.7
(8,9)	8472	12384	95	3764	1555.71	269.57	8092.4
(8,10)	9332	13656	104.33	4135	1715.14	296.71	8931.3
(8,11)	10192	14928	113.67	4507	1874.57	323.86	9770.2

Table 3
Numerical Comparison of indices for type 2 parallelogram

(m, n)	M_1	M_2	$^aM_2$	SDD	ISI	H	AZI
(4,4)	2360	3360	28.33	1113.33	424.29	76.43	2149.12
(4,5)	2836	4056	33.67	1324.67	511.71	91.57	2604.03
(4,6)	3312	4752	39	1536	599.14	106.71	3058.94
(4,7)	3788	5448	44.33	1747.33	686.57	121.86	3513.86
(4,8)	4264	6144	49.67	1958.67	774	137	3968.77
(4,9)	4740	6840	55	2170	861.43	152.14	4423.68
(4,10)	5216	7536	60.33	2381.33	948.86	167.29	4878.59
(8,9)	8564	12504	96.33	3815.33	1571.14	272.71	8163.33
(8,10)	9424	13776	105.67	4186.67	1730.57	299.86	9002.24
(8,11)	10284	15048	115	4558	1890	327	9841.15

Table 4
Numerical Comparison of indices for type 1 hexagonal

m	M_1	M_2	$^aM_2$	SDD	ISI	H	AZI
4	4560	6624	52	2056	833.14	145.71	4306.94
5	7140	10440	80	3170	1311.43	227.14	6823.68
6	10296	15120	114	4524	1897.72	326.57	9916.42
7	14028	20664	154	6118	2592	444	13585.15
8	18336	27072	200	7952	3394.26	579.43	17829.89
9	23220	34344	252	10026	4304.57	732.86	22650.62
10	28680	42480	310	12340	5322.86	904.29	28047.36
11	34716	51480	374	14894	6449.14	1093.71	34020.10
12	41328	61344	444	17688	7683.43	1301.14	40568.83
13	48516	72072	520	20722	9025.71	1526.57	47693.57

Table 5
Numerical Comparison of indices for type 2 hexagonal

m	M_1	M_2	$^aM_2$	SDD	ISI	H	AZI
4	4928	7104	57.33	2261.33	894.86	158.29	4590.59
5	7600	11040	86.67	3426.6	1388.57	242.86	7178.24
6	10848	15840	122	4832	1990.29	345.43	10341.89
7	14672	21504	163.33	6477.33	2700	466	14081.54
8	19072	28032	210.67	8362.67	3517.71	604.57	18397.18
9	24048	35424	264	10488	4443.43	761.14	23288.83
10	29600	43680	323.33	12853.33	5477.14	935.71	28756.48
11	35728	52800	388.67	15458.67	6618.86	1128.29	34800.13
12	42432	62784	460	18304	7868.57	1338.86	41419.78
13	49712	73632	537.33	21389.33	9226.23	1567.43	48615.42

Table 6
Numerical Comparison of indices for type 1 triangle

m	M_1	M_2	$^aM_2$	SDD	ISI	H	AZI
4	1554	2196	19	745	277.71	50.57	1395.84
5	2172	3096	26	1022	390.86	70.29	1982.29
6	2886	4140	34	1339	522	93	2664.58
7	3696	5328	43	1696	671.14	118.71	3442.94
8	4602	6660	53	2093	838.29	147.43	4317.31
9	5604	8136	64	2530	1023.43	179.14	5287.68
10	6702	9756	76	3007	1226.57	213.86	6354.05
11	7896	11520	89	3524	1447.71	251.57	7516.42
12	9186	13428	103	4081	1686.86	292.29	8774.78
13	10572	15480	118	4678	1944	336	10129.15

Table 7
Numerical Comparison of indices for type 2 triangle

m	M_1	M_2	$^aM_2$	SDD	ISI	H	AZI
4	1784	2496	22.33	873.33	316.29	58.43	1573.12
5	2448	3456	30	1176	437.14	79.71	2194.94
6	3208	4560	38.67	1518.67	576	104	2912.77
7	4064	5808	48.33	1901.33	732.86	131.29	3726.59
8	5016	7200	59	2324	907.71	161.57	4636.42
9	6064	8736	70.67	2786.67	1100.57	194.86	5642.24
10	7208	10416	83.33	3289.33	1311.43	231.14	6744.06
11	8448	12240	97	3832	1540.29	270.43	7941.89
12	9784	14208	111.67	4414.67	1787.14	312.71	9235.71
13	11216	16320	127.33	5037.33	2052	358	10625.54

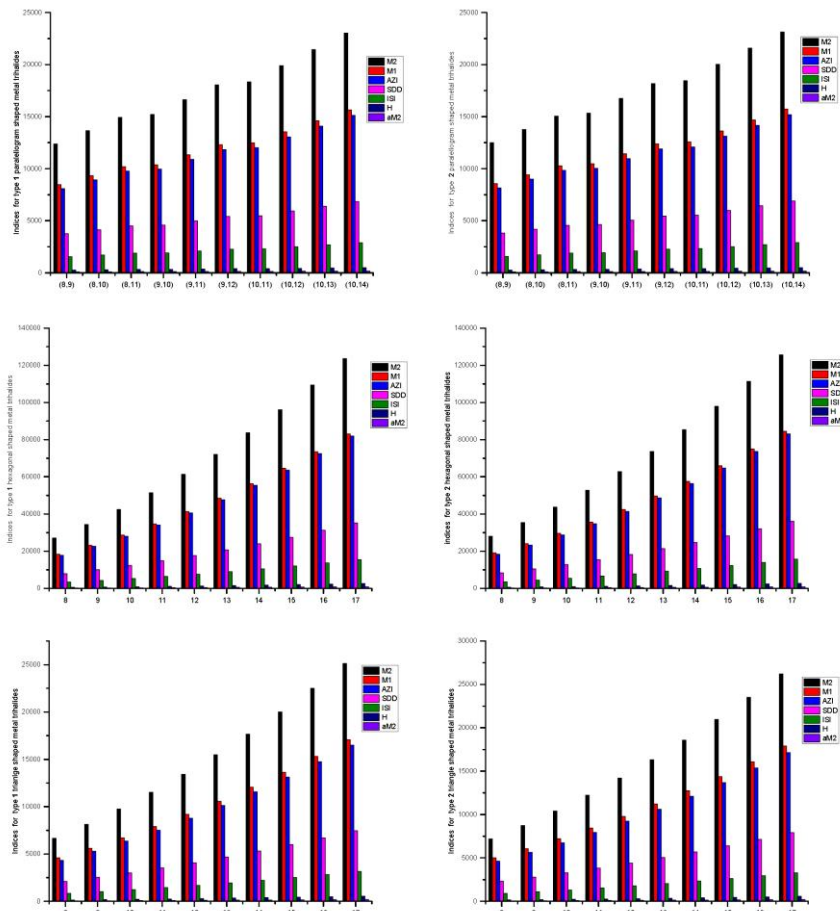


Figure 5
Comparison of indices for type 1 and 2 MX_3 .

4. Conclusion

The development of 2D novel MX_3 has revealed Dirac half-metallicity with topological spintronic properties, largely due to the intrinsic magnetic processes associated with 2D MX_3 . Additionally, the effects of orbital pair interactions contribute to significant spin-orbit coupling. As a result of this spin-orbit coupling combined with strong forces and high Curie temperatures, 2D materials like BiI_3 find important applications in room temperature radiation detectors, which exhibit unusual band gaps. The M-polynomial provides accurate and effective results for the topological indices of corresponding chemical compounds, which can then be used to correlate these compounds with their chemical properties and biological activities. The primary objective of this study is to compute and compare the M-polynomial for two types of MX_3 . This general

form is then employed to determine the degree-based topological indices of these MX_3 . A detailed graphical comparison of the M-polynomials and the topological indices of the MX_3 is provided. In particular, a comparison of the degree-based indices is conducted using 2D chart plots and numerical tables.

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