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Evaluation of some degree based topological indices of boron kagome lattice

Divyashree B. K. *

Department of Mathematics, Bangalore University, Bangalore, 560056, India.

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Abstract

The technique of securing information or data in the form of images, codes, merging words etc are closely related to the disciplines of cryptanalysis and cryptology. Analogous to this numerical encoding of chemical structure, connected to topological indices is also growing significantly in the field of chemical graph theory. One of the salient features of topological indices is to predict the characteristics prescribed by the molecule's chemical structure. In this paper, we calculate the topological indices of the two-dimensional Boron Kagome Lattice by M- polynomial. Further, the graphical representation of the M-polynomial and the topological indices are obtained.

Keywords: Boron Kagome Lattice; Reduced reciprocal randic; $\boldsymbol{SK}$ index; General sum-connectivity index; $\boldsymbol{SK_1}$ index; First Zagrab index; Forgotten index; $\boldsymbol{SK_2}$ index; Arithmetic geometric index; $\boldsymbol{SCI_\gamma}$ index

1. Introduction

Graph theory as various branches, in which Chemical graph theory plays a very important role where a chemical compound is represented by simple graph called molecular graph in which atoms are vertices and atomic bounds are edges of a molecule. In recent times we see another emerging field that is Cheminformatics, in which the relationship between structural property and quantitative structural activities are studied to predict biological activities of the structure.

In 1947 Weiner first introduced topological indices, it is a process in which the data related to chemical compounds is converted to some numerical values. These topological indices have many applications in the field of chemistry and graph theory, precisely in QSAR and QSPR studies. Topological indices are divided majorly in to eccentricity-based, degree-based, distance-based, spectrum-based, and so on. The degree-based topological indices are obtained by degrees of the vertices of the molecular graph of the corresponding chemical structures.

Graph polynomials encode the information of a graph and build up various algebraic methods to find out the hidden information of a graph. Several important graph algebraic polynomials have been introduced. Some of them are Hosoye polynomial [1], Matching polynomial [2], M-polynomial [3], and so on.

To compute the numerical values of the topological indices, there are multiple methods such as by using integrals or derivatives or by graph polynomials. We see similar type of works done in [4-6]. In [7], Gutman and Furtula established a reduced reciprocal index in 2015.The reduced reciprocal randic index is defined as

$$R(G) = \sqrt{(d_s - 1)(d_l - 1)}\,.$$

* Corresponding author: Divyashree BK
Department of Mathematics, Bangalore University, Bangalore, 560056, India.

In [6], Deutsch and Klawzar used the arithmetic geometric index which is defined as

$$AG_1(G) = \sum_{sl\in E(G)} \frac{d_s + d_l}{2\sqrt{d_s d_l}}$$

In 2016, Shegehalli and Kanabur used SK, SK_1, SK_2 indices which are defined as follows [8].

$$SK(G) = \sum_{sl\in E(G)} \frac{d_s + d_l}{2}$$

$$SK_1(G) = \sum_{sl\in E(G)} \frac{d_s d_l}{2}$$

$$SK_2(G) = \sum\nolimits_{sl\in E(G)} (\frac{d_s d_l}{2})^2$$

First Zagreb index which was defined as follows and was introduced in 2014 [9].

$$EM_1(G) = \sum_{sl\in E(G)} (d_{sl})^2$$

In [10], Du.et.al introduced sum connectivity index which is defined as

$$SCI(G) = \sum_{sl\in E(G)} \frac{1}{\sqrt{d_s + d_l}}$$

Du.et.al also introduced SCI_γ index which is defined as [12]

$$SCI_\gamma(G) = \sum_{sl\in E(G)} (d_s + d_l)^\gamma$$

In 2015, Gutman and Furtula introduced forgotten index which is defined as

$$F(G) = \sum_{sl\in E(G)} (d_s^2 + d_l^2)$$

The M-polynomial is introduced in 2015 [8] defined as $M_f(G,x,y) = \sum_{\mu\le s\le l\le \xi} f_{sl}\,(G)x^s y^l$

Where$\mu = \max\{\, d_i : i \in V(G)\}$, $\xi = \min\{d_i : i \in V(G)\}$ and $f_{sl}(G)$ is the set of all edges such that$\{d_g, d_h\} = \{s, l\}$.

Lately, many researchers have examined the M-polynomials of several graph structures. In [11], the M-polynomial of the two-dimensional three-layered single-walled titania nanotube lattice was studied by Raheem *et al.*, The topological indices through M-polynomial of book graphs were found by Khalaf *et al.*, [12]. Some other works related to M-polynomials was also found in [13,14]. In this paper, we compute the topological indices of Boron Kagome Lattice with the help of M-polynomial.

In Table 1, degree-dependent topological indices via M-polynomial are provided

Table 1 Molecular descriptors and M-polynomial expressions

	Topological Index	**Resulting from $\mathbf{M_f(G,x,y)}$**
1	Reduced reciprocal randic	$RRR(G) = D_x^{(1/2)} D_y^{(1/2)} Q_{y(-1)}\, Q_{x(-1)}[g(x,y)]_{x=y=1}$
2	Arithmetic geometric index	$AG_1(G) = (1/2)D_x J S_x^{(1/2)} S_y^{(1/2)}[g(x,y)]_{x=1}$
3	SK index	$SK(G) = (1/2)(D_x + D_y)\ [g(x,y)]_{x=y=1}$
4	SK_1 index	$SK_1(G) = (1/2)(D_x D_y)[g(x,y)]_{x=y=1}$
5	SK_2 index	$SK_2(G) = (1/4)(D_x^{\ 2})J[g(x,y)]_{x=y=1}$
6	First Zagrab index	$EM_1(G) = D_x^2 Q_{x(-2)} J[g(x,y)]_{x=1}$
7	General sum connectivity index	$SCI(G) = S_x^{(1/2)}\, J[g(x,y)]_{x=1}$
8	Forgotten index	$F(G) = (D_x^2 + D_y^2)\ [g(x,y)]_{x=y=1}$

Where

$$D_x g(x,y) = x\frac{\partial\big(g(x,y)\big)}{\partial x};\ D_y g(x,y) = y\frac{\partial\big(g(x,y)\big)}{\partial y};\ Jg(x,y) = \quad g(x,x);\quad Q_{x(\alpha)}g(x,y) = x^{\alpha}g(x,y);\ \ D_x^{(1/2)}\big(g(x,y)\big) = \sqrt{x\frac{\partial\big(g(x,y)\big)}{\partial x}}\sqrt{g(x,y)};\ \ D_y^{(1/2)}\big(g(x,y)\big) = \sqrt{y\frac{\partial\big(g(x,y)\big)}{\partial y}}\sqrt{g(x,y)};\quad S_x^{(1/2)}\big(g(x,y)\big) = \sqrt{\int_0^x \frac{g(t,y)}{t}dt}\sqrt{g(x,y)}\,;\quad S_y^{(1/2)}\big(g(x,y)\big) = \sqrt{\int_0^y \frac{g(x,t)}{t}dt}\sqrt{g(x,y)}$$

2. Boron kagome lattice

In this paper, the M-polynomial of Boron Kagome Lattice are found and this polynomial is used to derive few degree-based topological indices, let us denote Boron Kagome Lattice by $B_{KL}\{(m,n),x,y\}$. Here, we consider two-dimensional Boron Kagome Lattice (MgB_6) [27]. In the Figure 1(b), we see the structure of Boron Kagome Lattice (MgB_6). A triangular magnesium layer is sandwiched in between every set of Kagome layers. In the structure, the atoms of magnesium are placed at the centers of the hexagonal holes when viewed from the top. Between every two magnesium atoms there is no direct connection, although it is encircled by six boron atoms which sums up-to degree six. In the lattice structure we see Boron atoms are of degree-4.

As the result of covalent bond formation of the ionic bond between magnesium and boron and of Boron Kagome Lattice (MgB_6) we see the lattice structure cultivates the transfer of electrons and stabilizes the two-dimensional structure, this can be used as an electrode the field of nanoelectronics. Because of the superconductivity the Boron Kagome Lattice (MgB_6) can be used as a superconductor in addition to (MgB_2). This structure can be used for storing hydrogen energy which is one of the major applications of nano energy.

In the structure of Boron Kagome Lattice, the magnesium atoms are represented by green-colour and the yellow-colour are the Boron atoms of the lattice.

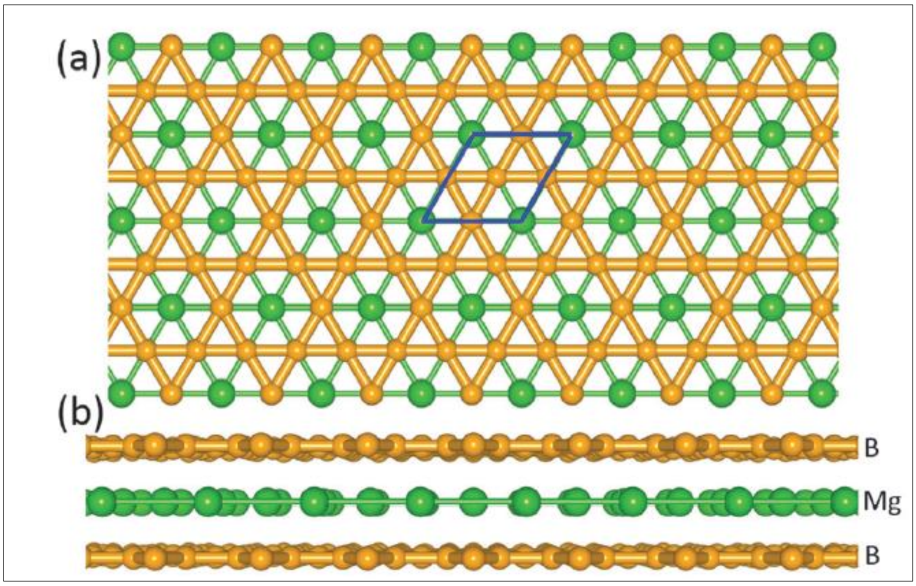

Figure 1 The structure of MgB_6. (a) is the top view and (b) is the side view

For the better comprehension of the structure, assigning some specific values to m and n are considered. In Figure 2, green-coloured edges denote the relation between atoms of Boron and Magnesium, the yellow-coloured edges denote the association of two Boron atoms.

In Figure 3, several colours have been used to distinguish the edge partitions like the association between 4-degree and 2-degree vertices and also three degree and three degree vertices, for grey colour, the edge partition of two degree and five vertices as green colour, orange for four-degree and three-degree vertices, the edge partition of six-degree and three-degree vertices as pink colour, for 4-degree and 4-degree vertices as yellow colour, five-degree and four-degree vertices as violet colour, six-degree and four-degree vertices as blue colour, six-degree and five-degree vertices as red colour and the edge partition of 6-degree and 6-degree vertices as black colour.

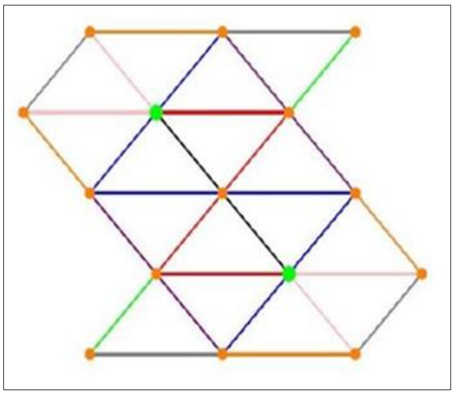

Figure 2 For m=1, n=1

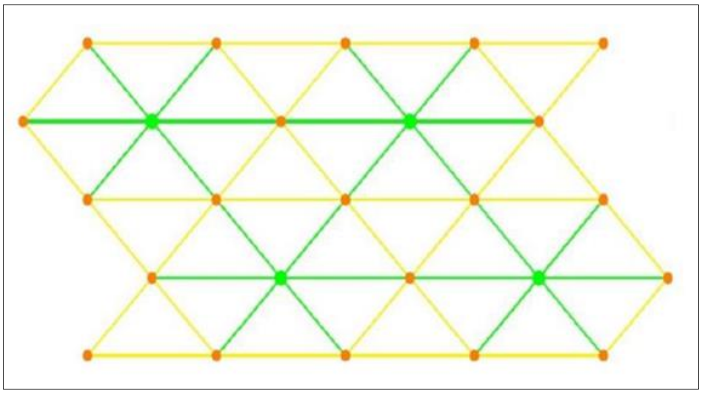

Figure 3 For m=1, n=2

3. Topological indices of boron kagome lattice

Theorem 1. Let $B_{KLM}(m,n)$ be the Boron Kagome Lattice. The M −polynomial is

$M_f(B_{KLM}(m,n)\,,x,y) = 2x^2y^4 + 2x^2\,y^5 + 2x^3y^3 + 4mx^3y^4 + (2m+2)x^3y^6 + (4n-4)x^4y^4 + 4mx^4y^5 + (8m + 8n - 10)x^4y^6 + (6m-2)x^5y^6 + (24mn - 20m - 10n + 8)x^6y^6$. Then,

- $RRR(G) = m\big(2\sqrt{10} + 8\sqrt{3} + 8\sqrt{15} + 5\sqrt{12} - 100\big) + n\big(8\sqrt{15} - 38\big) + 120mn + \big(2\sqrt{3} + 4\sqrt{6} + 2\sqrt{10} - 10\sqrt{15} - 4\sqrt{5} + 36\big)$.
- $AG_1(G) = m\left(\frac{3}{\sqrt{2}} + \frac{9}{\sqrt{5}} + \frac{20}{\sqrt{6}} + \frac{33}{\sqrt{30}} - 20\right) + n\left(4 + \frac{20}{\sqrt{6}} - 10\right) + 24mn + \left(\frac{3}{\sqrt{2}} + 6 + \frac{7}{\sqrt{10}} + \frac{7}{\sqrt{3}} + \frac{3}{\sqrt{2}} - \frac{25}{\sqrt{6}} - \frac{11}{\sqrt{30}}\right)$.
- $SK(G) = -6m - 4n + 144mn - 10$.
- $SK_1(G) = -92m - 52n + 432mn + 7$.
- $SK_2(G) = 744mn - 68m - 46n - (25.5)$.
- $EM_1(G) = 2400mn - 608m - 344n + 66$.
- $SCI(G) = 4\sqrt{3}mn + m\left(\frac{4}{\sqrt{7}} + 2 + \frac{8}{\sqrt{10}} + \frac{6}{\sqrt{11}} - \frac{10}{\sqrt{3}}\right) + n\left(\sqrt{2} + \frac{8}{\sqrt{10}} - \frac{5}{\sqrt{3}}\right) + \left(\frac{4}{\sqrt{6}} + \frac{2}{\sqrt{7}} - \sqrt{2} + \frac{2}{3} - \sqrt{10} - \frac{2}{\sqrt{11}} + \frac{4}{\sqrt{3}}\right)$.
- $F(G) = 1728mn - 304m - 176n + 30$.

Proof: Let $M_f(B_{KLM}(m,n)\,,x,y) = f(x,y)$

- Reduced reciprocal randic index is

$$D_y^{(1/2)}Q_{y(-1)}Q_{x(-1)}\big(f(x,y)\big) = 2\sqrt{3}xy^3 + 4xy^4 + 2\sqrt{2}x^2y^2 + 4\sqrt{3}x^2y^3 + (2m+2)\sqrt{5}x^2y^5 + (4n-4)\sqrt{3}x^3y^3 + 8mx^3y^4 + \sqrt{5}(8m+8n-10)x^3y^5 + (6m-2)\sqrt{5}x^4y^5 + \sqrt{5}(24mn-20m-10n+8)x^5y^5.$$

$$D_x^{(1/2)}D_y^{(1/2)}Q_{y(-1)}Q_{x(-1)}\big(f(x,y)\big) = 2\sqrt{3}xy^3 + 4xy^4 + 4x^2y^2 + 4\sqrt{6}x^2y^3 + (2m+2)\sqrt{10}x^2y^5 + (12n-12)x^3y^3 + 8\sqrt{3}mx^3y^4 + \sqrt{15}(8m+8n-10)x^3y^5 + (12m-4)\sqrt{5}x^4y^5 + 5(24mn-20m-10n+8)x^5y^5.$$

$$RRR(G) = D_x^{(1/2)}D_y^{(1/2)}Q_{y(-1)}\,Q_{x(-1)}[g(x,y)]_{x=y=1} = m\big(2\sqrt{10} + 8\sqrt{3} + 8\sqrt{15} + 5\sqrt{12} - 100\big) + n\big(8\sqrt{15} - 38\big) + 120mn + \big(2\sqrt{3} + 4\sqrt{6} + 2\sqrt{10} - 10\sqrt{15} - 4\sqrt{5} + 36\big).$$

- Arithmetic Geometric index is

$$S_x^{(1/2)}S_y^{(1/2)}\big(f(x,y)\big) = \frac{1}{\sqrt{2}}x^2y^4 + \frac{2}{\sqrt{10}}x^2\,y^5 + \frac{2}{3}x^3y^3 + \frac{2}{\sqrt{3}}x^3y^4 + \frac{\sqrt{2}(m+1)}{3}x^3y^6 + (n-1)x^4y^4 + \frac{2m}{\sqrt{5}}x^4y^5 + \frac{(4m+4n-5)}{\sqrt{6}}x^4y^6 + \frac{(6m-2)}{\sqrt{30}}x^5y^6 + \frac{(24mn-20m-10n+8)}{6}x^6y^6.$$

$$JS_x^{(1/2)}S_y^{(1/2)}\big(f(x,y)\big) = \left(\frac{1}{\sqrt{2}}+\frac{2}{3}\right)x^6 + \left(\frac{2}{\sqrt{10}}+\frac{2}{\sqrt{3}}\right)x^7 + (n-1)x^8 + \left(\frac{\sqrt{2}(m+1)}{3}+\frac{2m}{\sqrt{5}}\right)x^9 + \frac{(4m+4n-5)}{\sqrt{6}}x^{10} + \frac{(6m-2)}{\sqrt{30}}x^{11} + \frac{(24mn-20m-10n+8)}{6}x^{12}.$$

$$(1/2)D_xJS_x^{(1/2)}S_y^{(1/2)}\big(g(x,y)\big) = \left(\frac{3}{\sqrt{2}}+2\right)x^6 + \left(\frac{7}{\sqrt{10}}+\frac{7}{\sqrt{3}}\right)x^7 + (4n-4)x^8 + \frac{9}{2}\left(\frac{\sqrt{2}(m+1)}{3}+\frac{2m}{\sqrt{5}}\right)x^9 + \frac{5(4m+4n-5)}{\sqrt{6}}x^{10} + \frac{11(3m-1)}{\sqrt{30}}x^{11} + (24mn-20m-10n+8)x^{12}.$$

$$AG_1(G) = (1/2)D_xJS_x^{(1/2)}S_y^{(1/2)}[g(x,y)]_{x=1} = m\left(\frac{3}{\sqrt{2}}+\frac{9}{\sqrt{5}}+\frac{20}{\sqrt{6}}+\frac{33}{\sqrt{30}}-20\right) + n\left(4+\frac{20}{\sqrt{6}}-10\right) + 24mn + \left(\frac{3}{\sqrt{2}}+6+\frac{7}{\sqrt{10}}+\frac{7}{\sqrt{3}}+\frac{3}{\sqrt{2}}-\frac{25}{\sqrt{6}}-\frac{11}{\sqrt{30}}\right).$$

- ***SK* index is**

$$D_x\big(f(x,y)\big) = 4x^2y^4 + 4x^2y^5 + 6x^3y^3 + 12mx^3y^4 + 3(2m+2)x^3y^6 + 4(4n-4)x^4y^4 + 16mx^4y^5 + 4(8m+8n-10)x^4y^6 + 5(6m-2)x^5y^6 + 6(24mn-20m-10n+8)x^6y^6.$$

$$D_y\big(f(x,y)\big) = 8x^2y^4 + 10x^2y^5 + 6x^3y^3 + 16mx^3y^4 + 6(2m+2)x^3y^6 + 4(4n-4)x^4y^4 + 20mx^4y^5 + 6(8m+8n-10)x^4y^6 + 6(6m-2)x^5y^6 + 6(24mn-20m-10n+8)x^6y^6.$$

$$\frac{1}{2}(D_x+D_y)\big(f(x,y)\big) = 6x^2y^4 + 7x^2y^5 + 6x^3y^3 + 14mx^3y^4 + (9m+9)x^3y^6 + 4(4n-4)x^4y^4 + 18mx^4y^5 + 5(8m+8n-10)x^4y^6 + 11(3m-1)x^5y^6 + 6(24mn-20m-10n+8)x^6y^6.$$

$$SK(G) = (1/2)(D_x+D_y)\ [g(x,y)]_{x=y=1} = -6m-4n+144mn-10.$$

- ***SK*$_1$ index is**

$$\frac{1}{2}(D_xD_y)\big(f(x,y)\big) = 8x^2y^4 + 10x^2y^5 + 9x^3y^3 + 24mx^3y^4 + 9(2m+2)x^3y^6 + 8(4n-4)x^4y^4 + 40mx^4y^5 + 12(8m+8n-10)x^4y^6 + 15(6m-2)x^5y^6 + 18(24mn-20m-10n+8)x^6y^6.$$

$$SK_1(G) = (1/2)(D_xD_y)\ [g(x,y)]_{x=y=1} = -92m-52n+432mn+7.$$

- ***SK*$_2$ index is**

$$J\big(f(x,y)\big) = 4x^6 + (4m+2)x^7 + (4n-4)x^8 + (6m+2)x^9 + (8m+8n-10)x^{10} + (6m-2)x^{11} + (24mn-20m-10n+8)x^{12}.$$

$$(1/4)D_x^2J\big(f(x,y)\big) = 36x^6 + \frac{49}{4}(4m+2)x^7 + 16(4n-4)x^8 + \frac{81}{4}(6m+2)x^9 + 25(8m+8n-10)x^{10} + \frac{121}{4}(6m-2)x^{11} + 31(24mn-20m-10n+8)x^{12}.$$

$$SK_2(G) = (1/4)(D_x{}^2)J[g(x,y)]_{x=y=1} = 744mn-68m-46n-(25.5).$$

- **First zagrab index is**

$$Q_{x(-2)}J\big(f(x,y)\big) = 4x^4 + (4m+2)x^5 + (4n-4)x^6 + (6m+2)x^7 + (8m+8n-10)x^8 + (6m-2)x^9 + (24mn-20m-10n+8)x^{10}.$$

$$D_x^2Q_{x(-2)}J\big(f(x,y)\big) = 64x^4 + 25(4m+2)x^5 + 36(4n-4)x^6 + 49(6m+2)x^7 + 64\,(8m+8n-10)x^8 + 81(6m-2)x^9 + 100(24mn-20m-10n+8)x^{10}.$$

$$EM_1(G) = D_x^2Q_{x(-2)}J[g(x,y)]_{x=1} = 2400mn-608m-344n+66.$$

- **General sum connectivity index is**

$$S_x^{(1/2)}J\big(f(x,y)\big) = \frac{4}{\sqrt{6}}x^6 + \frac{1}{\sqrt{7}}(4m+2)x^7 + \frac{1}{2\sqrt{2}}(4n-4)x^8 + \frac{1}{3}(6m+2)x^9 + \frac{1}{\sqrt{10}}(8m+8n-10)x^{10} + \frac{(6m-2)}{\sqrt{11}}x^{11} + \frac{(24mn-20m-10n+8)}{2\sqrt{3}}x^{12}.$$

$$SCI(G) = S_x^{(1/2)} J[g(x,y)]_{x=1} = 4\sqrt{3}mn + m\left(\frac{4}{\sqrt{7}} + 2 + \frac{8}{\sqrt{10}} + \frac{6}{\sqrt{11}} - \frac{10}{\sqrt{3}}\right) + n\left(\sqrt{2} + \frac{8}{\sqrt{10}} - \frac{5}{\sqrt{3}}\right) + \left(\frac{4}{\sqrt{6}} + \frac{2}{\sqrt{7}} - \sqrt{2} + \frac{2}{3} - \sqrt{10} - \frac{2}{\sqrt{11}} + \frac{4}{\sqrt{3}}\right).$$

- **Forgotten index is**

$$D_x^2\big(f(x,y)\big) = 8x^2y^4 + 8x^2y^5 + 18x^3y^3 + 36mx^3y^4 + 9(2m+2)x^3y^6 + 16(4n-4)x^4y^4 + 64mx^4y^5 + 16(8m+8n-10)x^4y^6 + 25(6m-2)x^5y^6 + 36(24mn-20m-10n+8)x^6y^6.$$

$$D_y^2\big(f(x,y)\big) = 32x^2y^4 + 50x^2y^5 + 18x^3y^3 + 64mx^3y^4 + 36(2m+2)x^3y^6 + 16(4n-4)x^4y^4 + 100mx^4y^5 + 36(8m+8n-10)x^4y^6 + 36(6m-2)x^5y^6 + 36(24mn-20m-10n+8)x^6y^6.$$

$$(D_x^2 + D_y^2)\big(f(x,y)\big) = 40x^2y^4 + 58x^2y^5 + 36x^3y^3 + 100mx^3y^5 + 45(2m+2)x^3y^6 + 32(4n-4)x^4y^4 + 164mx^4y^5 + 52(8m+8n-10)x^4y^6 + 61(6m-2)x^5y^6 + 72(24mn-20m-10n+8)x^6y^6.$$

$$F(G) = (D_x^2 + D_y^2)\ [g(x,y)]_{x=y=1} = 1728mn - 304m - 176n + 30.$$

The topological values obtained through M-polynomial have different functioning with respect to the parameters x and y used. The values of M-polynomial can be modulated by the parameters x and y.

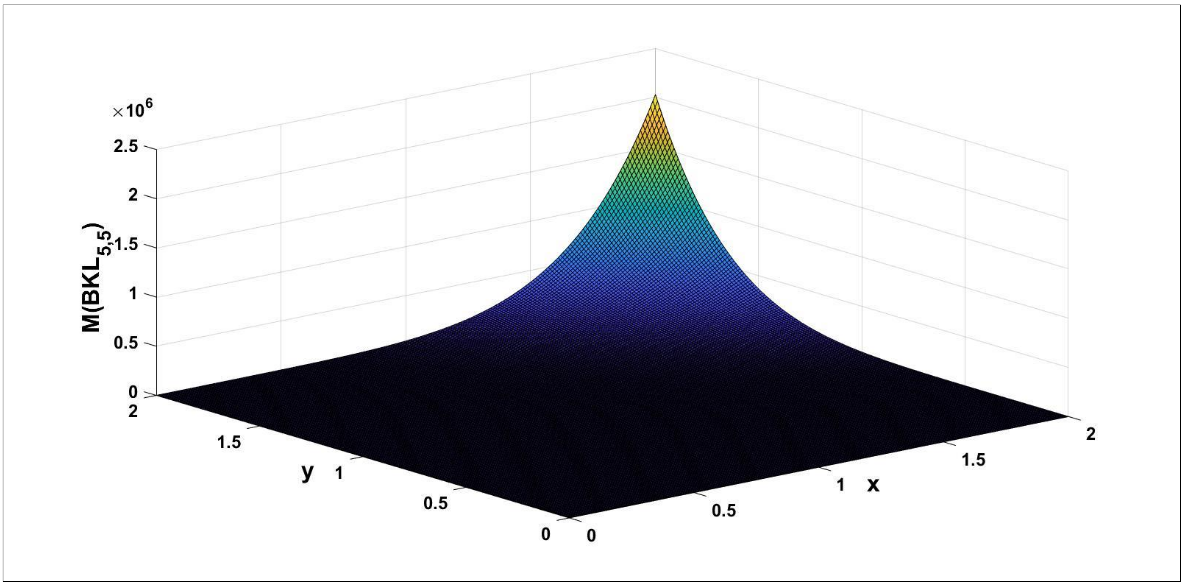

Figure 4 Plot of M-polynomial of Boron Kagome Lattice $\boldsymbol{B_{KLM}(5,5)}$

Now we plot the graphs of degree based topological indices of $\boldsymbol{B_{KLM}(5,5)}$.

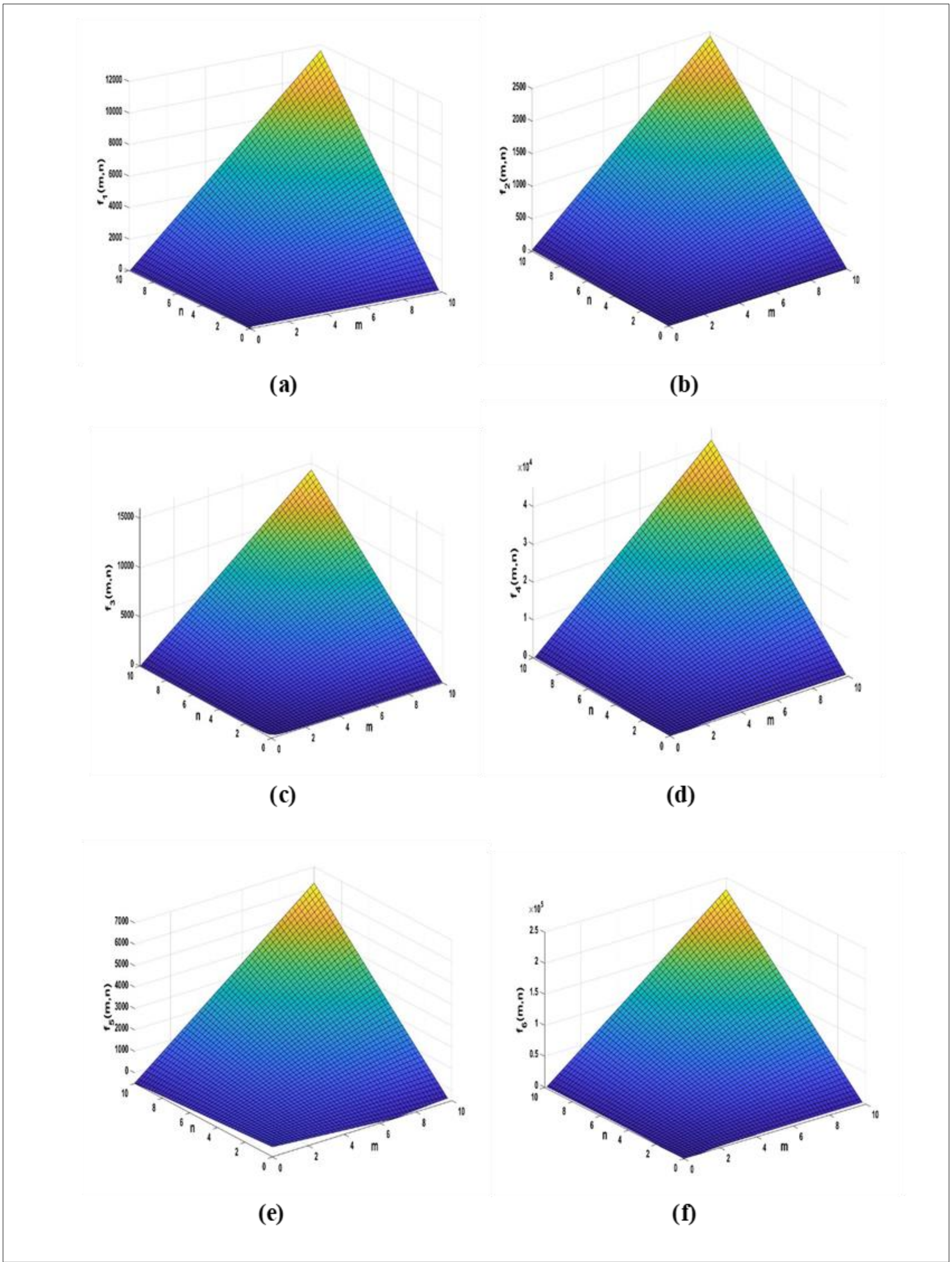

Figure 5 Plots of Topological indices of Boron Kagome Lattice. (a) $RRR(G)$.(b) $AG_1(G)$.(c) $SK(G)$.(d) $SK_1(G)$.(e) $SK_2(G)$.(f) $EM_1(G)$.(g) $SCI(G)$.(h) $F(G)$.

4. Conclusion

A topological index acts as a core instrument which maps every molecular structure to a mathematical number also it can be thought as a description of an entire molecular structure under testing. In this article, the degree based topological indices of Boron Kagome Lattice are calculated through M-polynomials. The graphs of these topological indices are plotted, which concludes that these indices are associated with structural parameters m and n as considered.

Compliance with ethical standards

Acknowledgments

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