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Topological Invariants of Hexagonal Cage Network by Using Algebraic Polynomials

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Abstract

In this article, we go beyond earlier limits in the analysis by using algebraic polynomials to compute the topological indices for hexagonal cage networks. We investigate hexagonal cage networks of different orders and copies by introducing M-Polynomials and Forgotten polynomials, and we derive novel closed formulae and conclusions for a broad range of topological indices. We also create an efficient technique to compute $\boldsymbol{HXC_n^m}$, a pivotal polynomial, as part of our work. In addition to computing, we apply algebraic polynomials to the analysis of these indices, providing more insights into their structural significance in hexagonal cage networks. This work illuminates the algebraic underpinnings of these intricate networks and broadens the scope of topological index computation, with implications for a variety of scientific domains. These polynomials allow us to calculate several features of the network, such as the first and second Zagreb, modified Zagreb, General Randić, inverse General Randić, harmonic, symmetric division, inverse sum, and so on. There are now new closed formulae and outcomes available. Additionally, we offer a technique for calculating the polynomial $\boldsymbol{HXC_n^m}$. We also use algebraic polynomials to analyses all of the aforementioned indices.

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1 Introduction and preliminary results

Suppose we have a structure that is made up of dots that are joined together with line segment, if there is no dot in that particular structure that is connected with a line segment to itself and there are no two dots that are joined by more than one-line segment, we call that particular structure a graph, the set of dots in that particular structure is called vertices and set of line joining the dots is called the edges [1].

A graph can be recognized by a numerical number, network, matrix which represent the whole graph. There are lots of ways for the given information on mutual connectors of atoms in molecules can measured. A diagrammatically representation, which one may be easily describe through graphs by organic chemists because of its closed resembles of structural formula [2]. A chemical graph is a labeled graph whose vertices correspond to the atoms of the compound and edges correspond to chemical bonds.

A topological index is parameter mathematically derived from graph structure. It is used to better under- stand the molecular structure. These indices are beneficial for the better study of properties of many chemical molecules. Lots of research have been conducted on topological indices of different classes of graphs like line graph, chemical molecular, nanotubes, nanotories and face- connected cube lattice [3, 4]. A topological index is a Mathematical formula that can be applied to any graph which models some molecular structure. From this index, it is possible to analyze Mathematical values and further investigation of some physio-chemical properties of molecule. Therefore, it is an efficient method in avoiding expensive and time-consuming laboratory experiments [5, 6].

These methods are based on graph-theoretical concepts and were first introduced by Harry Wiener during the years 1947-1948. Wiener investigated the physical and chemical properties of a series of (branched) alkanes such as boiling point at atmospheric pressure, heat of isomerization, and heat of vaporization [7]. He postulated that these properties depend solely on the number, kind, and structural arrangement of the atoms. In the case of alkane isomers, the kind and number of atoms is constant. Then the variations in the property in question depend solely on the structural arrangement of the atoms. He further assumed that these properties would satisfy a linear formula of the type

$$X = aW + bP + c \tag{1.1}$$

where a, b and c are two constants for a given isomeric group and W and P are two topological indices defined by Wiener and described below. All the way, in this paper we assume Γ to be finite, simple and connected network with $V(\Gamma)$ = Vertex set, $E = E(\Gamma)$ = Edge family and d_v = vertex degree.

Definition 1. For any graph $\Gamma = (V, E)$ the M-polynomial [6] is described as:

$$M(\Gamma; x, y) = f(x, y) = \sum_{i \le j} m_{ij}(\Gamma) x^i y^j$$

where $m_{ij}(\Gamma)$ represent number of edges $uv \in E(\Gamma)$ such that $\{d_u(\Gamma), d_v(\Gamma)\} = \{i, j\}$.

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Definition 2. Let $\Gamma = (V, E)$ be any graph, then formula for forgotten polynomial of Γ is given by:

$$F(\Gamma; x) = \sum_{uv \in E(\Gamma)} x^{[(d_u)^2 + (d_v)^2]}$$

The first and oldest topological index based on degree is the Randić index [8] denoted by $R\left(\frac{1}{2}\right)(G)$,

$$R\left(\frac{1}{2}\right)(G) = \sum_{uv \in E(G)} \frac{1}{\sqrt{d_u d_v}} \tag{1.2}$$

The general Randić index [9, 10] denoted by

$$R_\alpha(G) = \sum_{uv \in E(G)} [d(u)d(v)]^\alpha \tag{1.3}$$

and defined as where $\alpha = 1, \frac{1}{2}, -1, \frac{-1}{2}$

Another topological index the Zagreb index is denoted by $M_1(G)$ is very vital topological index and the founder of this index are Gutman and Rinajstic [11], defined as

$$MI(G) = \sum_{uv \in E(G)} [d(u) + d(v)]. \tag{1.4}$$

For more detail about this index one can see [12–15]. Estrada et al. [16] introduced one of the well-known connectivity topological index namely atom-bond connectivity (ABC) index [17] defined as

$$ABC(G) = \sum_{uv \in E(G)} \sqrt{\frac{d(u)d(v) - 2}{d(u)d(v)}} \tag{1.5}$$

Geometric index (GA) index has its own importance $[18 - 22]$, very important and well-known index defined as,

$$GA(G) = \sum_{uv \in E(G)} \frac{2\sqrt{d(u)d(v)}}{d(u) + d(v)} \tag{1.6}$$

Deutsch and Klavžar figured out some prominent topological indices which are achieved with the help of M polynomial [6] and are given in Table 1 given below.

Table 1: Formulae of some prominent topological descriptors depending on M-polynomial

Topological Descriptors	**Formulae based on M-polynomial**
First Zagreb index	$(D_x + D_y)f(x, y)$
Second Zagreb index	$(D_x D_y)f(x, y)$
Modified Second Zagreb index	$(S_x S_y)f(x, y)$

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General Randić index	$D_x^\alpha D_y^\alpha f(x,y)$
Inverse Randić index	$S_x^\alpha S_y^\alpha f(x,y)$
Symmetric Division Index	$(D_x S_y + S_x D_y) f(x,y)$
Harmonic Index	$2S_x J f(x,y)$
Inverse sum Index	$S_x J D_x D_y f(x,y)$
Augmented Zagreb Index	$S_x^3 Q_{-2} J D_x^3 D_y^3 f(x,y)$

where $D_x f = x\frac{\partial f}{\partial x}, D_y f = y\frac{\partial f}{\partial y}, S_x f = \int_0^x \frac{f(t,y)}{t} dt, S_y f = \int_0^y \frac{f(x,t)}{t} dt,$
$J(f(x,y)) = f(x,x), Q_\alpha f = x^\alpha f.$
All formulae presented in table 1 will be calculated for $x = y = 1$.

2 Main Results

We derive the topological indices of the generalized hexagonal cage network graph HXC_n^m of order n with m copies. In this work, the mathematical property of general Randić index and general Zagreb index. Also Zagreb index of some general chains are studied and hence their special cases are considered where n denotes the order of the hexagonal cage and then we derive some explicit expressions of the same for other degree based topological indices such as Zagreb indices, Hyper Zagreb index, redefined Zagreb index, general first Zagreb index, general Randić index, Atom Bond connectivity index is also studied for hexagonal cage network.

2.1 Hexagonal Cage network HXC_n^m drawing algorithm

Step-1: Find two hexagonal n-dimensional networks, which denoted as $HX_1(n)$, and $HX_2(n)$, respectively.

In $HX_1(n)$, each $HX_2(n)$, boundary vertex is connected to its mirror image vertex by an edge. The graph is called the hexagonal cage network of two layers, as shown in Figure 1.

In this paper $E(G)$ is used for the edge of the graph and $v(Q)$ is used for the vertex of the graph and d_r is the degree of the vertex $r \in V(G)$

Extend this hexagonal cage network for order n for m copies. That is generalize HXC_n^m for m copies. A hexagonal cage with order n and m copies can be seen in the above illustration. This indicates that the hexagonal rings in the cage are layered on top of one another in $n \times m$ layers. With gaps between the rings that permit movement between the layers, the layers are organized to give the impression of being a maze. There are numerous uses for hexagonal cages in computers, chemistry, and

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physics with order n and m copies. Physics has examined this structure as a model for several other systems, including Colloidal crystals are arrays of colloidal particles that self-assemble. It has been shown that hexagonal cage structures exist in colloidal crystals shaped like spheres, rods, and other shapes. Materials with a periodic structure that have the ability to regulate light propagation are called photonic crystals. Utilizing hexagonal cage architectures, photonic crystals with distinct optical characteristics have been produced. It has proven possible to develop artificial materials with unusual optical properties, such a negative refractive index, by using hexagonal cage arrangements. This may result in novel optical applications like super lenses and cloaking devices.

Hexagonal cage structures have been investigated in chemistry as a means of encasing and delivering molecules. New catalysts for chemical processes have been created using hexagonal cage architectures. see figure 1

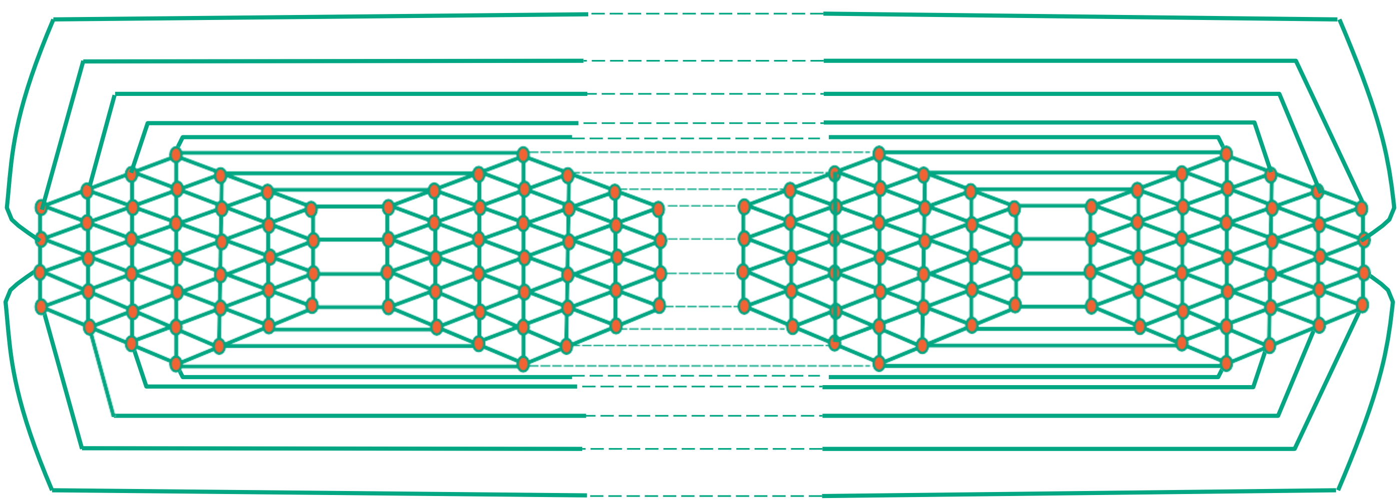

Figure 1: Generalized cage network

In this work, we formulate the different topological indices of Hexagonal cage network of order n with m copies. Let HXC_n^m be the hexagonal cage network taking m copies of HXC_n^m and joining each vertex of HXC_n^m, we get the hexagonal cage network graph of the HXC_n^m. The edge set of HXC_n^m can be partitioned into the following subsets.

$$E_1(HXC_n^m) = \{e = uv; d(u) = 4, d(v) = 5\},$$
$$E_2(HXC_n^m) = \{e = uv; d(u) = d(v) = 5\},$$
$$E_3(HXC_n^m) = \{e = uv; d(u) = 5, d(v) = 6\},$$
$$E_4(HXC_n^m) = \{e = uv; d(u) = 6, d(v) = 6\},$$

such that $|E_1(HXC_n^m| = 20 + 4m, |E_2(HXC_n^m)| = 6m + 6n - 30, |E_3(HXC_n^m| = 40m + 40n - 30$, and $|E_4(HXC_n^m)| = 94m + 94n - 516$.

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Theorem 2.1. Let HXC_n^m be the hexagonal network, then M and Forgotten Polynomials of of HXC_n^m are:

$$M(HX_n;x,y) = (20-4m)x^4y^5 + (6m+6n-30)x^5y^5 + (40m+40n-30)x^5y^6 + (94m+94n-516)x^6y^6$$
$$F(HX_n;x) = (20+4m)x^{41} + (6m+6n-30)x^{50} + (40m+40n-30)x^{61} + (94m+94n-30)x^{72}$$

Proof: We know total vertices and total edges of HX_n are given by $|V(HX_n)| = 3n^2-3n+1$ and $|E(HX_n)| = 9n^2-15n+6$ respectively. Table 2 presents edge partition of hexagonal network. We can rewrite

Table 2: Degrees based edge partitioning of a graph HX_n.

$(d_u,d_v): uv \in E(HX_n)$	(4,5)	(5,5)	(5,6)	(6,6)
Number of edges	20 + 4 m	6 m + 6n − 30	$40m+40n-30$	$94m+94n-516$

information given in table 2 in the following form.

$$E_1(HX_n) = \{uv \in E(HX_n): d_u = 4, d_v = 5\} \quad |E_1(HX_n)| = 20+4m$$
$$E_2(HX_n) = \{uv \in E(HX_n): d_u = 5, d_v = 5\} \quad |E_2(HX_n)| = 6m+6n-30$$
$$E_3(HX_n) = \{uv \in E(HX_n): d_u = 5, d_v = 6\} \quad |E_3(HX_n)| = 40m+40n-30$$
$$E_4(HX_n) = \{uv \in E(HX_n): d_u = 6, d_v = 6\} \quad |E_2(HX_n)| = 94m+94n-516$$

Using definition 1, we get

$$M(HX_n;x,y) = \sum_{i\le j} m_{ij}x^iy^j$$
$$= \sum_{4\le 5} m_{45}x^4y^5 + \sum_{5\le 5} m_{55}x^5y^5 + \sum_{5\le 6} m_{56}x^5y^6 + \sum_{6\le 6} m_{66}x^6y^6$$
$$= |E_1(HX_n)|x^4y^5 + |E_2(HX_n)|x^5y^5 + |E_3(HX_n)|x^5y^6 + |E_4(HX_n)|x^6y^6$$

$$M(HX_n;x,y) = (20+4m)x^4y^5 + (6m+6n-30)x^5y^5 + (40m+40n-30)x^5y^6 + (94m+94n - 516)x^6y^6$$

using the definition of Forgotten Polynomial, we get

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$$\begin{aligned} F(HX_n;x) &= \sum_{uv\in E(\Gamma)} x^{[(d_u)^2+(d_v)^2]} \\ &= \sum_{uv\in E_1(HX_n)} m_{45}x^{41} + \sum_{uv\in E_2(HX_n)} m_{55}x^{50} + \sum_{uv\in E_3(HX_n)} m_{56}x^{61} \\ &+ \sum_{uv\in E_4(HX_n)} m_{66}x^{72} \\ &= (20+4m)x^{41} + (6m+6n-30)x^{50} + (40m+40n-30)x^{61} + (94m+94n-516)x^{72} \end{aligned}$$

Theorem 2.2. For Hexagonal cage network of HXC_n^m, first Zagrab, second zagrab, and general Randić indices are given by:

1 $M_1(\,HXC_n^m) = 1664mn + 1628n - 6642$

2 $M_2(\,HXC_n^m) = 4814mn + 4734n - 19826$

3 $R_\alpha(\,HXC_n^m) = 20^{-\alpha}(20+4m) + 25^{-2\alpha}(6m+6n-30) + 30^{-\alpha}(40m+40n-30) + 6^{-2\alpha}(40m+40n-30)$

Now, using derivation formulae of topological indices over M-polynomial from table 1, we get

1 First Zagreb Index $= M_1(HX_n) = \left(D_x + D_y\right)f(x,y)\big|_{x=y=1} = 1664m + 1628n - 6642$

2 Second Zagreb Index $= M_2(HX_n) = D_yD_xf(x,y)\big|_{x=y=1} = 4814m + 4734n - 19826$

3 Generalized Randić Index $= R_\alpha(HX_n) = D_x^\alpha D_y^\alpha f(x,y)\big|_{x=y=1} = 20^{-\alpha}(20+4m)$

$$+25^{-2\alpha}(6m+6n-30) + 30^{-\alpha}(40m+40n-30) + 6^{-2\alpha}(40m+40n-30)$$

Proof: Let $M(HX_n;x,y) = f(x,y) = (20+4m)x^4y^5 + (6m+6n-30)x^5y^5 + (40m+40n-30)x^5y^6 + (94m+94n-516)x^6y^6$

First, we apply the operators, illustrated in derivation table 1, on M-polynomial function as follows.

$$\text{First Zagreb Index} = M_1(HX_n) = \left(D_x + D_y\right)f(x,y)\big|_{x=y=1} =$$

$$9(20+4m) + 10(6m+6n-30) + 11(40m+40n-30) + 12(94m+94n-516)$$

$$\text{First Zagreb Index} = M_1(HX_n) = 1664m + 1628n - 6642$$

$$M_2(HX_n) = D_yD_xf(x,y)\big|_{x=y=1} = 4814m + 4734n - 19826$$

$$M_2(G) = 20(20+4m)x^3y^4 + 25(6n+6m-30)x^4y^4 + 11(40m+40n-190)x^4y^5 + 12(94n+94m-516)x^5y^5$$
$$M_2(G) = 20(20+4m) + 25(6n+6m-30) + 11(40m+40n-190) + 12(94n+94m-516)$$

at x = y = 1

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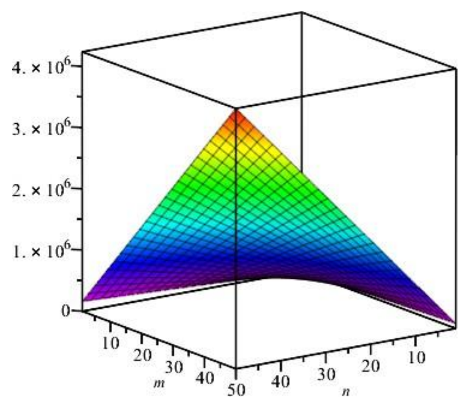
$$M_2(G) = 4814m + 4734n - 19826$$
$$M_2(G) = 4814m + 4734n - 19826$$

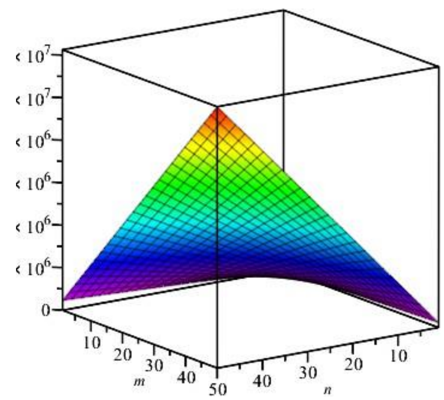
at x = y = 1

$$\begin{aligned} D_x^{\alpha} D_y^{\alpha} f(x,y) &= 20^{\alpha}(20+4m)x^4y^5 + 25^{2\alpha}(6n+6m-30)x^5y^5 + 30^{\alpha}(40m+40n-190)x^5y^6 \\ &+6^{2\alpha}(94n+94m-516)x^5y^6 20^{-\alpha}(20+4m)x^4y^5 + 25^{-2\alpha}(6n+6m-30)x^5y^5 \\ &+30^{-\alpha}(40m+40n-190)x^5y^6 + 6^{-2\alpha}(94n+94m-516)x^5y^6 \end{aligned}$$

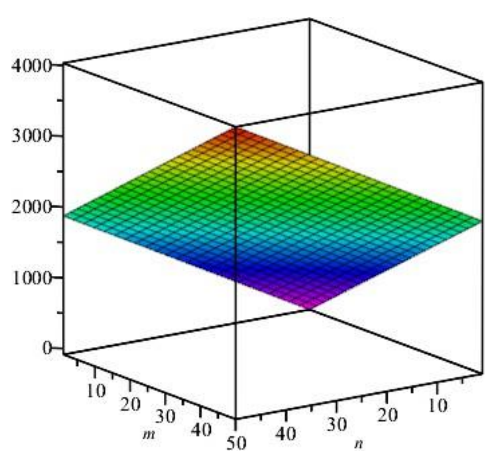
see Figure 2a, Figure 2b, Figure 2c



(a) Zagreb 1



(b) Zagreb 2



(c) General Randić

The number of copies, m raises the first Zagreb index. This indicates that when the number of copies rises,

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the cage gets increasingly branched. As the number of copies, m increases, the second Zagreb index drops. This implies that as the number of copies rises, the cage gets less complex. The Randić index of the hexagonal cage of order n and m copies are plotted in a three-dimensional (3D) graph, demonstrating a rise with both the cage's order (n) and number of copies(m). This indicates that as n and m increase, the cage gets more complex. These findings help to forecast the features of the hexagonal cage of order n and m copies as well as to comprehend its construction. For instance, the cage appears to be more porous because it branches out more as the order rises. It appears that the cage could be simpler to synthesize because it gets less complex as the number of copies rises. This may lead to the conclusion that a good model for a complicated system is the hexagonal cage with order n and m copies. Complex systems can self-organize due to their large number of interconnected components. Similar in structure, the hexagonal cage of order n and m copies consist of several interconnected hexagonal rings. It has the capacity to self-organize into many patterns and shapes.

Theorem 2.3. let HXC_n^m the hexagonal cage network work of order n with m copies then the modiefied second Zegrab index is given by

$$m_M^2(G) = S_x S_y f(x,y) \mid x = y = 1$$

and its final result of order n with m copies

$$m_M^2(G) = 53.40m + 49.20n - 1$$

Proof: let HXC_n^m the hexagonal cage network work of order n with m copies then the modiefied second Zegrab index is defined as

$$M(HX_n; x, y) = \sum_{i \le j} m_{ij} x^i y^j$$

$$= \sum_{4 \le 5} m_{45} x^4 y^5 + \sum_{5 \le 5} m_{55} x^5 y^5 + \sum_{5 \le 6} m_{56} x^5 y^6 + \sum_{6 \le 6} m_{66} x^6 y^6$$

$$= |E_1(HX_n)| x^4 y^5 + |E_2(HX_n)| x^5 y^5 + |E_3(HX_n)| x^5 y^6 + |E_4(HX_n)| x^6 y^6$$

$$M(HX_n; x, y) = (20 + 4m) x^4 y^5 + (6m + 6n - 30) x^5 y^5 + (40m + 40n - 30) x^5 y^6 + (94m + 94n - 516) x^6 y^6$$

Now we first find

$$S_x = \int_0^x \frac{f(x,y)}{x} dx$$

$$M(HX_n; x, y) = (20 + 4m) x^4 y^5 + (6m + 6n - 30) x^5 y^5 + (40m + 40n - 30) x^5 y^6 + (94m + 94n - 516) x^6 y^6$$

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$$\int_0^x \frac{f(x,y)}{x} dx$$
$$= \int_0^x (20+4m)x^4y^5 + (6m+6n-30)x^5y^5 + (40m+40n-30)x^5y^6 + (94m+94n-516)x^6y^6 dx$$
$$= \frac{1}{4}(20+4m)x^4y^5 + \frac{1}{5}(6m+6n-30)x^4y^5 + \frac{1}{5}(40m+40n-30)x^4y^6 + \frac{1}{5}(94m+94n-516)x^5y^6$$
$$= (5+m)x^4y^5 + \frac{1}{5}(6m+6n-30)x^4y^5 + (8m+8n-6)x^5y^5 + \frac{1}{5}(94m+94n-516)x^6y^6$$
$$= (m+5)x^4y^5 + \frac{1}{5}(6m+6n-30)x^4y^5 + (8m+8n-6)x^5y^5 + \frac{1}{5}(94m+94n-516)x^6y^6$$

Now we first find

$$S_y = \int_0^x \frac{f(x,y)}{y} dx$$

$$M(HX_n; x, y) = (20+4m)x^4y^5 + (6m+6n-30)x^5y^5 + (40m+40n-30)x^5y^5 + (94m+94n-516)x^5y^5$$

$$\int_0^y \frac{f(x,y)}{y} dx$$
$$= \int_0^y (20+4m)x^3y^4 + (6m+6n-30)x^4y^4 + (40m+40n-30)x^4y^4 + (94m+94n-516)x^5y^4 dx$$
$$= \frac{1}{5}(20+4m)x^3y^5 + \frac{1}{5}(6m+6n-30)x^4y^5 + \frac{1}{5}(40m+40n-30)x^5y^5 + \frac{1}{5}(94m+94n-516)x^5y^5$$
$$m_M^2(G) = S_x S_y f(x,y) \mid x = y = 1$$

$$m_M^2(G) = (m+5)x^4y^5 + \frac{1}{5}(6m+6n-30)x^4y^5 + (8m+8n-6)x^5y^5 + \frac{1}{5}(94m+94n-516)x^6y^6$$
$$\frac{1}{5}(20+4m)x^3y^5 + \frac{1}{5}(6m+6n-30)x^4y^5 + \frac{1}{5}(40m+40n-30)x^5y^5 + \frac{1}{5}(94m+94n-516)x^5y^5$$

$$m_M^2(G) = S_x S_y f(x,y) \mid x = y = 1$$
$$m_M^2(G) = \frac{16021}{300} + \frac{14761}{300} + 1$$

The 3D plot of modified second Zagreb index is in figure, also can be seen that dependent variables used in the above index on the involved parameters.

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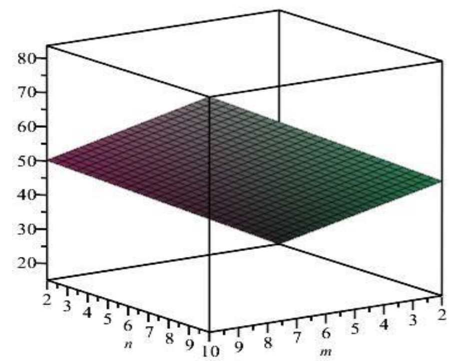

(a) Modified Zagreb

This could lead to the conclusion that the complexity of the hexagonal cage of order n and m copies can be accurately determined by the modified Zagreb index. Since the modified Zagreb index is a topological index, it is determined solely by the graph's structure and does not take into account the particular kinds of atoms or bonds that are there. It can therefore be used as a helpful tool to compare the complexity of various graphs.

Theorem 2.4. let HXC_n^m the hexagonal cage network work of order n with m copies then the inverse General Randić index is

$$RR_\alpha(G) = \left(S_x^\alpha S_y^\alpha\right)M(G,x,y)\big|_{x=y=1} = \frac{334}{5}m + \frac{226}{5}n - \frac{1147}{5}$$

Proof. let HXC_n^m the hexagonal cage network work of order n with m copies then the inverse General Randić index is defined as

$$RR_\alpha(G) = \left(S_x^\alpha S_y^\alpha\right)M(G,x,y) \mid x = y = 1$$

$$M(HX_n;x,y) = \sum_{i \le j} m_{ij}x^i y^j$$
$$= \sum_{4\le5} m_{45}x^4y^5 + \sum_{5\le5} m_{55}x^5y^5 + \sum_{5\le6} m_{56}x^5y^6 + \sum_{6\le6} m_{66}x^6y^6$$
$$= |E_1(HX_n)|x^4y^5 + |E_2(HX_n)|x^5y^5 + |E_3(HX_n)|x^5y^6 + |E_4(HX_n)|x^6y^6$$

$$M(HX_n;x,y) = (20+4m)x^4y^5 + (6m+6n-30)x^5y^5 + (40m+40n-30)x^5y^6 + (94m+94n-516)x^6y^6$$

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Now we first find

$$S_x = \int_0^x \frac{f(x,y)}{x} dx$$

$$M(HX_n; x, y) = (20 + 4m)x^4y^5 + (6m + 6n - 30)x^5y^5 + (40m + 40n - 30)x^5y^6 + (94m + 94n - 516)x^6y^6$$

$$\int_0^x \frac{f(x,y)}{x} dx$$
$$= \int_0^x (20 + 4m)x^4y^5 + (6m + 6n - 30)x^5y^5 + (40m + 40n - 30)x^5y^6 + (94m + 94n - 516)x^6y^6 dx$$
$$= \frac{1}{4}(20 + 4m)x^4y^5 + \frac{1}{5}(6m + 6n - 30)x^4y^5 + \frac{1}{5}(40m + 40n - 30)x^4y^6 + \frac{1}{5}(94m + 94n - 516)x^5y^6$$
$$= (5 + m)x^4y^5 + \frac{1}{5}(6m + 6n - 30)x^4y^5 + (8m + 8n - 6)x^5y^5 + \frac{1}{5}(94m + 94n - 516)x^6y^6$$
$$= (m + 5)x^4y^5 + \frac{1}{5}(6m + 6n - 30)x^4y^5 + (8m + 8n - 6)x^5y^5 + \frac{1}{5}(94m + 94n - 516)x^6y^6$$

Now we first find

$$S_y = \int_0^x \frac{f(x,y)}{y} dx$$

$$M(HX_n; x, y) = (20 + 4m)x^4y^5 + (6m + 6n - 30)x^5y^5 + (40m + 40n - 30)x^5y^5 + (94m + 94n - 516)x^5y^5$$

$$\int_0^y \frac{f(x,y)}{y} dx = \int_0^y (20 + 4m)x^3y^4 + (6m + 6n - 30)x^4y^4 + (40m + 40n - 30)x^4y^4 + (94m + 94n - 516)x$$
$$= \frac{1}{5}(20 + 4m)x^3y^5 + \frac{1}{5}(6m + 6n - 30)x^4y^5 + \frac{1}{5}(40m + 40n - 30)x^5y^5 + \frac{1}{5}(94m + 94n - 51$$

$$m_M^2(G) = S_xS_yf(x,y) \mid x = y = 1$$

$$RR_\alpha(G) = (S_xS_y)M(G,x,y) = (m + 5)x^4y^5 + \frac{1}{5}(6m + 6n - 30)x^4y^5 + (8m + 8n - 6)x^5y^5$$
$$+ \frac{1}{5}(94m + 94n - 516)x^6y^6 \frac{1}{5}(20 + 4m)x^3y^5 + \frac{1}{5}(6m + 6n - 30)x^4y^5$$
$$+ \frac{1}{5}(40m + 40n - 30)x^5y^5 + \frac{1}{5}(94m + 94n - 516)x^5y^5$$

taking both sides α, we get

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$$RR_\alpha(G) = \left(S_x^\alpha S_y^\alpha\right)M(G,x,y) = (m+5)x^4y^5 + \frac{1}{5}(6m+6n-30)x^4y^5 + (8m+8n-6)x^5y^5 + \frac{1}{5}(94m+94n-516)x^6y^6\frac{1}{5}(20+4m)x^3y^5 + \frac{1}{5}(6m+6n-30)x^4y^5 + \frac{1}{5}(40m+40n-30)x^5y^5 + \frac{1}{5}(94m+94n-516)x^5y^5$$

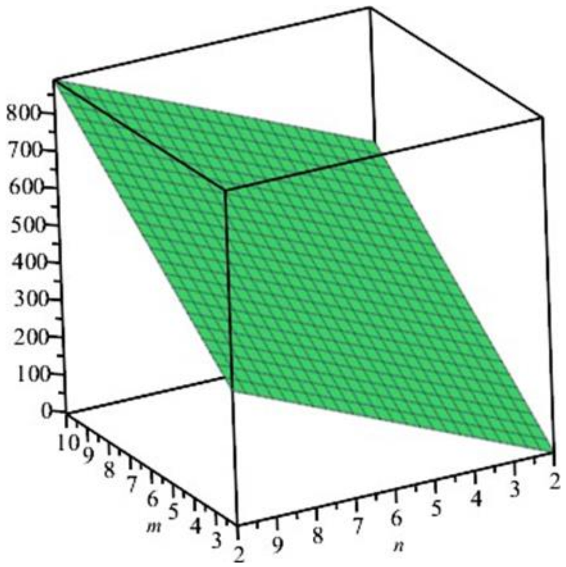
$$RR_\alpha(G) = \left(S_x^\alpha S_y^\alpha\right)M(G,x,y) = \left(m+5+4+\frac{4}{5}\right)x^4y^5 + \left(\frac{6}{5}m+\frac{6}{5}n-6+\frac{6}{5}+\frac{6}{5}n-5\right)x^5y^6 + (8m+8n-6+8m+8n-6)x^5y^6 + \left(\frac{94}{5}m+\frac{94}{5}n-\frac{516}{5}+\frac{94}{5}m+\frac{94}{5}n-\frac{516}{5}\right)x^5y^5$$

$$RR_\alpha(G) = \left(S_x^\alpha S_y^\alpha\right)M(G,x,y)\Big|_{x=y=1} = \frac{54}{5}m + \frac{12}{5}m + \frac{12}{5}n - 11 + 16m + 16n - 12 + \frac{188}{5}m + \frac{188}{5}n - \frac{1032}{5}$$

$$RR_\alpha(G) = \left(S_x^\alpha S_y^\alpha\right)M(G,x,y)\Big|_{x=y=1} = \frac{334}{5}m + \frac{226}{5}n - \frac{1147}{5}$$

The 3D plot of inverse general Randić index is shown in the figure, also can be seen that dependent variables used in the above index on the involved parameters.

Figures Modified the second Zagreb
index plotted in 3D Inverse Randić
index plotted in 3D



(a) Inverse Randić

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Theorem 2.5. let HXC_n^m the hexagonal cage network work of order n with m copies then the Symetric index is

$$SSD(G) = \left|D_x\delta_y + \delta_x D_y\right|_{x=y=1}$$

anditsfinalresultis

$$SSD(G) = \frac{17889}{100}m + \frac{17289}{100}n - 557$$

Proof.

$$\int_0^y \frac{f(x,y)}{y}dx = \int_0^y (20+4m)x^3y^4 + (6m+6n-30)x^4y^4 + (40m+40n-30)x^4y^4 + (94m+94n-516)x$$

$$= \frac{1}{5}(20+4m)x^4y^5 + \frac{1}{5}(6m+6n-30)x^4y^5 + \frac{1}{5}(40m+40n-30)x^5y^5 + \frac{1}{5}(94m+94n-51$$

Now

$$D_x\delta_y = 4(20+4m)x^3y^4 + 5(6m+6n-30)x^4y^5 + 5(40m+40n-30)x^4y^6 + 6(94m+94n-516)x^5y^5$$

$$S_x = \int_0^x \frac{f(x,y)}{x}dx$$

$$M(HX_n;x,y) = (20+4m)x^4y^5 + (6m+6n-30)x^5y^5 + (40m+40n-30)x^5y^6 + (94m + 94n - 516)x^6y^6$$

$$\int_0^x \frac{f(x,y)}{x}dx$$

$$= \int_0^x (20+4m)x^4y^5 + (6m+6n-30)x^5y^5 + (40m+40n-30)x^5y^6 + (94m+94n-516)x^6y^6dx$$

$$= \frac{1}{4}(20+4m)x^4y^5 + \frac{1}{5}(6m+6n-30)x^4y^5 + \frac{1}{5}(40m+40n-30)x^4y^6 + \frac{1}{5}(94m+94n-516)x^5y^6$$

$$= (5+m)x^4y^5 + \frac{1}{5}(6m+6n-30)x^4y^5 + (8m+8n-6)x^5y^5 + \frac{1}{5}(94m+94n-516)x^6y^6$$

$$= (m+5)x^4y^5 + \frac{1}{5}(6m+6n-30)x^4y^5 + (8m+8n-6)x^5y^5 + \frac{1}{5}(94m+94n-516)x^6y^6$$

$$\delta_x D_y = 5(m+5)x^4y^4 + \frac{1}{5}(6m+6n-30)x^5y^4 + 6(8m+8n-6)x^5y^5 + 6(94m + 94n - 516)x^6y^5$$

$$SSD(G) = \left|D_x\delta_y + \delta_x D_y\right|_{x=y=1} = [4(20+4m)x^3y^4 + 5(6m+6n-30)x^4y^5 + 5(40m+40n-30)x^4y^6$$
$$+6(94m+94n-516)x^5y^5]\left[(m+5)x^4y^5 + \frac{1}{5}(6m+6n-30)x^4y^5 + (8m+8n-6)x^5y^5 + \frac{1}{5}(94m+94n-516)x^6y^6\right]$$

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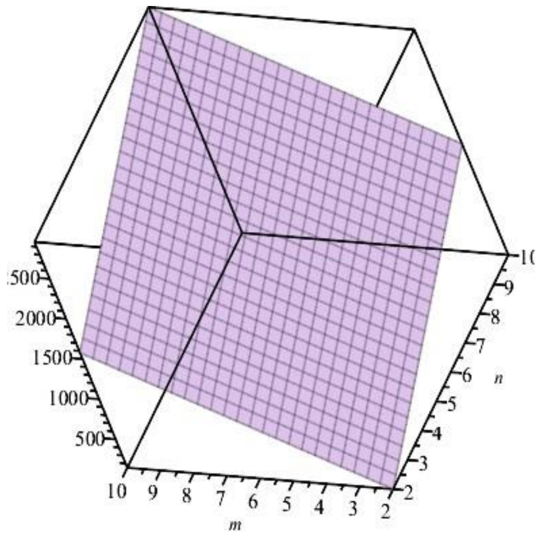
$$SSD(G) = \left|D_x\delta_y + \delta_x D_y\right|_{x=y=1} = \frac{17889}{100}m + \frac{17289}{100}n - 557$$

The 3D plot of symmetric division index is shown in the figure, also can be seen that dependent variables used in the above index on the involved parameters.



(a) Inverse Randić

Figures index plotted in 3D.

Theorem 2.6. let HXC_n^m the hexagonal cage network work of order n with m copies then the Harmonic index is defined as

$$H(G) = 2\delta_x JM(G;x,y)|_{x=y=1}$$
$$H(G) = 2\delta_x JM(G;x,y)|_{x=y=1}$$
$$H(G) = 288m + 280n - 1112$$

Proof.

$$M(HX_n;x,y) = (20+4m)x^4y^5 + (6m+6n-30)x^5y^5 + (40m+40n-30)x^5y^5 + (94m+94n-516)x^5y^5$$

$$Jf(x,y) = Jf(x,x)Jf(x,y) = (20+4m)x^9 + (6m+6n-30)x^{10} + (40m+40n-30)x^{11} + (94m+94n-516)x^{12}$$

$$\delta_x = \int_0^x \frac{f(x,y)}{x}dx = \frac{1}{7}(20+4m)x^7 + \frac{1}{10}(6m+6n-30)x^{10} + \frac{1}{11}(40m+40n-30)x^{11} + \frac{1}{12}(94m+94n-516)x^{12}$$

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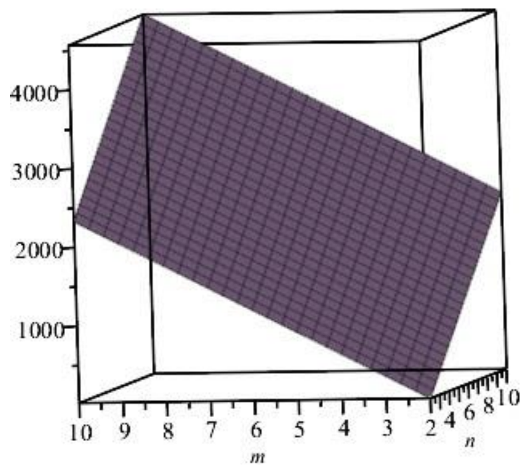
$$H(G) = 2\delta_x JM(G;x,y)|_{x=y=1} = 2(20+4m) + 2(6m+6n-30) + 2(40m+40n-30) + 2(94m+94n-516)$$

$$H(G) = 2\delta_x JM(G;x,y)|_{x=y=1} = 2(20+4m) + 2(6m+6n-30) + 2(40m+40n-30) + 2(94m+94n-516) \ldots$$

$$H(G) = 2\delta_x JM(G;x,y)|_{x=y=1} = 288m + 280n - 1112$$



(a) Inverse Randić

Theorem 2.7. let, HXC_n^m the hexagonal cage network work of order n with m copies then the Inverse sum index is defined as

$$I(G) = \delta_x D_X D_Y M(G;x,y)|_{x=y=1}$$

$$I(G) = 5054m + 4974n - 20006$$

Proof.

$$M(HX_n;x,y) = (20+4m)x^4y^5 + (6m+6n-30)x^5y^5 + (40m+40n-30)x^5y^6 + (94m+94n-516)x^6y^6$$

$$D_y = 5(20+4m)x^4y^5 + 5(6m+6n-30)x^5y^5 + 6(40m+40n-30)x^5y^6 + 6(94m+94n-516)x^6y^6$$

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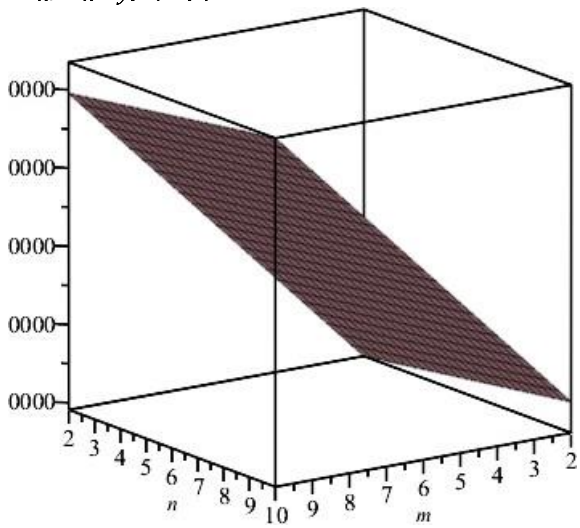
$$D_x D_y = 20(20+4m)x^9 + 25(6m+6n-30)x^{10} + 36(40m+40n-30)x^{11} + 36(94m+94n-516)x^{12}$$

$$S_x = \int_0^x \frac{f(x,y)}{x} dx$$

$$\delta_x J D_x D_y f(x,y) = \frac{20(20+4m)x^9}{9} + 25\frac{(6m+6n-30)x^{10}}{10} + 36\frac{(40m+40n-30)x^{11}}{11} + 36\frac{(94m+94n-516)x^{12}}{12}$$

$$\delta_x J D_x D_y f(x,y) = 5054m + 497n - 20006$$



(a) Inverse Randić

Conclusion

We study the closed-form M-Polynomials for n-order hexagonal cage networks with m copies in this paper. We analyse a large collection of popular topological indices, such as the Randić index and the first, second, and third Zagreb indices. We have made significant contributions to the field of hexagonal cage networks by developing a number of closed-form indices, including the General Randić index, Inverse General Randić index, Symmetric division index, Harmonic index, and Inverse sum index. These indices have provided new insights into the physical, chemical, and biological characteristics of hexagonal cage networks, such as their strength, boiling point, fracture toughness, and heat of formation.

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Furthermore, we offer computer-aided evaluations of these indices along with corresponding parameters, emphasizing their robust associations with molecular structures.

Data Availability

In this article, no data were utilized.

Authors Contributions

All authors contributed equally.

Conflicts of Interest

Authors have no conflict of interest.

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