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Algebraic Properties for Molecular Structure of Magnesium Iodide

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ABSTRACT

As an inorganic chemical, magnesium iodide has a significant crystalline structure. It is a complex and multi-functional substance that has the potential to be used in a wide range of medical advancements. Molecular graph theory, on the other hand, provides a sufficient and cost-effective method of investigating chemical structures and networks. M-polynomial is a relatively new method for studying chemical networks and structures in molecular graph theory. It displays numerical descriptors in algebraic form and highlights molecular features in the form of a polynomial function. We present a polynomials display of magnesium iodide structure and calculate several M-polynomials in this paper, particularly the M-polynomials of the augmented Zagreb index, inverse sum index, hyper Zagreb index and for the symmetric division index.

1 Introduction

The chemical formula MX_2 is referred to a chemical compound named magnesium iodide. It has numerous commercial uses and is also valuable to get different organic synthesis, noted that MX_2 or magnesium iodide is an inorganic compound. Nanopowder, submicron, high impurity and volumes are the availability measures of MX_2. It is a very useful asset in internal medicine. Magnesium iodide may be produced by reacting hydro-iodic acid with magnesium carbonate, magnesium hydroxide, and magnesium oxide. Magnesium iodide is made up of a unique C_4-graph pattern, according to molecular graph theory. Multiple heptagons are connected to each other, having each C_4-graph inside [1]. For a better understanding of the magnesium iodide molecular graph, we labeled the parameters as follows: m is the number of C_4's of upper sides in a row, and n is the number of lower side $C4$ in heptagons. The magnesium iodide graph is required to preserve the relationship of m for even and odd values of

separately with the relation of $m = 2\,(n+1)$, and $m = 2n+1$, respectively, for all values of $n \in \mathbb{Z}$ with $n \geq 1$.

In this article, we studied some M-polynomials of magnesium iodide structure for both cases of m. The studied M-polynomials are defined below in Definitions 1.1 to 1.5, with their other fundamentals. Moreover, for a graph χ and their polynomial parameters are $\mathfrak{x}$, $\mathfrak{y}$, while $\xi_\mathfrak{a}$ is the degree of a vertex $\mathfrak{a}$ and defined by the counting of edges attached to a vertex $\mathfrak{a}$.

Definition 1.1. The most famous and first, Hosoya polynomials were introduced by [2] in 1988, and in 2015, Modified-polynomial, also known as M-polynomial, is introduced by [3]. This form of the polynomial has a closed relationship to degree-based topological indices. Topological indices from M-polynomials of a graph may be obtained using a specific format. This M-polynomial may be defined as follows:

$$M\,(\chi;\mathfrak{x},\mathfrak{y}) = \sum_{i \leq j} m_{i,j}\,(\chi)\,\mathfrak{x}^i \mathfrak{y}^j, \tag{1}$$

where $m_{i,j}\,(\chi)$ is the number of edges of graph χ such that $i \leq j$, are the notation of degrees of a vertex.

Definition 1.2. The symmetric division index SDI of a graph χ was introduced by [4] in 2010. Following are the symmetric division index and its M-polynomials.

$$SDI\,(\chi) = \sum_{\mathfrak{ab} \in E(\chi)} \frac{\xi_\mathfrak{a}^2 + \xi_\mathfrak{b}^2}{\xi_\mathfrak{a} \times \xi_\mathfrak{b}}, \tag{2}$$

$$P_{SDI}(\chi) = \left(D_\mathfrak{x} S_\mathfrak{y} + D_\mathfrak{y} S_\mathfrak{x}\right) (M\,(\chi;\mathfrak{x},\mathfrak{y})), \tag{3}$$

where $D_\mathfrak{x}$, $D_\mathfrak{y}$, $S_\mathfrak{y}$, $S_\mathfrak{x}$ are differential and integral operators defined in the Eqs. (10) to (15).

Definition 1.3. Shirdel et al. [5,6] introduced hyper Zagreb index, and given below are topological descriptor and its M-polynomial.

$$HM\,(\chi) = \sum_{\mathfrak{ab} \in E(\chi)} [\xi_\mathfrak{a} + \xi_\mathfrak{b}]^2, \tag{4}$$

$$P_{HM}(\chi) = 2S_\mathfrak{x} J\,(M\,(\chi;\mathfrak{x},\mathfrak{y})). \tag{5}$$

Definition 1.4. Inverse sum index introduced by [7], and its M-polynomials [8], given below are formulations of its indices and M-polynomial.

$$IS\,(\chi) = \sum_{\mathfrak{ab} \in E(\chi)} \frac{\xi_\mathfrak{a} \xi_\mathfrak{b}}{\xi_\mathfrak{a} + \times \xi_\mathfrak{b}}, \tag{6}$$

$$P_{IS}(\chi) = S_\mathfrak{x} J D_\mathfrak{x} D_\mathfrak{y}\,(M\,(\chi;\mathfrak{x},\mathfrak{y})). \tag{7}$$

Definition 1.5. Furtula et al. [9] defined augmented Zagreb index and given below are formulation of index and its M-polynomial.

$$AZI\,(\chi) = \sum_{\mathfrak{ab} \in E(\chi)} \left(\frac{\xi_\mathfrak{a} \times \xi_\mathfrak{b}}{\xi_\mathfrak{a} + \xi_\mathfrak{b} - 2}\right)^3, \tag{8}$$

$$P_{AZI}(\chi) = S_\mathfrak{x}^3 Q_{-2} J D_\mathfrak{x}^3 D_\mathfrak{y}^3\,(M\,(\chi;\mathfrak{x},\mathfrak{y})). \tag{9}$$

where

$$D_{\mathfrak{x}}\left(f\left(\mathfrak{x}, \mathfrak{y}\right)\right) \quad = \mathfrak{x}\frac{\partial f\left(\mathfrak{x}, \mathfrak{y}\right)}{\partial \mathfrak{x}}, \tag{10}$$

$$D_{\mathfrak{y}}\left(f\left(\mathfrak{x}, \mathfrak{y}\right)\right) = \mathfrak{x}\frac{\partial f\left(\mathfrak{x}, \mathfrak{y}\right)}{\partial \mathfrak{y}}, \tag{11}$$

$$S_{\mathfrak{x}}\left(f\left(\mathfrak{x}, \mathfrak{y}\right)\right) = \int_{0}^{\mathfrak{x}}\frac{f\left(z, \mathfrak{y}\right)}{z}dz, \tag{12}$$

$$S_{\mathfrak{y}}\left(f\left(\mathfrak{x}, \mathfrak{y}\right)\right) = \int_{0}^{\mathfrak{y}}\frac{f\left(\mathfrak{x}, z\right)}{z}dz, \tag{13}$$

$$J\left(f\left(\mathfrak{x}, \mathfrak{y}\right)\right) = f\left(\mathfrak{x}, \mathfrak{x}\right), \tag{14}$$

$$Q_{a}\left(f\left(\mathfrak{x}, \mathfrak{y}\right)\right) = \mathfrak{x}^{a}f\left(\mathfrak{x}, \mathfrak{y}\right). \tag{15}$$

The researchers in [3] introduced the concept, in combination with numerical descriptors (known as topological indices [10–13]), an algebraic graph theory. The concept is known as the M-polynomials of the graph. It has fundamentals from topological indices. For some basic and important topological indices, we refer to see the articles [14–17]. This subject has been extensively researched in the last half-decade, and there is a wealth of material accessible. We will review a few of the most current papers on this topic.

The study of M-polynomials on nanotubes are available for h-naphthenic nanotube [18], various nanostructures studied in [19], and VC_5C_7-type of nanotubes are discussed in [20]. Generalized classes and families of the graph are studied with different M-polynomials in [15,21,22], various benzenoid structures are showcased in [23], M-polynomials interaction with statistics probability concept are available in [24]. Metal organic chemical network's M-polynomials are studied in [25,26]. M-polynomials concept is also studied for various computer related networks and found in [27,28].

The M-polynomials are figured out for the magnesium iodide or MX_2 structure for both even and odd cases of parameter m, and such M-polynomials named of augmented Zagreb index, inverse sum index, hyper Zagreb index and the symmetric division index.

2 Results on the M-Polynomials of Magnesium Iodide

Given in this section are some important results of this research work. The idea totally depends on the structural values of the MX_2 or magnesium iodide graph, which is defined in Table 1 (for $m = odd$) and Table 2 (for $n = even$).

Table 1: Edge partition of $I(m, n)$ $m = 2n + 1$

(ξ_a, ξ_b)	Frequency	Set of edges
$(1, 3)$	1	E_1
$(1, 4)$	1	E_2
$(1, 6)$	$n + 5$	E_3
$(2, 3)$	2	E_4
$(2, 4)$	2	E_5

(Continued)

Table 1 (continued)

(ξ_a, ξ_b)	Frequency	Set of edges
$(2,5)$	8	E_6
$(2,6)$	$2n+8$	E_7
$(3,3)$	$3n$	E_8
$(3,4)$	1	E_9
$(3,5)$	12	E_{10}
$(3,6)$	$27n-13$	E_{11}

Case 1: For the odd values of m with given $n \geq 1$. Let $m = 2n+1$ and $n \in \mathbb{Z}$.

Theorem 2.1. Let $I_{m,n}$ be a magnesium iodide graph, with $m = 2n+1$, $n \geq 1$, shown in Fig. 1. Then, its M-polynomial is

$$M\left(I_{m,n}, \mathfrak{x}, \mathfrak{y}\right) = \mathfrak{x}\left[\mathfrak{y}^3 + \mathfrak{y}^4 + (n+5)\,\mathfrak{y}^6\right] + 2\mathfrak{x}^2\left[\mathfrak{y}^3 + \mathfrak{y}^4 + 4\mathfrak{y}^5 + (n+4)\,\mathfrak{y}^6\right] + \mathfrak{x}^3\left[3n\mathfrak{y}^3 + \mathfrak{y}^4 + 12\mathfrak{y}^5 + (27n-13)\,\mathfrak{y}^6\right]. \tag{16}$$
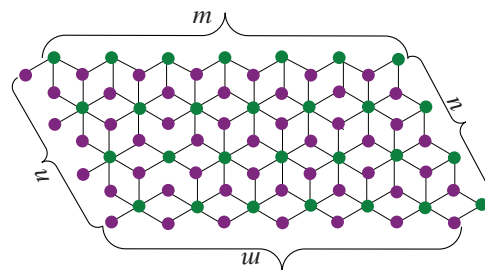

Figure 1: Magnesium iodide graph for $n = 4$ and $m = 7$

Proof. The construction of magnesium iodide graph from its structure, which is found in Fig. 1. It has six type of vertices, evaluated from the figure and these vertices are described in the vertex set as:

$$\vee_1 = \left\{a \in V\left(I_{m,n}\right) : \xi_a = 1\right\}, \quad \vee_2 = \left\{a \in V\left(I_{m,n}\right) : \xi_a = 2\right\}$$
$$\vee_3 = \left\{a \in V\left(I_{m,n}\right) : \xi_a = 3\right\}, \quad \vee_4 = \left\{a \in V\left(I_{m,n}\right) : \xi_a = 4\right\}$$
$$\vee_5 = \left\{a \in V\left(I_{m,n}\right) : \xi_a = 5\right\}, \quad \vee_6 = \left\{a \in V\left(I_{m,n}\right) : \xi_a = 6\right\}.$$

The same figure also shows the information of its edge types. It contains eleven types of edges in total and these are described as:

$$\Xi_{1,3} = \left\{ab \in E(I_{m,n}) : \xi_a = 1, \xi_b = 3\right\}, \quad \Xi_{1,4} = \left\{ab \in E(I_{m,n}) : \xi_a = 1, \xi_b = 4\right\}$$
$$\Xi_{1,6} = \left\{ab \in E(I_{m,n}) : \xi_a = 1, \xi_b = 6\right\}, \quad \Xi_{2,3} = \left\{ab \in E(I_{m,n}) : \xi_a = 2, \xi_b = 3\right\}$$
$$\Xi_{2,4} = \left\{ab \in E(I_{m,n}) : \xi_a = 2, \xi_b = 4\right\}, \quad \Xi_{2,5} = \left\{ab \in E(I_{m,n}) : \xi_a = 2, \xi_b = 5\right\}$$
$$\Xi_{2,6} = \left\{ab \in E(I_{m,n}) : \xi_a = 2, \xi_b = 6\right\}, \quad \Xi_{3,3} = \left\{ab \in E(I_{m,n}) : \xi_a = 3, \xi_b = 3\right\}$$
$$\Xi_{3,4} = \left\{ab \in E(I_{m,n}) : \xi_a = 3, \xi_b = 4\right\}, \quad \Xi_{3,5} = \left\{ab \in E(I_{m,n}) : \xi_a = 3, \xi_b = 5\right\}$$
$$\Xi_{3,6} = \left\{ab \in E(I_{m,n}) : \xi_a = 3, \xi_b = 6\right\}.$$

The cardinality of these edge partitions are $\left|\Xi_{1,3}\right| = \left|\Xi_{1,4}\right| = \left|\Xi_{3,4}\right| = 1, \left|\Xi_{2,3}\right| = \left|\Xi_{2,4}\right| = 2, \left|\Xi_{1,6}\right| = n + 5, \left|\Xi_{2,5}\right| = 8, \left|\Xi_{2,6}\right| = 2(n+4), \left|\Xi_{3,3}\right| = 3n, \left|\Xi_{3,5}\right| = 12$, and $\left|\Xi_{3,6}\right| = 27n - 13$. Then from the Definition 1.1, the M-polynomial of $I_{m,n}$ is

$$M\left(I_{m,n}; \mathfrak{x}, \mathfrak{y}\right) = \sum_{i \leq j} m_{i,j}\left(I_{m,n}\right) \mathfrak{x}^i \mathfrak{y}^j$$

$$= \left|\Xi_{1,3}\right|\left(I_{m,n}\right) x^1 y^3 + \left|\Xi_{1,4}\right|\left(I_{m,n}\right) x^1 y^4 + \left|\Xi_{1,6}\right|\left(I_{m,n}\right) x^1 y^6$$

$$+ \left|\Xi_{2,3}\right|\left(I_{m,n}\right) x^2 y^3 + \left|\Xi_{2,4}\right|\left(I_{m,n}\right) x^2 y^4 + \left|\Xi_{2,5}\right|\left(I_{m,n}\right) x^2 y^5$$

$$+ \left|\Xi_{2,6}\right|\left(I_{m,n}\right) x^2 y^6 + \left|\Xi_{3,3}\right|\left(I_{m,n}\right) x^3 y^3 + \left|\Xi_{3,4}\right|\left(I_{m,n}\right) x^3 y^4$$

$$+ \left|\Xi_{3,5}\right|\left(I_{m,n}\right) x^3 y^5 + \left|\Xi_{3,6}\right|\left(I_{m,n}\right) x^3 y^6,$$

$$= \mathfrak{x}\left[\mathfrak{y}^3 + \mathfrak{y}^4 + (n+5)\mathfrak{y}^6\right] + 2\mathfrak{x}^2\left[\mathfrak{y}^3 + \mathfrak{y}^4 + 4\mathfrak{y}^5 + (n+4)\mathfrak{y}^6\right]$$

$$+ \mathfrak{x}^3\left[3n\mathfrak{y}^3 + \mathfrak{y}^4 + 12\mathfrak{y}^5 + (27n - 13)\mathfrak{y}^6\right]. \tag{17}$$

The 3D plot shown in the Fig. 2, is the general M-polynomial of magnesium iodide graph, for a particular value with $n = 7$ and $m = 15$.
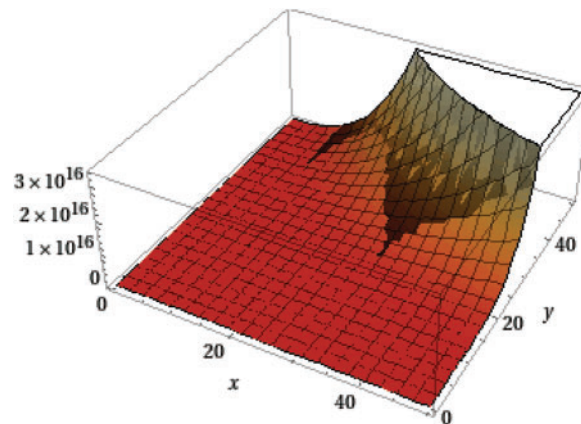

Figure 2: Graphical plot of M-polynomial of magnesium iodide graph

Lemma 2.1. Let $I_{m,n}$ be a magnesium iodide graph, with $m = 2n + 1, n \geq 1$, Then the differential operators are

$$D_{\mathfrak{x}}\left[M\left(I_{m,n}; \mathfrak{x}, \mathfrak{y}\right)\right] = \mathfrak{x}\left[\mathfrak{y}^3 + \mathfrak{y}^4 + (n+5)\mathfrak{y}^6\right] + 4\mathfrak{x}^2\left[\mathfrak{y}^3 + \mathfrak{y}^4 + 4\mathfrak{y}^5 + (n+4)\mathfrak{y}^6\right]$$

$$+ 3\mathfrak{x}^3\left[3n\mathfrak{y}^3 + \mathfrak{y}^4 + 12\mathfrak{y}^5 + (27n - 13)\mathfrak{y}^6\right]. \tag{18}$$

$$D_{\mathfrak{y}}\left[M\left(I_{m,n}; \mathfrak{x}, \mathfrak{y}\right)\right] = \mathfrak{x}\left[3\mathfrak{y}^3 + 4\mathfrak{y}^4 + 6(n+5)\mathfrak{y}^6\right] + 2\mathfrak{x}^2\left[3\mathfrak{y}^3 + 4\mathfrak{y}^4 + 20\mathfrak{y}^5 + 3(2n+8)\mathfrak{y}^6\right]$$

$$+ \mathfrak{x}^3\left[9n\mathfrak{y}^3 + 4\mathfrak{y}^4 + 60\mathfrak{y}^5 + 6(27n - 13)\mathfrak{y}^6\right]. \tag{19}$$

Proof. Differentiate Eq. (16) with respect to $\mathfrak{x}$ and multiply the result with $\mathfrak{x}$, we get the $D_{\mathfrak{x}}\left[M\left(I_{m,n}; \mathfrak{x}, \mathfrak{y}\right)\right]$. Similarly, differentiate Eq. (16) with respect to $\mathfrak{y}$ and multiply the result with $\mathfrak{y}$, we get the $D_{\mathfrak{y}}\left[M\left(I_{m,n}; \mathfrak{x}, \mathfrak{y}\right)\right]$.

Lemma 2.2. Let $I_{m,n}$ be a magnesium iodide graph, with $m = 2n + 1$, $n \geq 1$. Then the integral operators are

$$S_{\mathfrak{x}}\left[M\left(I_{m,n}; \mathfrak{x}, \mathfrak{y}\right)\right] = \mathfrak{x}\left[\mathfrak{y}^3 + \mathfrak{y}^4 + (n + 5)\,\mathfrak{y}^6\right] + \mathfrak{x}^2\left[\mathfrak{y}^3 + \mathfrak{y}^4 + 4\mathfrak{y}^5 + (n + 4)\,\mathfrak{y}^6\right]$$

$$+ \frac{1}{3}\mathfrak{x}^3\left[3n\mathfrak{y}^3 + \mathfrak{y}^4 + 12\mathfrak{y}^5 + (27n - 13)\,\mathfrak{y}^6\right]. \tag{20}$$

$$S_{\mathfrak{y}}\left[M\left(I_{m,n}; \mathfrak{x}, \mathfrak{y}\right)\right] = \mathfrak{x}\left[\frac{1}{3}\mathfrak{y}^3 + \frac{1}{4}\mathfrak{y}^4 + \frac{(n + 5)}{6}\mathfrak{y}^6\right] + \mathfrak{x}^2\left[\frac{2}{3}\mathfrak{y}^3 + \frac{1}{2}\mathfrak{y}^4 + \frac{8}{5}\mathfrak{y}^5 + \frac{(n + 4)}{3}\mathfrak{y}^6\right]$$

$$+ \mathfrak{x}^3\left[n\mathfrak{y}^3 + \frac{1}{4}\mathfrak{y}^4 + \frac{12}{5}\mathfrak{y}^5 + \frac{(27n - 13)}{6}\mathfrak{y}^6\right]. \tag{21}$$

Proof. As we know that from Eq. (12), $S_{\mathfrak{x}}\left[M\left(I_{m,n}; \mathfrak{x}, \mathfrak{y}\right)\right] = \int_0^{\mathfrak{x}} \frac{M(Im,n;t,\mathfrak{y})}{t}dt$ uses the general M-polynomial for the $I_{m,n}$ from Eq. (16) in it. After simplification, we obtain $S_{\mathfrak{x}}\left[M\left(I_{m,n}; \mathfrak{x}, \mathfrak{y}\right)\right]$. Similarly, from Eq. (13), $S_{\mathfrak{y}}\left[M\left(I_{m,n}; \mathfrak{x}, \mathfrak{y}\right)\right] = \int_0^{\mathfrak{y}} \frac{M(Im,n;\mathfrak{x},t)}{t}dt$ uses the general M-polynomial for the $I_{m,n}$ from Eq. (16) in it. After simplification, we obtain $S_{\mathfrak{y}}\left[M\left(I_{m,n}; \mathfrak{x}, \mathfrak{y}\right)\right]$.

Lemma 2.3. Let $I_{m,n}$ be a magnesium iodide graph, with $m = 2n + 1$, $n \geq 1$. Then the Eq. (16) is

$$J\left[M\left(I_{m,n}; \mathfrak{x}, \mathfrak{y}\right)\right] = \mathfrak{x}^4 + 3\mathfrak{x}^5 + (3n + 2)\,\mathfrak{x}^6 + (n + 8)\,\mathfrak{x}^7 + 2\,(n + 10)\,\mathfrak{x}^8 + (27n - 13)\,\mathfrak{x}^9.$$

Proof. By implementing the operator stated in the Eq. (14) on the main equation defined in Eq. (16), we get the $J\left[M\left(I_{m,n}; \mathfrak{x}, \mathfrak{y}\right)\right]$.

Theorem 2.2. Let $I_{m,n}$ be a magnesium iodide graph, with $m = 2n + 1$, $n \geq 1$, and P_{SDI} is the M-polynomial of symmetric division index. Then $P_{SDI}\left(I_{m,n}\right)$ is

$$P_{SDI}\left(I_{m,n}\right) = \mathfrak{x}\left[\frac{10}{3}\mathfrak{y}^3 + \frac{17}{4}\mathfrak{y}^4 + \frac{(41 + n)}{6}\mathfrak{y}^6\right] + \mathfrak{x}^2\left[\frac{13}{3}\mathfrak{y}^3 + 5\mathfrak{y}^4 + \frac{116}{5}\mathfrak{y}^5 + \frac{20\,(n + 4)}{3}\mathfrak{y}^6\right]$$

$$+ \frac{10}{3}\mathfrak{x}^3\left[10n\mathfrak{y}^3 + \frac{17}{4}\mathfrak{y}^4 + \frac{312}{5}\mathfrak{y}^5 + \frac{37\,(27n - 13)}{6}\mathfrak{y}^6\right]. \tag{22}$$

Proof. The M-polynomial of symmetric division index, given in the Definition 1.2, and the formulas for our structure $I_{m,n}$ can be written as: $P_{SDI}(I_{m,n}) = \left(D_{\mathfrak{x}}S_{\mathfrak{y}} + D_{\mathfrak{y}}S_{\mathfrak{x}}\right)(M\left(\chi; \mathfrak{x}, \mathfrak{y}\right))$. Lemmas 2.1 and 2.2 are the operators and here we used these to find our results for $I_{m,n}$. We will obtain the M-polynomial of symmetric division index for $I_{m,n}$ after some algebraic simplifications as

$$P_{SDI}\left(I_{m,n}\right) = \mathfrak{x}\left[\frac{10}{3}\mathfrak{y}^3 + \frac{17}{4}\mathfrak{y}^4 + \frac{(41 + n)}{6}\mathfrak{y}^6\right] + \mathfrak{x}^2\left[\frac{13}{3}\mathfrak{y}^3 + 5\mathfrak{y}^4 + \frac{116}{5}\mathfrak{y}^5 + \frac{20\,(n + 4)}{3}\mathfrak{y}^6\right]$$

$$+ \frac{10}{3}\mathfrak{x}^3\left[10n\mathfrak{y}^3 + \frac{17}{4}\mathfrak{y}^4 + \frac{312}{5}\mathfrak{y}^5 + \frac{37\,(27n - 13)}{6}\mathfrak{y}^6\right].$$

The 3D plot shown in the Fig. 3, is the symmetric division index M-polynomial of magnesium iodide graph, for a particular value with $n = 7$ and $m = 15$.
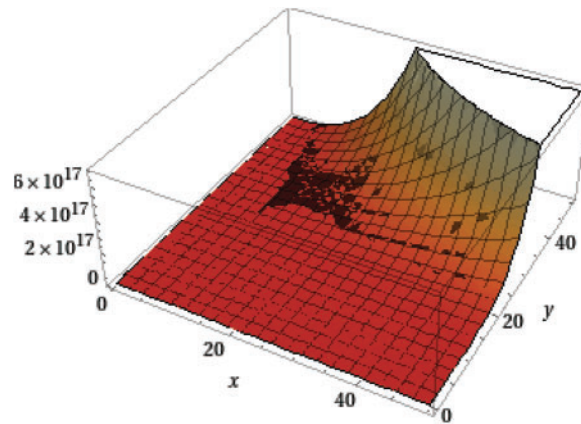
Figure 3: Graphical plot of SDI M-polynomial of magnesium iodide graph

Theorem 2.3. Let $I_{m,n}$ be a magnesium iodide graph, with $m = 2n + 1$, $n \geq 1$, and P_{HM} is the M-polynomial of hyper Zagreb index. Then $P_{HM}\left(I_{m,n}\right)$ is

$$P_{HM}\left(I_{m,n}\right) = \frac{1}{2}\mathfrak{x}^4 + \frac{6}{5}\mathfrak{x}^5 + \frac{(3n+2)}{3}\mathfrak{x}^6 + 4\mathfrak{x}^7 + \frac{(n+10)}{2}\mathfrak{x}^8 + \frac{2(27n-13)}{9}\mathfrak{x}^9. \tag{23}$$

Proof. The M-polynomial of hyper Zagreb index, given in the Definition 1.3, and the formulas for our structure $I_{m,n}$ can be written as: $P_{HM}(I_{m,n}) = 2S_{\mathfrak{x}}J\left(M\left(\chi;\mathfrak{x},\mathfrak{y}\right)\right)$. Lemmas 2.2 and 2.3 are the operators and here we used these to find our results for $I_{m,n}$. We will obtain the M-polynomial of symmetric division index for $I_{m,n}$ after some algebraic simplifications as:

$$P_{HM}\left(I_{m,n}\right) = \frac{1}{2}\mathfrak{x}^4 + \frac{6}{5}\mathfrak{x}^5 + \frac{(3n+2)}{3}\mathfrak{x}^6 + 4\mathfrak{x}^7 + \frac{(n+10)}{2}\mathfrak{x}^8 + \frac{2(27n-13)}{9}\mathfrak{x}^9.$$

The 2D plot shown in the Fig. 4, is the hyper Zagreb M-polynomial of magnesium iodide graph. Moreover, all the 2D plots show the M-polynomials of different index containing $\mathfrak{x}$ values on horizontal scale with different values of $n \in \{2, 3, \ldots, 10\}$.
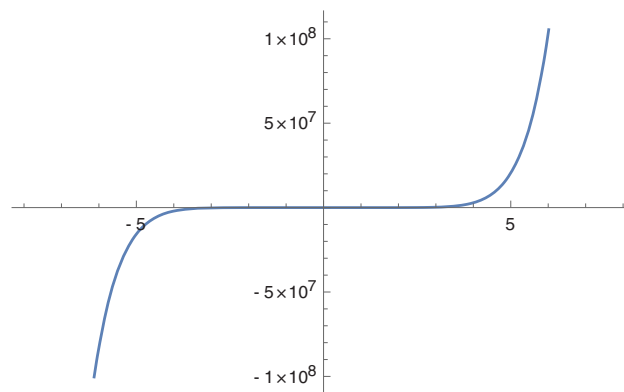

Figure 4: Graphical plot of HM M-polynomial of magnesium iodide graph

Theorem 2.4. Let $I_{m,n}$ be a magnesium iodide graph, with $m = 2n + 1$, $n \geq 1$, and P_{IS} is the M-polynomial of inverse sum index. Then $P_{IS}(I_{m,n})$ is

$$P_{IS}(I_{m,n}) = \frac{3}{4}\mathfrak{x}^4 + 2\mathfrak{x}^5 + \frac{(9n+8)}{6}\mathfrak{x}^6 + \frac{(6n+74)}{7}\mathfrak{x}^7 + \frac{(3n+27)}{2}\mathfrak{x}^8 + \frac{2(27n-13)}{3}\mathfrak{x}^9. \tag{24}$$

Proof. The M-polynomial of inverse sum index, given in the Definition 1.4, and the formulas for our structure $I_{m,n}$ can be written as: $P_{IS}(I_{m,n}) = S_{\mathfrak{x}}JD_{\mathfrak{x}}D_{\mathfrak{y}}(M(\chi;\mathfrak{x},\mathfrak{y}))$. Lemmas 2.1, 2.2 and 2.3 are the operators and here we used these to find our results for $I_{m,n}$. We will obtain the M-polynomial of symmetric division index for $I_{m,n}$ after some algebraic simplifications as

$$P_{IS}(I_{m,n}) = \frac{3}{4}\mathfrak{x}^4 + 2\mathfrak{x}^5 + \frac{(9n+8)}{6}\mathfrak{x}^6 + \frac{(6n+74)}{7}\mathfrak{x}^7 + \frac{(3n+27)}{2}\mathfrak{x}^8 + \frac{2(27n-13)}{3}\mathfrak{x}^9.$$

The 2D plot shown in the Fig. 5, is the inverse sum M-polynomial of magnesium iodide graph, for a particular value with $n = 7$ and $m = 15$.
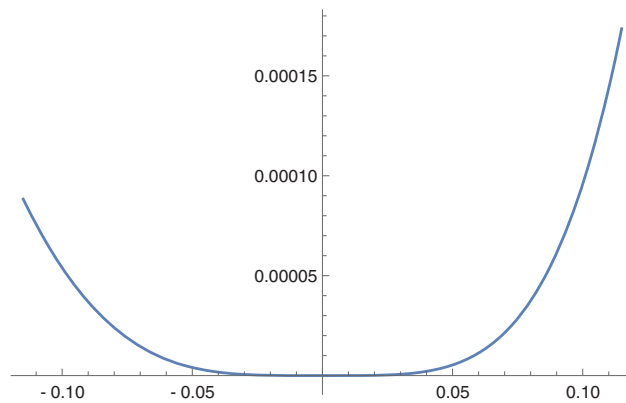

Figure 5: Graphical plot of IS M-polynomial of magnesium iodide graph

Theorem 2.5. Let $I_{m,n}$ be a magnesium iodide graph, with $m = 2n + 1$, $n \geq 1$, and P_{AZI} is the M-polynomial of augmented Zagreb index. Then $P_{AZI}(I_{m,n})$ is

$$P_{AZI}(I_{m,n}) = \frac{27}{8}\mathfrak{x}^2 + \frac{118}{27}\mathfrak{x}^3 + \frac{(243n+128)}{64}\mathfrak{x}^4 + \frac{(216n+1644)}{125}\mathfrak{x}^5 + \frac{(432n+3228)}{216}\mathfrak{x}^6$$
$$+ \frac{216(27n-13)}{343}\mathfrak{x}^7. \tag{25}$$

Proof. The M-polynomial of augmented Zagreb index, given in the Definition 1.5, and the formulas for our structure $I_{m,n}$ can be written as: $P_{AZI}(I_{m,n}) = S_{\mathfrak{x}}^3 Q_2 J D_{\mathfrak{x}}^3 D_{\mathfrak{y}}^3 (M(\chi;\mathfrak{x},\mathfrak{y}))$. Lemmas 2.1, 2.2 and 2.3 are the operators and here we used these to find our results for $I_{m,n}$. We will obtain the M-polynomial of symmetric division index for $I_{m,n}$ after some algebraic simplifications as

$$P_{AZI}(I_{m,n}) = \frac{27}{8}\mathfrak{x}^2 + \frac{118}{27}\mathfrak{x}^3 + \frac{(243n+128)}{64}\mathfrak{x}^4 + \frac{(216n+1644)}{125}\mathfrak{x}^5 + \frac{(432n+3228)}{216}\mathfrak{x}^6 + \frac{216(27n-13)}{343}\mathfrak{x}^7.$$

The 2D plot shown in the Fig. 6, is the augmented Zagreb index M-polynomial of magnesium iodide graph, for a particular value with $n = 7$ and $m = 15$.

Case 2: For the even values of m with given $n \geq 1$. Let $m = 2(n + 1)$ and $n \in \mathbb{Z}$.

Theorem 2.6. Let $I_{m,n}$ be a magnesium iodide graph, with $m = 2\,(n+1)$, $n \geq 1$, shown in the Fig. 1. Then, its M-polynomial is

$$M\left(I_{m,n}, x, y\right) = \mathfrak{x}\left[\mathfrak{y}^3 + \mathfrak{y}^5 + (n+5)\,\mathfrak{y}^6\right] + \mathfrak{x}^2\left[5\mathfrak{y}^2 + 6\mathfrak{y}^3 + 2\mathfrak{y}^5 + (2n+8)\,\mathfrak{y}^6\right]$$
$$+ \mathfrak{x}^3\left[(3n+1)\,\mathfrak{y}^3 + 2\mathfrak{y}^5 + (27n+7)\,\mathfrak{y}^6\right]. \tag{26}$$
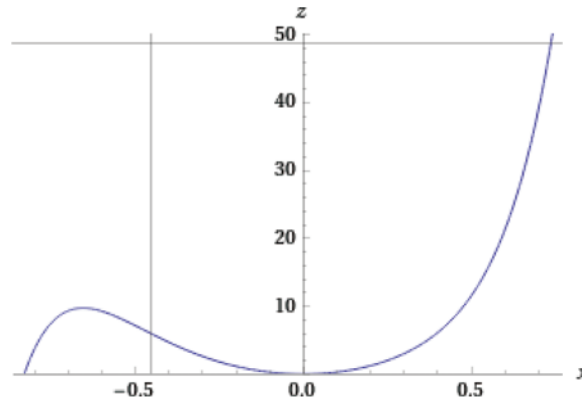

Figure 6: Graphical plot of AZI M-polynomial of magnesium iodide graph

Proof. The construction of magnesium iodide graph from its structure is found in Fig. 1. It has five types of vertices, evaluated from the figure and these vertices are described in the vertex set as

$$\underset{1}{\vee} = \left\{a \in V\left(I_{m,n}\right) : \xi_a = 1\right\}, \quad \underset{2}{\vee} = \left\{a \in V\left(I_{m,n}\right) : \xi_a = 2\right\}$$

$$\underset{3}{\vee} = \left\{a \in V\left(I_{m,n}\right) : \xi_a = 3\right\}, \quad \underset{5}{\vee} = \left\{a \in V\left(I_{m,n}\right) : \xi_a = 5\right\}$$

$$\underset{6}{\vee} = \left\{a \in V(I_{m,n}) : \xi_a = 6\right\}.$$

The same figure is also shown the information of its edge types. It contains ten types of edges in total and these are described as

$$\begin{aligned}
\Xi_{1,3} &= \left\{ab \in E(I_{m,n}) : \xi_a = 1, \xi_b = 3\right\}, & \Xi_{1,5} &= \left\{ab \in E(I_{m,n}) : \xi_a = 1, \xi_b = 5\right\} \\
\Xi_{1,6} &= \left\{ab \in E(I_{m,n}) : \xi_a = 1, \xi_b = 6\right\}, & \Xi_{2,2} &= \left\{ab \in E(I_{m,n}) : \xi_a = 2, \xi_b = 2\right\} \\
\Xi_{2,3} &= \left\{ab \in E(I_{m,n}) : \xi_a = 2, \xi_b = 3\right\}, & \Xi_{2,5} &= \left\{ab \in E(I_{m,n}) : \xi_a = 2, \xi_b = 5\right\} \\
\Xi_{2,6} &= \left\{ab \in E(I_{m,n}) : \xi_a = 2, \xi_b = 6\right\}, & \Xi_{3,3} &= \left\{ab \in E(I_{m,n}) : \xi_a = 3, \xi_b = 3\right\} \\
\Xi_{3,5} &= \left\{ab \in E(I_{m,n}) : \xi_a = 3, \xi_b = 5\right\}, & \Xi_{3,6} &= \left\{ab \in E(I_{m,n}) : \xi_a = 3, \xi_b = 6\right\}.
\end{aligned}$$

The cardinality of these edge partitions are $\left|\Xi_{1,3}\right| = \left|\Xi_{1,5}\right| = 1, \left|\Xi_{2,5}\right| = \left|\Xi_{3,5}\right| = 2, \left|\Xi_{1,6}\right| = n+5, \left|\Xi_{2,2}\right| = 5, \left|\Xi_{2,3}\right| = 6, \left|\Xi_{2,6}\right| = 2\,(n+4), \left|\Xi_{3,3}\right| = 3n+1$, and $\left|\Xi_{3,6}\right| = 27n+7$. Then from the

definition 1.1, the M-polynomial of $I_{m,n}$ is

$$M\left(I_{m,n}; \mathfrak{x}, \mathfrak{y}\right) = \sum_{i \leq j} m_{i,j}\left(I_{m,n}\right) \mathfrak{x}^i \mathfrak{y}^j$$

$$= \left|\Xi_{1,3}\right|\left(I_{m,n}\right) x^1 y^3 + \left|\Xi_{1,5}\right|\left(I_{m,n}\right) x^1 y^5 + \left|\Xi_{1,6}\right|\left(I_{m,n}\right) x^1 y^6$$

$$+ \left|\Xi_{2,2}\right|\left(I_{m,n}\right) x^2 y^2 + \left|\Xi_{2,3}\right|\left(I_{m,n}\right) x^2 y^3 + \left|\Xi_{2,5}\right|\left(I_{m,n}\right) x^2 y^5$$

$$+ \left|\Xi_{2,6}\right|\left(I_{m,n}\right) x^2 y^6 + \left|\Xi_{3,3}\right|\left(I_{m,n}\right) x^3 y^3 + \left|\Xi_{3,5}\right|\left(I_{m,n}\right) x^3 y^5$$

$$+ \left|\Xi_{3,6}\right|\left(I_{m,n}\right) x^3 y^6,$$

$$= \mathfrak{x}\left[\mathfrak{y}^3 + \mathfrak{y}^5 + (n+5)\,\mathfrak{y}^6\right] + \mathfrak{x}^2\left[5\mathfrak{y}^2 + 6\mathfrak{y}^3 + 2\mathfrak{y}^5 + 2\,(n+4)\,\mathfrak{y}^6\right]$$

$$+ \mathfrak{x}^3\left[(3n+1)\,\mathfrak{y}^3 + 2\mathfrak{y}^5 + (27n+7)\,\mathfrak{y}^6\right]. \tag{27}$$

Table 2: Edge partition of $I(m,n)$ for $m = 2\,(n+1)$

(ξ_a, ξ_b)	Frequency	Set of edges
$(1, 3)$	1	E_1
$(1, 5)$	1	E_2
$(1, 6)$	$n+5$	E_3
$(2, 2)$	2	E_4
$(2, 3)$	2	E_5
$(2, 5)$	8	E_6
$(2, 6)$	$2n+8$	E_7
$(3, 3)$	$3n$	E_8
$(3, 5)$	1	E_9
$(3, 6)$	12	E_{10}

The 3D plot shown in the Fig. 7, is the general M-polynomial of magnesium iodide graph, for a particular value with $n = 7$ and $m = 16$.

Lemma 2.4. Let $I_{m,n}$ be a magnesium iodide graph, with $m = 2\,(n+1)$, $n \geq 1$, then the differential operators are

$$D_{\mathfrak{x}}\left[M\left(I_{m,n}; \mathfrak{x}, \mathfrak{y}\right)\right] = \mathfrak{x}\left[\mathfrak{y}^3 + \mathfrak{y}^5 + (n+5)\,\mathfrak{y}^6\right] + 2\mathfrak{x}^2\left[5\mathfrak{y}^2 + 6\mathfrak{y}^3 + 2\mathfrak{y}^5 + 2\,(n+4)\,\mathfrak{y}^6\right]$$

$$+ 3\mathfrak{x}^3\left[(3n+1)\,\mathfrak{y}^3 + 2\mathfrak{y}^5 + (27n+7)\,\mathfrak{y}^6\right]. \tag{28}$$

$$D_{\mathfrak{y}}\left[M\left(I_{m,n}; \mathfrak{x}, \mathfrak{y}\right)\right] = \mathfrak{x}\left[3\mathfrak{y}^3 + 5\mathfrak{y}^4 + 6\,(n+5)\,\mathfrak{y}^6\right] + 2\mathfrak{x}^2\left[5\mathfrak{y}^2 + 9\mathfrak{y}^3 + 5\mathfrak{y}^5 + 6\,(n+4)\,\mathfrak{y}^6\right]0$$

$$+ \mathfrak{x}^3\left[3\,(3n+1)\,\mathfrak{y}^3 + 10\mathfrak{y}^5 + 6\,(27n+7)\,\mathfrak{y}^6\right]. \tag{29}$$

Proof. Differentiate Eq. (26) with respect to $\mathfrak{x}$ and multiply the result with $\mathfrak{x}$, we get the $D_{\mathfrak{x}}\left[M\left(I_{m,n}; \mathfrak{x}, \mathfrak{y}\right)\right]$. Similarly, differentiate Eq. (26) with respect to $\mathfrak{y}$ and multiply the result with $\mathfrak{y}$, we get the $D_{\mathfrak{y}}\left[M\left(I_{m,n}; \mathfrak{x}, \mathfrak{y}\right)\right]$.
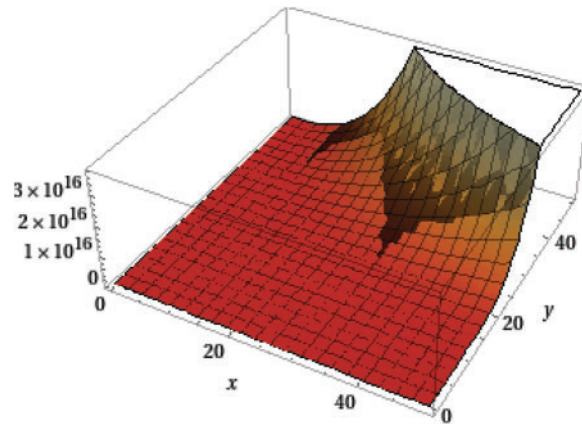
Figure 7: Graphical plot of M-polynomial of magnesium iodide graph

Lemma 2.5. Let $I_{m,n}$ be a magnesium iodide graph, with $m = 2n + 1$, $n \geq 1$. Then the integral operators are

$$S_{\mathfrak{x}}\left[M\left(I_{m,n}; \mathfrak{x}, \mathfrak{y}\right)\right] = \mathfrak{x}\left[\mathfrak{y}^3 + \mathfrak{y}^5 + (n+5)\,\mathfrak{y}^6\right] + \frac{1}{2}\mathfrak{x}^2\left[5\mathfrak{y}^2 + 6\mathfrak{y}^3 + 2\mathfrak{y}^5 + 2\,(n+4)\,\mathfrak{y}^6\right]$$

$$+ \frac{1}{3}\mathfrak{x}^3\left[(3n+1)\,\mathfrak{y}^3 + 2\mathfrak{y}^5 + (27n+7)\,\mathfrak{y}^6\right]. \tag{30}$$

$$S_{\mathfrak{y}}\left[M\left(I_{m,n}; \mathfrak{x}, \mathfrak{y}\right)\right] = \mathfrak{x}\left[\frac{1}{3}\mathfrak{y}^3 + \frac{1}{5}\mathfrak{y}^5 + \frac{(n+5)}{6}\mathfrak{y}^6\right] + \mathfrak{x}^2\left[\frac{5}{2}\mathfrak{y}^2 + 2\mathfrak{y}^3 + \frac{2}{5}\mathfrak{y}^5 + \frac{(n+4)}{3}\mathfrak{y}^6\right]$$

$$+ \mathfrak{x}^3\left[\frac{(3n+1)}{3}\mathfrak{y}^3 + \frac{2}{5}\mathfrak{y}^5 + \frac{(27n+7)}{6}\mathfrak{y}^6\right]. \tag{31}$$

Proof. As we know that from Eq. (12), $S_{\mathfrak{x}}\left[M\left(I_{m,n}; \mathfrak{x}, \mathfrak{y}\right)\right] = \int_0^{\mathfrak{x}} \frac{M(Im,n;t,\mathfrak{y})}{t} dt$ uses the general M-polynomial for the $I_{m,n}$ from Eq. (26) in it. After simplification, we obtain $S_{\mathfrak{x}}\left[M\left(I_{m,n}; \mathfrak{x}, \mathfrak{y}\right)\right]$. Similarly, from Eq. (13), $S_{\mathfrak{y}}\left[M\left(I_{m,n}; \mathfrak{x}, \mathfrak{y}\right)\right] = \int_0^{\mathfrak{y}} \frac{M(Im,n;\mathfrak{x},t)}{t} dt$ uses the general M-polynomial for the $I_{m,n}$ from Eq. (26) in it. After simplification, we obtain $S_{\mathfrak{y}}\left[M\left(I_{m,n}; \mathfrak{x}, \mathfrak{y}\right)\right]$.

Lemma 2.6. Let $I_{m,n}$ be a magnesium iodide graph, with $m = 2\,(n+1)$, $n \geq 1$. Then the Eq. (26) is

$$J\left[M\left(I_{m,n}; \mathfrak{x}, \mathfrak{y}\right)\right] = 6\mathfrak{x}^4 + 6\mathfrak{x}^5 + (3n+2)\,\mathfrak{x}^6 + (n+7)\,\mathfrak{x}^7 + 2\,(n+5)\,\mathfrak{x}^8 + (27n+7)\,\mathfrak{x}^9.$$

Proof. By implementing the operator stated in the Eq. (14) on the main equation defined in 11, we get the $J\left[M\left(I_{m,n}; \mathfrak{x}, \mathfrak{y}\right)\right]$.

Theorem 2.7. Let $I_{m,n}$ be a magnesium iodide graph, with $m = 2\,(n+1)$, $n \geq 1$, and P_{SDI} is the M-polynomial of symmetric division index. Then $P_{SDI}\left(I_{m,n}\right)$ is

$$P_{SDI}\left(I_{m,n}\right) = \mathfrak{x}\left[\frac{2}{3}\mathfrak{y}^3 + \frac{2}{5}\mathfrak{y}^5 + \frac{n+5}{3}\mathfrak{y}^6\right] + \mathfrak{x}^2\left[\frac{25}{4}\mathfrak{y}^2 + 5\mathfrak{y}^3 + \mathfrak{y}^5 + \frac{5\,(n+4)}{6}\mathfrak{y}^6\right]$$

$$+ \mathfrak{x}^3\left[\frac{246n+81}{3}\mathfrak{y}^3 + \frac{182}{5}\mathfrak{y}^5 + \frac{3429n+889}{6}\mathfrak{y}^6\right]. \tag{32}$$

Proof. The M-polynomial of symmetric division index, given in the Definition 1.2, and the formulas for our structure $I_{m,n}$ can be written as: $P_{SDI}(I_{m,n}) = (D_\mathfrak{x} S_\mathfrak{y} + D_\mathfrak{y} S_\mathfrak{x})(M(\chi;\mathfrak{x},\mathfrak{y}))$. Lemmas 2.4 and 2.5 are the operators and here we used these to find our results for $I_{m,n}$. We will obtain the M-polynomial of symmetric division index for $I_{m,n}$ after some algebraic simplifications as

$$P_{SDI}(I_{m,n}) = \mathfrak{x}\left[\frac{2}{3}\mathfrak{y}^3 + \frac{2}{5}\mathfrak{y}^5 + \frac{n+5}{3}\mathfrak{y}^6\right] + \mathfrak{x}^2\left[\frac{25}{4}\mathfrak{y}^2 + 5\mathfrak{y}^3 + \mathfrak{y}^5 + \frac{5(n+4)}{6}\mathfrak{y}^6\right]$$

$$+ \qquad \mathfrak{x}^3\left[\frac{246n+81}{3}\mathfrak{y}^3 + \frac{182}{5}\mathfrak{y}^5 + \frac{3429n+889}{6}\mathfrak{y}^6\right].$$

The 3D plot shown in the Fig. 8, is the symmetric division index M-polynomial of magnesium iodide graph, for a particular value with $n = 7$ and $m = 16$.

Theorem 2.8. Let $I_{m,n}$ be a magnesium iodide graph, with $m = 2(n+1)$, $n \geq 1$, and P_{HM} is the M-polynomial of hyper Zagreb index. Then $P_{HM}(I_{m,n})$ is

$$P_{HM}(I_{m,n}) = 6\mathfrak{x}^4 + \frac{12}{5}\mathfrak{x}^5 + \frac{3n+2}{3}\mathfrak{x}^6 + \frac{2(n+7)}{7}\mathfrak{x}^7 + \frac{n+5}{2}\mathfrak{x}^8 + \frac{2(27n+7)}{9}\mathfrak{x}^9. \qquad (33)$$

Proof. The M-polynomial of hyper Zagreb index, given in the Definition 1.3, and the formulas for our structure $I_{m,n}$ can be written as: $P_{HM}(I_{m,n}) = 2S_\mathfrak{x} J(M(G;\mathfrak{x},\mathfrak{y}))$. Lemmas 2.5 and 2.6 are the operators and here we used these to find our results for $I_{m,n}$. We will obtain the M-polynomial of symmetric division index for $I_{m,n}$ after some algebraic simplifications as

$$P_{HM}(I_{m,n}) = 6\mathfrak{x}^4 + \frac{12}{5}\mathfrak{x}^5 + \frac{3n+2}{3}\mathfrak{x}^6 + \frac{2(n+7)}{7}\mathfrak{x}^7 + \frac{n+5}{2}\mathfrak{x}^8 + \frac{2(27n+7)}{9}\mathfrak{x}^9.$$
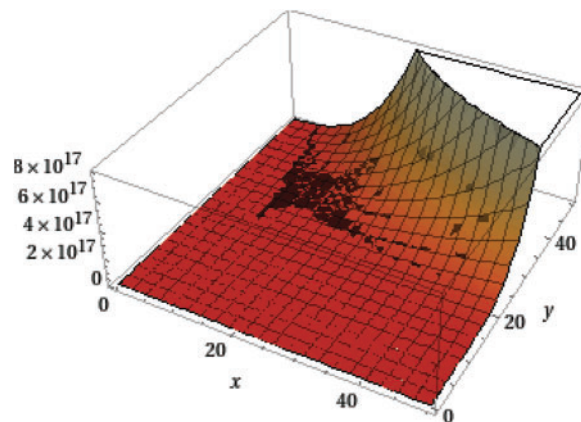

Figure 8: Graphical plot of SDI M-polynomial of magnesium iodide graph

The 2D plot shown in the Fig. 9, is the hyper Zagreb M-polynomial of magnesium iodide graph, for a particular value with $n = 7$ and $m = 16$.

Theorem 2.9. Let $I_{m,n}$ be a magnesium iodide graph, with $m = 2(n+1)$, $n \geq 1$, and P_{IS} is the M-polynomial of inverse index. Then $P_{IS}(I_{m,n})$ is

$$P_{IS}(I_{m,n}) = \frac{23}{4}\mathfrak{x}^4 + \frac{41}{5}\mathfrak{x}^5 + \frac{3(3n+1)}{2}\mathfrak{x}^6 + \frac{(6n+50)}{7}\mathfrak{x}^7 + \frac{(12n+63)}{4}\mathfrak{x}^8 + 2(27n+7)\mathfrak{x}^9. \qquad (34)$$
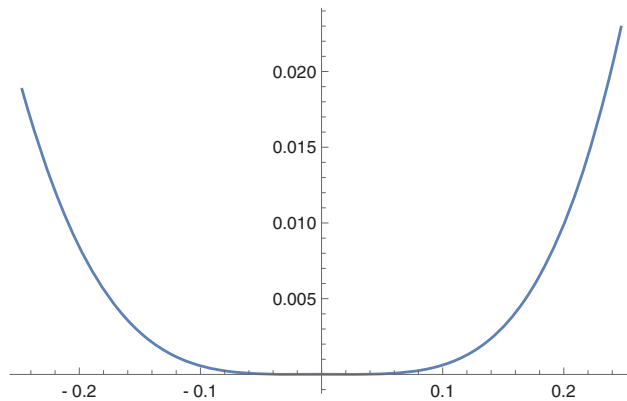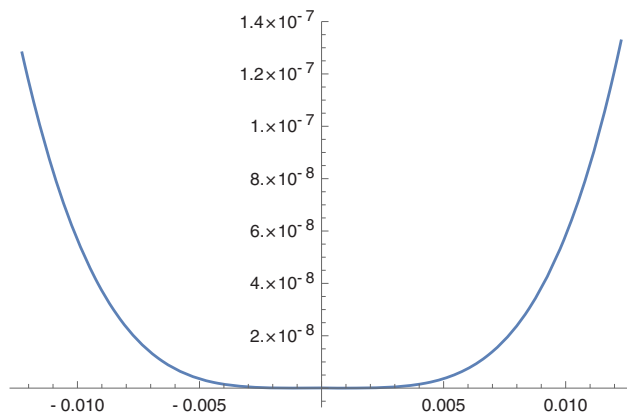
Figure 9: Graphical plot of HM M-polynomial of magnesium iodide graph

Proof. The M-polynomial of inverse sum index, given in the Definition 1.4, and the formulas for our structure $I_{m,n}$ can be written as: $P_{IS}(I_{m,n}) = S_{\mathfrak{x}}JD_{\mathfrak{x}}D_{\mathfrak{y}}(M(\chi;\mathfrak{x},\mathfrak{y}))$. Lemmas 2.4, 2.5 and 2.6 are the operators and here we used these to find our results for $I_{m,n}$. We will obtain the M-polynomial of symmetric division index for $I_{m,n}$ after some algebraic simplifications as

$$P_{IS}\left(I_{m,n}\right) = \frac{23}{4}\mathfrak{x}^4 + \frac{41}{5}\mathfrak{x}^5 + \frac{3(3n+1)}{2}\mathfrak{x}^6 + \frac{(6n+50)}{7}\mathfrak{x}^7 + \frac{(12n+63)}{4}\mathfrak{x}^8 + 2(27n+7)\mathfrak{x}^9.$$

The 2D plot shown in the Fig. 10, is the inverse sum M-polynomial of magnesium iodide graph, for a particular value with $n = 7$ and $m = 16$.

Figure 10: Graphical plot of IS M-polynomial of magnesium iodide graph

Theorem 2.10. Let $I_{m,n}$ be a magnesium iodide graph, with $m = 2(n+1)$, $n \geq 1$, and P_{AZI} is the M-polynomial of augmented Zagreb index. Then $P_{AZI}(I_{m,n})$ is

$$P_{AZI}\left(I_{m,n}\right) = \frac{347}{8}\mathfrak{x}^2 + 48\mathfrak{x}^3 + \frac{(2187n+854)}{64}\mathfrak{x}^4 + \frac{(216n+3080)}{125}\mathfrak{x}^5 + \frac{(576n+3429)}{36}\mathfrak{x}^6$$

$$+ \frac{5832(27n+7)}{343}\mathfrak{x}^7. \tag{35}$$

Proof. The M-polynomial of augmented Zagreb index, given in the Definition 1.5, and the formulas for our structure $I_{m,n}$ can be written as: $P_{AZI}(I_{m,n}) = S_\mathfrak{x}^3 Q_2 J D_\mathfrak{x}^3 D_\mathfrak{y}^3 (M(\chi; \mathfrak{x}, \mathfrak{y}))$. Lemmas 2.4, 2.5 and 2.6 are the operators and here we used these to find our results for $I_{m,n}$. We will obtain the M-polynomial of symmetric division index for $I_{m,n}$ after some algebraic simplifications as

$$P_{AZI}(I_{m,n}) = \frac{347}{8}\mathfrak{x}^2 + 48\mathfrak{x}^3 + \frac{(2187n + 854)}{64}\mathfrak{x}^4 + \frac{(216n + 3080)}{125}\mathfrak{x}^5 + \frac{(576n + 3429)}{36}\mathfrak{x}^6 + \frac{5832(27n + 7)}{343}\mathfrak{x}^7.$$

The 2D plot shown in the Fig. 11, is the augmented Zagreb index M-polynomial of magnesium iodide graph, for a particular value with $n = 7$ and $m = 16$.
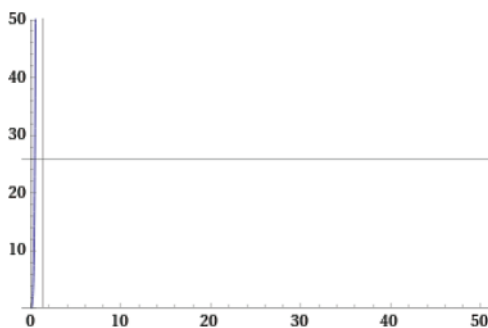

Figure 11: Graphical plot of AZI M-polynomial of magnesium iodide graph

3 Conclusion

The M-polynomial of a structure delivers the polynomial or abstract function of a chemical network or structure. To add up some algebraic properties of magnesium iodide or MX_2 structure, we computed the M-polynomials of augmented Zagreb index, inverse sum index, hyper Zagreb index and the symmetric division index are figured out for the magnesium iodide or MX_2 structure, for both even and odd cases of parameter m.

Conflicts of Interest: The authors declare that they have no conflicts of interest to report regarding the present study.

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