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Topological Aspects Investigated from M-Polynomial of γ-Sheet of Boron Clusters

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Abstract

In this paper, we have taken the γ-sheet of molecular graph transformed from the chemical compound of boron clusters. After the conversion of graph into planar, finite, simple and connected with the help of various mathematical techniques, we have investigated M-Polynomials (MP) and topological invariants (TI). Different topological invariants such as first and second Zagreb, second modified Zagreb, general Randic, reciprocal general Randic, symmetric, harmonic, and inverse sum are determined from the M-Polynomial. We have also determined the atomic bond connectivity, geometric-arithmetic index and general harmonic index, first Gourava, second Gourava, first hyper-Gourava and second hyper-Gourava indices. We have also discussed the graphical behaviors of the above-mentioned structure.

Keywords: M-Polynomials, Topological indices, γ-sheet of Boron clusters, Molecular structure, Vertex, Edge

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1. Introduction

In these days different forms of boron clusters which is now available in novel clusters [1] that is infect best substitute of carbon fullerenes and nanotubes. These substitutes have so many characteristics. Science the element near to carbon in periodic Table, boron has a vital role in due to its electron deficiency and thermal characteristic. It does not react at ambient temperature and has a small covalent radius, directed covalent bonds. It's so many types cannot be determined yet, except of solid boron or prediction of novel nanostructures. In [2], currently published a paper on spherical boron clusters B_n.

This study of graph theory has been enhanced to chemical compounds and networks which lead us to the idea of chemical graph theory. So, with the combination of chemistry and graph theory a new branch called chemical graph theory (CGT) was invented. It gives the idea of graph theory to characterize molecular structures [3]. Our approach is the modeling of chemical compound by choosing its molecular structures, conversion into planar graph and then analyzing it by using topological invariants. Topological invariants have many structural properties and wide range of uses in structural chemistry. "A topological index is used to determine the chemical, physical, biological properties of a chemical compound". It has lot off uses in field of chemistry, biology, information, quantitative structure-activity relationship", etc. [3-7]. Gutman and Trinajstic' [8] in 1972 define first and second Zagreb indices. Later on, many modified and various Zagreb indices were invented, like modified Zagreb index [9], Augmented Zagreb index [10] etc. Augmented Zagreb index is most effective in the study of heat formation of octanes and heptanes. Randic in 1975 introduced degree-based invariants Randic´ index, which has so many applications in drug create [11]. Generalized form of Randic index [12] was also introduced. New form of the Randic index, called Harmonic index was defined by Siemion Fajtlowicz [13]. In chemical graph theory, there exist so many topological invariants [14-15]. The uses of these structural invariants in many fields are remarkable [16] and a lot of peoples working on this idea to invent new invariants that links with the structural properties of a chemical compound more accurately [17-19]. Idea of M-Polynomial was given by Deutschand Klavžar [20], which indeed give us a polynomial by using it we can, find various topological invariants. In this paper, many invariants of molecular graph of the chemical compound of γ-sheet of boron clusters are determined by using M-Polynomial formula. The molecular graphs of the chemical compound of γ-sheet of boron clusters is shown in Figure 1. Atomic bond connectivity index in 1998 was defined as [21].

$$ABC(B_1) = \sum_{\alpha\beta \in E(R)} \sqrt{\frac{d_\alpha + d_\beta - 2}{d_\alpha d_\beta}} \quad 1.1$$

Geometric arithmetic index is defined as [22],

$$GA(B_1) = \sum_{\alpha\beta \in E(R)} \frac{2\sqrt{d_\alpha d_\beta}}{d_\alpha + d_\beta} \quad 1.2$$

General harmonic index in 1998 was defined as [23],

$$H_r(B_1) = \sum_{\alpha\beta \in E(R)} \left(\frac{2}{d_\alpha + d_\beta}\right)^r \quad 1.3$$

Kalli gave the idea of first and second Gourava indices and defined as [24],

$$GO_1(B_1) = \sum_{\alpha\beta \in E(R)} \left[\left(d_\alpha + d_\beta\right) + \left(d_\alpha d_\beta\right)\right] \quad 1.4$$

$$GO_2(B_1) = \sum\nolimits_{\alpha\beta \in E(R)} \left[\left(d_\alpha + d_\beta\right)\left(d_\alpha d_\beta\right)\right] \quad 1.5$$

Kalli gave the idea of first hyper Gourava and second hyper Gourava indices as [25],

$$HGO_1(B_1) = \sum_{\alpha\beta \in E(R)} \left[\left(d_\alpha + d_\beta\right) + \left(d_\alpha d_\beta\right)\right]^2 \quad 1.6$$

$$HGO_2(B_1) = \sum_{\alpha\beta \in E(R)} \left[\left(d_\alpha + d_\beta\right)\left(d_\alpha d_\beta\right)\right]^2. \quad 1.7$$

1. Material and Methods

First of all, we obtain the transformed pattern of molecular structures of γ-sheet of boron clusters named as B_1. Further, we gave the idea of M-Polynomial and topological indices for B_1 by conversion of graphs into planar, finite, simple and connected graphs with the help of various mathematical techniques. Moreover, we describe the edge partition which depend upon degree-based vertices and then determine indices.

2. Results and Discussion

3.

Definition: For a graph G the M-Polynomial is defined as,

$$M(G;\ l,m) = \sum_{a \le b} m_{ab}\, l^a m^b.$$

Where a is the minimum degree among all vertices and b is the maximum degree such that $a \le b$.

3.1. M-Polynomial for Boron Clusters

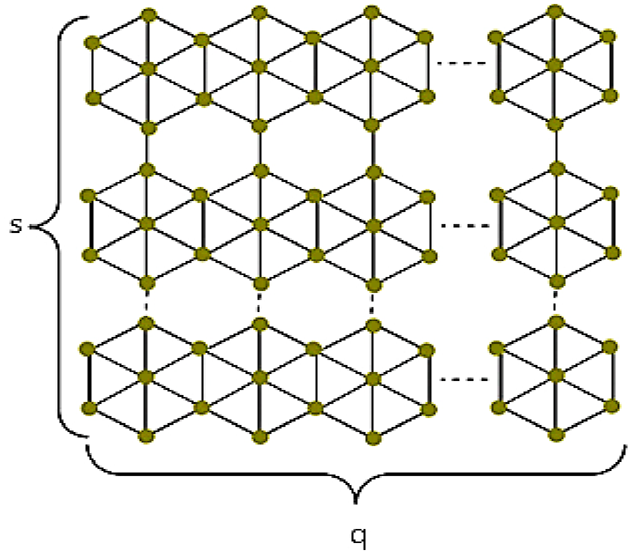


Figure 1. γ-sheet of Boron Clusters

Table 1: Edge partitions

Types of edges	Count of edges
$(3, 3)$	$2s + 4$
$(3, 4)$	$4s - 4$
$(3, 5)$	$4q - 4$
$(3, 6)$	$2q + 4s$
$(4, 4)$	$q(s - 1)$
$(4, 5)$	$4(q - 1)(s - 1)$
$(4, 6)$	$2q(s - 1)$
$(5, 5)$	$(q - 1)\ s$
$(5, 6)$	$4(q - 1)\ s$
Total number of edges	$12qs - q + s$

3.1.1 Theorem

M-Polynomial for γ-sheet of boron clusters is

$$M(B_1;\ l,m) = (2s+4)l^3m^3 + (4s-4)l^3m^4 + (4q-4)l^3m^5 + (2q+4s)l^3m^6 + q(s-1))l^4m^4 + 4(q-1)(s-1))l^4m^5 + 2q(s-1)l^4m^6 + s(q-\ 1)l^5m^5 + 4s(q-1)l^5m^6.$$

Proof: By definition of M-Polynomial and using Table 1,

$$M(B_1; l,m) = \sum_{a \le b} m_{ab}\, l^a m^b$$

$$= \sum_{3\le 3} m_{33} l^3\, m^3 + \sum_{3\le 4} m_{34} l^3\, m^4 + \sum_{3\le 5} m_{35} l^3\, m^5 + \sum_{3\le 6} m_{36} l^3\, m^6 + \sum_{4\le 4} m_{44} l^4\, m^4 + \sum_{4\le 5} m_{45} l^4\, m^5 + \sum_{4\le 6} m_{46} l^4\, m^6 + \sum_{5\le 5} m_{55} l^5\, m^5 + \sum_{5\le 6} m_{56} l^5\, m^6$$

$$= |E_{3,3}|l^3m^3 + |E_{3,4}|l^3m^4 + |E_{3,5}|l^3m^5 + |E_{3,6}|l^3m^6 + |E_{4,4}|l^4m^4 + |E_{4,5}|l^4m^5 + |E_{4,6}|l^4m^6 + |E_{5,5}|l^5m^5 + |E_{5,6}|l^5m^6$$
$$= (2s+4)l^3m^3 + (4s-4)l^3m^4 + (4q-4)l^3m^5 + (2q+4s)l^3m^6 + q(s-1)l^4m^4 + 4(q-1)(s-1))l^4m^5 + 2q(s-1)l^4m^6 + s(q-1)l^5m^5 + 4s(q-1)l^5m^6.$$

Table 2: Investigation of degree-based topological descriptors from M-Polynomials

Topological index	Derivation from $M(W_1;\ u, v)$
First Zagreb	$(D_l + D_m)M(B_1; l, m)\|l = m = 1$
Second Zagreb	$(D_l D_m)M(B_1; l, m)\|l = m = 1$
Second modified Zagreb	$(S_l^{\eta} S_m^{\eta})M(B_1; l, m)\|l = m = 1$
General Randic	$(D_l^{\eta} D_m^{\eta})M(B_1; l, m)\|l = m = 1$
Reciprocal general Randic	$(S_l^{\eta} S_m^{\eta})M(B_1; l, m)\|l = m = 1$
Symmetric division	$(S_m D_l + S_l D_m)M(B_1; l, m)\|l = m = 1$
Harmonic	$2S_l\, J(M(B_1; l, m)\|l = m = 1$
Inverse sum	$S_l J D_l D_m(f(l, m))\|l = m = 1$

Where $D_l = l\frac{\partial f(l,\ m)}{\delta l}$, $D_m = m\frac{\partial f(l,\ m)}{\delta m}$, $S_l = \int_0^l \frac{f(t,\ m)}{t}dt$, $S_m = \int_0^m \frac{f(l,\ t)}{t}dt$, $J(f(l,m)) = f(l, l)$.

3.1.2 Theorem

M-Polynomial of γ-sheet of boron clusters is

$$M(B_1;\ l,m) = (2s+4)l^3m^3 + (4s-4)l^3m^4 + (4q-4)l^3m^5 + (2q+4s)l^3m^6 + q(s-1))l^4m^4 + 4(q-1)(s-1))l^4m^5 + 2q(s-1)l^4m^6 + s(q-1)l^5m^5 + 4s(q-1)l^5m^6.$$

Then, first Zagreb $M_1(B_1)$, second Zagreb $M_2(B_1)$, second modified Zagreb$M_2^m(B_1)$, general Randic $R_\eta\ (B_1)$, $\eta \in N$, reciprocal general Randic $RR_\eta\ (B_1)$, $\eta \in N$ and symmetric division $SDD(B_1)$ indices are obtained from M-Polynomial as follows:

$$M_1(B_1) = 14q - 36s + 150qs - 38$$
$$M_2(B_1) = -48q - 99s + 289qs + 32$$
$$M_2^m(B_1) = \frac{415}{360}q + \frac{91}{225}s + \frac{191}{1200}qs + \frac{2}{45}.$$
$$R_\eta(B_1) = 9^\eta(2s+4) + 12^\eta(4s-4) + 15^\eta(4q-4) + 18^\eta(2q+4s) + 16^\eta q(s-1) + 20^\eta(4)(q-1)(s-1)) + 24^\eta(2)q(s-1) + 25^\eta s(q-1) + 30^\eta(4)s(q-1)$$
$$RR_\eta(B_1) = \frac{2s+4}{9^\eta} + \frac{(4s-4)}{12^\eta} + \frac{(4q-4)}{15^\eta} + \frac{(2q+4s)}{18^\eta} + \frac{q(s-1)}{16^\eta} + \frac{4(q-1)(s-1))}{20^\eta} + \frac{2q(s-1)}{24^\eta} + \frac{s(q-1)}{25^\eta} + \frac{4s(q-1)}{30^\eta}$$
$$SDD(B_1) = -\frac{13}{10}q + \frac{201}{45}s + \frac{74}{3}qs - \frac{6}{5}.$$

Proof: Let $f(l,m) = M(B_1; l,m)$ be the M-Polynomial for γ-sheet of boron cluster B_1. Then,

$$M(B_1;\ l,m) = (2s+4)l^3m^3 + (4s-4)l^3m^4 + (4q-4)l^3m^5 + (2q+4s)l^3m^6 + q(s-1))l^4m^4 + 4(q-1)(s-1)l^4m^5 + 2q(s-1)l^4m^6 + s(q-1)l^5m^5 + 4s(q-1)l^5m^6.$$

All partial derivatives and integral are calculated, by putting the values from Table 1 and Table 2,

$$D_l f(l,m) = 3(2s+4)l^3m^3 + 3(4s-4)l^3m^4 + 3(4q-4)l^3m^5 + 3(2q+4s)l^3m^6 + 4q(s-1))l^4m^4 + 16(q-1)(s-1)l^4m^5 + 8q(s-1)l^4m^6 + 5s(q-1)l^5m^5 + 20s(q-1)l^5m^6.$$

$$D_m f(l,m) = 3(2s+4)l^3m^3 + 4(4s-4)l^3m^4 + 5(4q-4)l^3m^5 + 6(2q+4s)l^3m^6 + 4q(s-1))l^4m^4 + 20(q-1)(s-1)l^4m^5 + 12q(s-1)l^4m^6 + 5s(q-1)l^5m^5 + 24s(q-1)l^5m^6.$$

$$D_l D_m f(l,m) = 9(2s+4)l^3m^3 + 12(4s-4)l^3m^4 + 15(4q-4)l^3m^5 + 18(2q+4s)l^3m^6 + 16q(s-1))l^4m^4 + 80(q-1)(s-1)l^4m^5 + 48q(s-1)l^4m^6 + 25s(q-1)l^5m^5 + 120s(q-1)l^5m^6.$$

$$S_l S_m f(l,m) = \frac{2s+4}{9}l^3m^3 + \frac{(4s-4)}{12}l^3m^4 + \frac{(4q-4)}{15}l^3m^5 + \frac{(2q+4s)}{18}l^3m^6 + \frac{q(s-1)}{16}l^4m^4 + \frac{4(q-1)(s-1)}{20}l^4m^5 + \frac{2q(s-1)}{24}l^4m^6 + \frac{s(q-1)}{25}l^5m^5 + \frac{4s(q-1)}{30}l^5m^6.$$

$$D_l^\eta D_m^\eta f(l,m) = 9^\eta(2s+4)l^3m^3 + 12^\eta(4s-4)l^3m^4 + 15^\eta(4q-4)l^3m^5 + 18^\eta(2q+4s)l^3m^6 + 16^\eta q(s-1)l^4m^4 + 20^\eta(4)(q-1)(s-1)l^4 + 24^\eta(2)q(s-1)l^4m^6 + 25^\eta s(q-1)l^5m^5 + 30^\eta(4)s(q-1)l^5m^6\ .$$

$$S_l^\eta S_m^\eta f(l,m) = \frac{2s+4}{9^\eta}l^3m^3 + \frac{(4s-4)}{12^\eta}l^3m^4 + \frac{(4q-4)}{15^\eta}l^3m^5 + \frac{(2q+4s)}{18^\eta}l^3m^6 + \frac{q(s-1)}{16^\eta}l^4m^4 + \frac{4(q-1)(s-1)}{20^\eta}l^4m^5 + \frac{2q(s-1)}{24^\eta}l^4m^6 + \frac{s(q-1)}{25^\eta}l^5m^5 + \frac{4s(q-1)}{30^\eta}l^5m^6.$$

$$S_mD_lf(l,m) = \frac{3(2s+4)}{3}l^3m^3 + \frac{3(4s-4)}{4}l^3m^4 + \frac{3(4q-4)}{5}l^3m^5 + \frac{3(2q+4s)}{6}l^3m^6 + \frac{4q(s-1)}{4}l^4m^4 + \frac{16(q-1)(s-1)}{5}l^4m^5 + \frac{8q(s-1)}{6}l^4m^6 + \frac{5s(q-1)}{5}l^5m^5 + \frac{20s(q-1)}{6}l^5m^6.$$

$$S_lD_mf(l,m) = \frac{3(2s+4)}{3}l^3m^3 + \frac{4(4s-4)}{3}l^3m^4 + \frac{5(4q-4)}{3}l^3m^5 + \frac{6(2q+4s)}{3}l^3m^6 + \frac{4q(s-1)}{4}l^4m^4 + \frac{20(q-1)(s-1)}{4}l^4m^5 + \frac{12q(s-1)}{4}l^4m^6 + \frac{5s(q-1)}{5}l^5m^5 + \frac{24s(q-1)}{5}l^5m^6.$$

Hence,

$$M_1(B_1) = (D_l+D_m)f(l,m)|l=1=m = -36s + 14q + 150qs$$

$$M_2(B_1) = D_lD_mf(l,m)|l=1=m = -48q - 99s + 289qs + 32$$

$$M_2{}^m(B_1) = S_lS_m\, f(l,m)|l=1=m$$

$$M_2^m(B_1) = \frac{91}{225}s + \frac{415}{360}q + \frac{191}{1200}qs + \frac{2}{45}.$$

$$R_\eta(B_1) = D^\eta{}_l D^\eta{}_m f(l,m)|l=1=m$$

$$R_\eta(B_1) = 9^\eta(2s+4) + 12^\eta(4s-4) + 15^\eta(4q-4) + 18^\eta(2q+4s) + 16^\eta q(s-1) + 20^\eta(4)(q-1)(s-1) + 24^\eta(2)q(s-1) + 25^\eta s(q-1) + 30^\eta(4)s(q-1)$$

$$RR_\eta(B_1) = S_l{}^\eta S_m{}^\eta f(l,m)|l=1=m` = \frac{2s+4}{9^\eta} + \frac{(4s-4)}{12^\eta} + \frac{(4q-4)}{15^\eta} + \frac{(2q+4s)}{18^\eta} + \frac{q(s-1)}{16^\eta} + \frac{4(q-1)(s-1))}{20^\eta} + \frac{2q(s-1)}{24^\eta} + \frac{s(q-1)}{25^\eta} + \frac{4s(q-1)}{30^\eta}.$$

$$SDD = (S_mD_l + S_lD_m)f(l,m)|l=1=m = -\frac{13}{10}q + \frac{201}{45}s + \frac{74}{3}qs - \frac{6}{5}.$$

3.1.3 Theorem

M-Polynomial of γ-sheet boron cluster is

$$M(B_1;\, l,m) = (2s+4)l^3m^3 + (4s-4)l^3m^4 + (4q-4)l^3m^5 + (2q+4s)l^3m^6 + q(s-1))l^4m^4 + 4(q-1)(s-1))l^4m^5 + 2q(s-1)l^4m^6 + s(q-1)l^5m^5 + 4s(q-1)l^5m^6.$$

Then, harmonic index $H(B_1)$ and inverse sum index $I(B_1)$ are calculated from M-Polynomial as follows:

$$H(B_1) = -\frac{1}{15}q + \frac{1}{3}s + \frac{73}{90}qs + \frac{37}{180}$$

$$I(B_1) = -\frac{77}{90}q - \frac{6155}{1386}s + \frac{28807}{990}qs + \frac{506}{63}.$$

Proof: By using Table 2 we have,

$$H(B_1) = 2S_l\,J\big(f(l,m)\big)|l=1=m = -\frac{1}{15}q + \frac{1}{3}s + \frac{73}{90}qs + \frac{37}{180}$$

$$I(B_1) = S_l\,JD_lD_m\big(f(l,m)\big)|l=1=m = -\frac{77}{90}q - \frac{6155}{1386}s + \frac{28807}{990}qs + \frac{506}{63}.$$

3.1.4 Theorem

For B_1, the atomic bond connectivity $ABC(B_1)$, geometric arithematic index $GA(B_1)$ and general harmonic index $H_r(B_1)$ are determined as follows.

$$(a)\ ABC(B_1) = (2s+4)\sqrt{\frac{4}{9}} + (4s-4)\sqrt{\frac{5}{12}} + (4q-4)\sqrt{\frac{2}{5}} + (2q+4s)\sqrt{\frac{7}{18}} + q(s-1)\left[\sqrt{\frac{3}{8}} + \frac{2}{\sqrt{3}}\right] + 4(q-1)(s-1)\sqrt{\frac{7}{20}} + s(q-1)\left[\frac{2\sqrt{2}}{5} + \frac{4\sqrt{3}}{10}\right]$$

$$(b)\ GA(B_1) = (2s+4) + (4s-4)\frac{4\sqrt{3}}{7} + (4q-4)\frac{1}{\sqrt{2}} + (2q+4s)\frac{2\sqrt{2}}{3} + q(s-1)\left[1 + \frac{4\sqrt{6}}{5}\right] + (q-1)(s-1)\frac{16\sqrt{5}}{9} + s(q-1)\left[1 + \frac{8\sqrt{30}}{11}\right]$$

$$(c)\ H_r(B_1) = (2s+4)\left(\frac{1}{3}\right)^r + (4s-4)\left(\frac{2}{7}\right)^r + (4q-4)\left(\frac{1}{4}\right)^r + (2q+4s)\left(\frac{2}{9}\right)^r + q(s-1)\left(\frac{1}{4}\right)^r + 4(q-1)(s-1)\left(\frac{2}{9}\right)^r + 2q(s-1)\left(\frac{1}{5}\right)^r + s(q-1)\left(\frac{1}{5}\right)^r + 4(q-1)s\left(\frac{2}{11}\right)^r.$$

Proof:

(a) By using equation 1.1 we have,

$$ABC(B_1) = \sum_{\alpha\beta\in E(R)} \sqrt{\frac{d_\alpha + d_\beta - 2}{d_\alpha d_\beta}}.$$

Putting the values from Table 1.

$$ABC(B_1) = (2s+4)\sqrt{\frac{3+3-2}{3\times 3}} + (4s-4)\sqrt{\frac{3+4-2}{3\times 4}} + (4q-4)\sqrt{\frac{3+5-2}{3\times 5}} + (2q+4s)\sqrt{\frac{3+6-2}{3\times 6}} + q(s-1)\sqrt{\frac{4+4-2}{4\times 4}} + 4(q-1)(s-1))\sqrt{\frac{4+5-2}{4\times 5}} + 2q(s-1)\sqrt{\frac{4+6-2}{4\times 6}} + s(q-1)\sqrt{\frac{5+5-2}{5\times 5}} + 4(q-1)s\sqrt{\frac{5+6-2}{5\times 6}}.$$

$$ABC(B_1) = (2s+4)\sqrt{\frac{4}{9}} + (4s-4)\sqrt{\frac{5}{12}} + (4q-4)\sqrt{\frac{2}{5}} + (2q+4s)\sqrt{\frac{7}{18}} + q(s-1)\left[\sqrt{\frac{3}{8}} + \frac{2}{\sqrt{3}}\right] + 4(q-1)(s-1)\sqrt{\frac{7}{20}} + (q-1)s\left[\frac{2\sqrt{2}}{5} + \frac{4\sqrt{3}}{10}\right].$$

(b) By using equation 1.2 we have,

$$GA(B_1) = \sum_{\alpha\beta\in E(R)} \frac{2\sqrt{d_\alpha d_\beta}}{d_\alpha + d_\beta}.$$

Putting the values from Table 1.

$$GA(B_1) = (2s+4)\frac{2\sqrt{3\times 3}}{3+3} + (4s-4)\frac{2\sqrt{3\times 4}}{3+4} + (4q-4)\frac{2\sqrt{3\times 5}}{3+5} + (2q+4s)\frac{2\sqrt{3\times 6}}{3+6} + q(s-1)\frac{2\sqrt{4\times 4}}{4+4} + 4(q-1)(s-1)\frac{2\sqrt{4\times 5}}{4+5} + 2q(s-1)\sqrt{\frac{4+6-2}{4\times 6}} + s(q-1)\sqrt{\frac{5+5-2}{5\times 5}} + 4(q-1)s\sqrt{\frac{5+6-2}{5\times 6}}$$

$$= (2s+4) + (4s-4)\frac{4\sqrt{3}}{7} + (4q-4)\frac{1}{\sqrt{2}} + (2q+4s)\frac{2\sqrt{2}}{3} + q(s-1)\left[1 + \frac{4\sqrt{6}}{5}\right] + (q-1)(s-1)\frac{16\sqrt{5}}{9} + (q-1)s\left[1 + \frac{8\sqrt{30}}{11}\right].$$

(c) By using equation 1.3 we have,

$$H_r(B_1) = \sum_{\alpha\beta\in E(R)} \left(\frac{2}{d_\alpha + d_\beta}\right)^r.$$

Putting the values from Table 1.

$$H_r(B_1) = (2s+4)\left(\frac{2}{3+3}\right)^r + (4s-4)\left(\frac{2}{3+4}\right)^r + (4q-4)\left(\frac{2}{3+5}\right)^r + (2q+4s)\left(\frac{2}{3+6}\right)^r + q(s-1)\left(\frac{2}{4+4}\right)^r + 4(q-1)(s-1)\left(\frac{2}{4+5}\right)^r + 2q(s-1)\left(\frac{2}{4+6}\right)^r + s(q-1)\left(\frac{2}{5+5}\right)^r + 4(q-1)s\left(\frac{2}{5+6}\right)^r.$$

$$H_r(B_1) = (2s+4)\left(\frac{1}{3}\right)^r + (4s-4)\left(\frac{2}{7}\right)^r + (4q-4)\left(\frac{1}{4}\right)^r + (2q+4s)\left(\frac{2}{9}\right)^r + q(S-1)\left(\frac{1}{4}\right)^r + 4(q-1)(s-1))\left(\frac{2}{9}\right)^r + 2q(s-1)\left(\frac{1}{5}\right)^r + s(q-1)\left(\frac{1}{5}\right)^r + 4(q-1)s\left(\frac{2}{11}\right)^r.$$

3.1.5 Theorem

For B_1, first Gourava, second Gourava, first hyper Gourava, and second hyper Gourava indices are determined as:

(a) $GO_1(B_1) = -62q - 101s + 407qs + 8$

(b) $GO_2(B_1) = -396q - 1198s + 2898qs - 8$

(c) $HGO_1(B_1) = -2450q - 6275s + 13973qs + 476$

(d) $HGO_2(B_1) = -151096q - 488668s + 759284qs + 55440.$

Proof:

(a) From equation 1.4 and using Table 3 we have,

$$GO_1(B_1) = \sum_{\alpha\beta\in E(R)} [(d_\alpha + d_\beta) + (d_\alpha d_\beta)]$$
$$= (2s+4)[(3+3)+(3\times 3)] + (4s-4)[(3+4)+(3\times 4)] + (4q-4)[(3+5)+(3\times 5)] + (2q+4s)[(3+6)+(3\times 6)] + q(s-1)[(4+4)+(4\times 4)] + 4(q-1)(s-1)[(4+5)+(4\times 5)] + 2q(s-1)[(4+6)+(4\times 6)] + s(q-1)[(5+5)+(5\times 5)] + 4(q-1)s[(5+6)+(5\times 6)]$$

$GO_1(B_1) = -62q - 101s + 407qs + 8.$

(b) From equation 1.5 and using Table 1 we have,

$$GO_2(B_1) = \sum_{\alpha\beta\in E(R)} [(d_\alpha + d_\beta)(d_\alpha d_\beta)]$$
$$= (2s+4)[(3+3)\times(3\times 3)] + (4s-4)[(3+4)\times(3\times 4)] + (4q-4)[(3+5)\times(3\times 5)] + (2q+4s)[(3+6)\times(3\times 6)] + q(s-1)[(4+4)\times(4\times 4)] + 4(q-1)(s-1)[(4+5)\times(4\times 5)] + 2q(s-1)[(4+6)\times(4\times 6)] + s(q-1)[(5+5)\times(5\times 5)] + 4(q-1)s[(5+6)\times(5\times 6)]$$

$GO_2(B_1) = -396q - 1198s + 2898qs - 8.$

(c) From equation 1.6 and using Table 3 we have,

$$HGO_1(B_1) = \sum_{\alpha\beta\in E(R)} [(d_\alpha + d_\beta) + (d_\alpha d_\beta)]^2$$
$$= (2s+4)[(3+3)+(3\times 3)]^2 + (4s-4)[(3+4)+(3\times 4)]^2 + (4q-4)[(3+5)+(3\times 5)]^2 + (2q+4s)[(3+6)+(3\times 6)]^2 + q(s-1)[(4+4)+(4\times 4)]^2 + 4(q-1)(s-1)[(4+5)+(4\times 5)]^2 + 2q(s-1)[(4+6)+(4\times 6)]^2 + s(q-1)[(5+5)+(5\times 5)]^2 + 4(q-1)s[(5+6)+(5\times 6)]^2.$$

$HGO_1(B_1) = -2450q - 6275s + 13973qs + 476$

(d) From equation 1.7 and using Table 1 we have,

$$HGO_2(B_1) = \sum_{\alpha\beta\in E(R)} [(d_\alpha + d_\beta)(d_\alpha d_\beta)]^2$$
$$= (2s+4)[(3+3)(3\times 3)]^2 + (4s-4)[(3+4)(3\times 4)]^2 + (4q-4)[(3+5)(3\times 5)]^2 + (2q+4s)[(3+6)(3\times 6)]^2 + q(s-1)[(4+4)(4\times 4)]^2 + 4(q-1)(s-1)[(4+5)(4\times 5)]^2 + 2q(s-1)[(4+6)(4\times 6)]^2 + s(q-1)[(5+5)(5\times 5)]^2 + 4(q-1)s[(5+6)(5\times 6)]^2.$$

4. Potential Applications for Chemists

Topological invariants [26-29] are very effective to calculate the chemical, physical, biological properties of a chemical compound. It has so many uses in chemistry, information, biology, quantitative structure-property relationships, online networking software, access of cheap price service facilities give us chance of generating secure social grid that led to effective social unity through shared subgraphs, industries, electronics, and medicines. In the following Table 3, we have some experimental physicochemical properties that are verified by our study.

Table 3: The experimented values for boron cluster are given below:

Chemical compound: Boron	BP	VP	ST	MP	D	MM
	2550	2140	1726	2076	2.3	10.81

The values of the linear regression for all topological indices can be computed by the formula given below,

$Y = a + bX.$ 1.8

Where Y is the chemical properties of the compound and X is the computed value of the topological indices, a and b are determined by the formula of regression coefficients. Thus, by using formula 1.8 and first Zagreb index $M_1(B_1)$, we have,

$BP = 2550 + (0)M_1(B_1)$, with $b = 0$ in 1.8.

This implies that $BP = 2550$ which indeed shows that BP determined from the regression model is same as the actual experimental BP as shown in Table 3.

Moreover,

$MP = 2076 + (0)M_1(B_1)$, with $b = 0$ in 1.8.

This implies that $MP = 2076$. Thus, experimental MP is equal to the actual MP(see Table 3). Similarly, by using formula 1.8 all other components VP, ST, D and MM for boron can be calculated.

In all cases actual and experimental values will be same. Continuing in this way, one can find all others values of linear regression of remaining topological indices i.e., $M_2(B_1)$, $M_2^m(B_1)$, $R_\eta\ (B_1)$, $RR_\eta\ (B_1)$, $SDD(B_1)$, $H(B_1)$, $I(B_1)$.

Table 4: M-Polynomial for $B_1\ at\ l = 1 = m$

Topological index	M-Polynomial for Boron clusters $(G = B_1)\ \vert l = 1 = m$
$M_1(G)$	$14q - 36s + 150qs - 38$

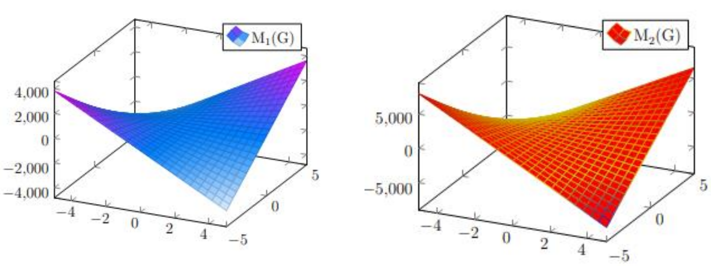
$M_2(G)$	$-48q - 99s + 289qs + 32$
$M_2^m(G)$	$\frac{415}{360}q + \frac{91}{225}s + \frac{191}{1200}qs + \frac{2}{45}$
$R_\eta(G)$	$9^\eta(2s+4) + 12^\eta(4s-4) + 15^\eta(4q-4) + 18^\eta(2q+4s) + 16^\eta q(s-1) + 20^\eta(4)(q-1)(s-1)) + 24^\eta(2)q(s-1) + 25^\eta s(q-1) + 30^\eta(4)s(q-1)$
$RR_\eta(G)$	$\frac{2s+4}{9^\eta} + \frac{(4s-4)}{12^\eta} + \frac{(4q-4)}{15^\eta} + \frac{(2q+4s)}{18^\eta} + \frac{q(s-1)}{16^\eta} + \frac{4(q-1)(s-1))}{20^\eta} + \frac{2q(s-1)}{24^\eta} + \frac{s(q-1)}{25^\eta} + \frac{4s(q-1)}{30^\eta}$
$SDD(G)$	$-\frac{13}{10}q + \frac{201}{45}s + \frac{74}{3}qs - \frac{6}{5}$
$H(G)$	$-\frac{1}{15}q + \frac{1}{3}s + \frac{73}{90}qs + \frac{37}{180}$
$I(G)$	$-\frac{77}{90}q - \frac{6155}{1386}s + \frac{28807}{990}qs + \frac{506}{63}$
$ABC(G)$	$(2s+4)\sqrt{\frac{4}{9}} + (4s-4)\sqrt{\frac{5}{12}} + (4q-4)\sqrt{\frac{2}{5}} + (2q+4s)\sqrt{\frac{7}{18}} + q(s-1)\left[\sqrt{\frac{3}{8}} + \frac{2}{\sqrt{3}}\right] + 4(q-1)(s-1)\sqrt{\frac{7}{20}} + (q-1)s\left[\frac{\sqrt{8}}{5} + \frac{4\sqrt{3}}{10}\right]$
$GA(G)$	$(2s+4) + (4s-4)\frac{4\sqrt{3}}{7} + (4q-4)\frac{1}{\sqrt{2}} + (2q+4s)\frac{2\sqrt{2}}{3} + (s-1)\left[1 + \frac{4\sqrt{6}}{5}\right] + (q-1)(s-1)\frac{16\sqrt{5}}{9} + (q-1)s\left[1 + \frac{8\sqrt{30}}{11}\right]$
$H_r(G)$	$(2s+4)\left(\frac{1}{3}\right)^r + (4s-4)\left(\frac{2}{7}\right)^r + (4q-4)\left(\frac{1}{4}\right)^r + (2q+4s)\left(\frac{2}{9}\right)^r + q(S-1)\left(\frac{1}{4}\right)^r + 4(q-1)(s-1)\left(\frac{2}{9}\right)^r + 2q(s-1)\left(\frac{1}{5}\right)^r + s(q-1)\left(\frac{1}{5}\right)^r + 4(q-1)s\left(\frac{2}{11}\right)^r$
$GO_1(G)$	$-62q - 101s + 407qs + 8$
$GO_2(G)$	$-396q - 1198s + 2898qs - 8$
$HGO_1(G)$	$-2450q - 6275s + 13973qs + 476$
$HGO_2(G)$	$-151096q - 488668s + 759284qs + 55440$

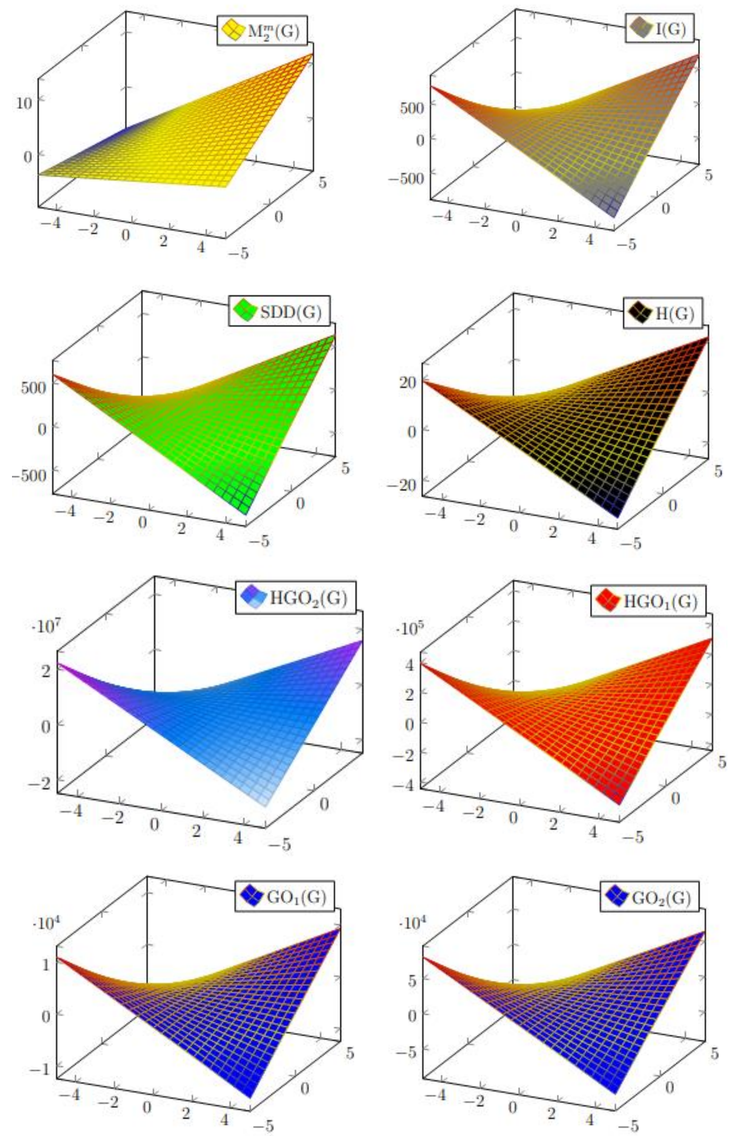
5. Graphical Analysis

We have depicted the behaviors of M-Polynomial at $l = 1 = m$ graphically for the boron cluster networks. It explores how the M-polynomial changes its behavior with the increase in network size and structure. Graphical representation of M-Polynomial for boron clusters (B_1) is shown below.

6. Graphical Behavior of Some M-Polynomials for B_1

By using Table 4, we have computed and depicted the graphical behaviors of ten M-Polynomials for B_1 at $l = 1 = m$ below.





7. Novelty

The γ-sheet of molecular graph transformed from the chemical compound of boron clusters has been taken in this article. And after converting of graph into planar, finite, simple and connected with the help of various mathematical techniques, we have investigated M-Polynomials (MP) and topological invariants (TI) to see their graphical behaviors and real-life applications in the field of pharmaceutical industry.

8. Conclusions

We have computed the M-Polynomial for the molecular structure of the chemical compound of γ-sheet of boron clusters. The results show which properties have most impression on invariants, and so to suppose whether it is feasible to plan system for administrative purpose that are more effective in regards of the efficiency of information pass. We have also investigated different topological indices like $M_1(B_1)$, $M_2(B_1)$, $M_2^m(B_1)$, R_η (B_1), RR_η (B_1), $SDD(B_1)$, $H(B_1)$, $I(B_1)$. Graphical behaviors of the γ-sheet of boron clusters have also been discussed.

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References

[1] B. Ihsan. (1997). Systematic ab initio investigation of bare boron clusters: m-Determination of the geometry and electronic structures of B_n. Physics Reviews. B. 55(24): 16426-16438.

[2] R.N. Grimes. (2004). Boron clusters come of age. Journal of Chemical Education. 81(5): 657.

[3] D. Bonchev. (1991). Chemical graph theory: introduction and fundamentals. (1). CRCPress.

[4] H. Wiener. (1947). Structural determination of paraffin boiling points. Journal of the American chemical society. 69(1): 17-20.

[5] M. Randic´. (1993). Novel molecular descriptor for structure-property studies. Chemical Physics Letters. 211(4-5): 478-483.

[6] M. Randic´. (1975). Characterization of molecular branching. Journal of the American Chemical Society. 97(23): 6609-6615.

[7] S. Shirakol, M. Kalyanshetti, and S.M. Hosamani. (2019). QSPR analysis of certain distance based topological indices. Applied Mathematics and Nonlinear Sciences. 4(2): 371- 386.

[8] I. Gutman, and N. Trinajstic´. (1972). Graph theory and molecular orbitals. Total Φ-electron energy of alternant hydrocarbons. Chemical Physics Letters. 17(4): 535-538.

[9] J. Hao. (2011). Theorems about Zagreb indices and modified Zagreb indices. MATCH Communications in Mathematial and in Computer Chemistry. 65: 659-670.

[10] B. Furtula, A. Graovac and D. Vukicˇevic´. (2010). Augmented Zagreb index. Journal of Mathematical Chemistry. 48(2): 370-380.

[11] B. Bollobás and P. Erdös. (1998). Graphs of extremal weights. Ars combinatoria. 50: 225.

[12] X. Li and Y. Shi. (2008). A survey on the Randic index. MATCH Communications in Mathematics and in Computer Chemistry. 59(1): 127-156.

[13] S. Fajtlowicz. (1987). On Conjectures of Grafitti II. Congr. Number. 60: 189-197.

[14] M.H. Aftab, M. Rafaqat and M. Hussain. (2022). Topological Invariants for the General Structure of Grape Seed Proanthocyanidins. Punjab University Journal of Mathematics. 54(1): 45-53.

[15] M.H. Aftab, M. Rafaqat and M. Hussain. (2021). On the computation of topological indices or molecular structures of subdivided aztec diamonds. Journal of Combinatorial Mathematics. 2: 13-20.

[16] M. Eliasi and D. Vukicevic. (2013). Comparing the multiplicative Zagreb indices. MATCH Communications in Mathematics and Computer Chemistry. 69: 765-773.

[17] A. Ali, B. Furtula, I. Redžepovic´ and I. Gutman. (2022). Atom-bond sum-connectivity index. Journal of Mathematical Chemistry. 60(10): 2081-2093.

[18] S. Amin, M.A. Rehman, A. Naseem, I. Khan and M. Abdulalem. (2022). Treatment of COVID-19 Patients Using Some New Topological Indices. Journal of Chemistry.

[19] M.H. Aftab, I. Siddique, J.K.K. Asamoah, H.A.W. Khalifa and M. Hussain. (2022). Multiplicative Attributes Derived from Graph Invariants for Saztec4 Diamond. Journal of Mathematics. Article ID 9148581. 1-7.

[20] E. Deutsch, and S. Klavžar. (2014). M-polynomial and degree-based topological indices. Ar Xiv preprint ar Xiv. 1407-1592.

[21] E. Estrada, L. Torres, L. Rodriguez and I. Gutman. (1998). An atom-bond connectivity index modelling the enthalpy of formation of alkanes. Indian Journal of Chemistry. 37: 849–855.

[22] Y.Y. Yuan, B. Zhou, B. and N. Trinajstic. (2010). On geometric-arithmetic index. Journal of Mathematical Chemistry. 47: 833–841.

[23] L. Yan, W. Gao and J. Li. (2015). General harmonic index and general sum connectivity index of polyomino chains and nanotubes. Journal of Computational and Theoretical Nanoscience. 12: 3940–3944.

[24] V.R. Kulli. (2017). The gourava indices and coindices of graphs. Annals of Pure and Applied Mathematics. 14: 33-38.

[25] V.R. Kulli. (2017). On hyper-gourava indices and coindices. International Journal of Mathematical Archieve. 1-8.

[26] K. Jebreen, M.H. Aftab, Z. Hussain, M.N. Tufail, M.I. Sowaity and H. Kanj. (2023). Consolidated Extremal Combinatorics Results among the Class of Degree-Based Graphs to Zagreb Indices with the Given. European Chemical Bulletin. 12(12): 818-835.

[27] I. Ali, N.M. diaa, M.H. Aftab, M.W. Raheed, K. Jebreen, H. Kanj. (2023). Topological Effects of Chiral Pamam Dendrimer for the Treatment of Cancer. Transylvanian Review. 31(2): 1-14.
[28] K. Jebreen, M.H. Aftab, M.I. Sowaity, B. Sharada, A.M. Naji, M. Pavithra. (2022). Eccentric Harmonic Index for the Cartesian Product of Graphs. Journal of Mathematics. 2022: 1-9.
[29] M.H. Aftab, K. Jebreen, M.I. Sowaity and M. Hussain. (2022). Analysis of eigenvalues for molecular structures. Computers, Materials & Continua. 73(1): 1225-1236.