

Research Article

Degree-Based Topological Indices of Boron B₁₂

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Topological index sometimes called molecular descriptor is a numerical value which associates a chemical composition for correlating chemical structure with numerous physical properties, chemical reactivity, or biological activity. In this paper, we study some topological indices of boron and try to correlate the physicochemical properties such as freezing points, boiling points, melting points, infrared spectrum, electronic parameters, viscosity, and density of chemical graphs. We discuss these topological indices, and some of them are mentioned here such as Randic index, the first general Zagreb index, the general sum connectivity index, hyper-Zagreb index (HM), the atom-bond connectivity index (ABC), the geometric-arithmetic index (GA), the harmonic index (*H*), and the forgotten index (*F*).

1. Introduction and Applications

A chemical graph theory is an outlet of mathematical chemistry which applied graph theory to the molecular structure of chemical compounds. Topological index is a part of chemical graph theory which correlates the physicochemical properties such as freezing point, boiling point, melting point, infrared spectrum, electronic parameters, viscosity, and density of the underlying chemical graphs. The reader can find bulk of papers on topological indices which have been in print so far [1–5].

A graph can be recognized by a polynomial, a matrix, a sequence of numbers, or a numeric number which represents the whole graph, and these representations are designed to be uniquely defined for that graph. Topological indices are major tools for analyzing many physicochemical properties of molecules without performing any testing. Some most significant types of topological indices of graphs are distance-based topological indices, degree-based topological indices, and spectrum-based topological indices. One of the most investigated categories of topological indices used in mathematical chemistry is called degree-based

topological indices, which are defined in terms of the degrees of the vertices of a graph.

Topological index is a graph invariant which characterizes the topology of the molecular structure and converts the molecular graph into a real number that predicts some physicochemical properties such as freezing point, boiling point, and melting point. Nowadays, a biological testing of chemical compounds is too much expensive. It requires a very large laboratory and advanced equipment to test these compounds. This process is costly and time-consuming. Due to this factor, pharmaceutical companies are very eager to find such new ideas or methods by which cost could be reduced. One can reduce the cost in which no need of laboratories and no need of equipment, but just need to study the certain chemical structure using topological indices

Topological indices are of different types such as degree-based topological indices, distance-based topological indices, and spectrum-based topological indices. The notion of topological index was discovered in 1947 when Harold Wiener was working on the boiling point of paraffin. He named this index as path number. Later on, the path number

was renamed as the Wiener index, and then the theory of topological index started. The Wiener index is the first and the most studied topological index. Wiener index is defined as the sum of distances among all the sets of vertices in G [6]. Among all the types of topological indices, degree-based topological indices play an extensive role in chemical graph theory [7]. That motivated us to study the chemical structure of boron B_{12} under this phenomenon.

B_{12} is a two-dimensional icosahedral network. A recent study of high-pressure solid boron affirmed that the icosahedral B_{12} -containing structures are quite universal [8]. On the other hand, previous experimental and theoretical studies of free-standing boron clusters have shown that the B_{12} structure is unstable in the gas phase [9, 10]. The (n, m) unit of boron B_{12} structure is given in the figure, where “ n ” represents the number of rows and “ m ” represents the number of columns of the boron B_{12} structure.

Let G be a simple graph with order p and size q . Let d_v represent the degree of the vertex v and is defined as the number of edges incident on v . Let S_v represent the sum of the degree of all the neighbors of v [11]. Graph theory is closely connected to the computer science, applied mathematics, optimization theory, web designing, operation research, biology, and chemistry.

The general Randić connectivity index of G is defined as

$$R_\alpha(G) = \sum_{rs \in E(G)} (d_r d_s)^\alpha, \quad (1)$$

where α represents a real number. If α is $-1/2$, then $R_{-1/2}(G)$ is said to be the Randić connectivity index of G . Gutman and Trinajstić presented the first general Zagreb index in 1972 [12]:

$$M_\alpha(G) = \sum_{r \in V(G)} (d_r)^\alpha. \quad (2)$$

In 2010, the general sum connectivity index $\chi_\alpha(G)$ has been invented:

$$\chi_\alpha(G) = \sum_{rs \in E(G)} (d_r + d_s)^\alpha. \quad (3)$$

The ABC index was presented by Estrada and Torres et al. in [13]. The ABC index of graph G is expressed as

$$ABC(G) = \sum_{rs \in E(G)} \sqrt{\frac{d_r + d_s - 2}{d_r d_s}}. \quad (4)$$

Das announced the geometric-arithmetic (GA) index in [14, 15]. The geometric-arithmetic index denoted by GA for graph G is presented by

$$GA(G) = \sum_{rs \in E(G)} \frac{2\sqrt{d_r d_s}}{d_r + d_s}. \quad (5)$$

In 2013, the hyper-Zagreb index has been introduced by Shirdel et al. as

$$HM(G) = \sum_{rs \in E(G)} (d_r + d_s)^2. \quad (6)$$

In 2012, Zhang introduced the harmonic index. It is defined as follows [16]:

$$H(G) = \sum_{rs \in E(G)} \frac{2}{(d_r + d_s)}. \quad (7)$$

After working on the Zagreb index, in 2015, Furtula and Gutman introduce the forgotten index $F(G)$:

$$F(G) = \sum_{rs \in E(G)} (d_r^2 + d_s^2). \quad (8)$$

Ghorbani and Azimi proposed two new types of Zagreb indices of a graph G in 2012. PM_1 is the first multiple Zagreb index, and PM_2 is the second multiple Zagreb index [6]:

$$PM_1(G) = \prod_{rs \in E(G)} (d_r + d_s), \quad (9)$$

$$PM_2(G) = \prod_{rs \in E(G)} (d_r \times d_s), \quad (10)$$

$M_1(G, p)$ and $M_2(G, p)$, the first Zagreb polynomial and the second Zagreb polynomial [12, 17], respectively, are defined as

$$M_1(G, p) = \sum_{rs \in E(G)} p^{(d_r + d_s)}, \quad (11)$$

$$M_2(G, p) = \sum_{rs \in E(G)} p^{(d_r \times d_s)}. \quad (12)$$

Recently, Furtula et al. proposed the second Zagreb index:

$$RM_2(G) = \sum_{rs \in E(G)} (d_r - 1)(d_s - 1). \quad (13)$$

After the success of the ABC index, Furtula et al. put forward its modified version in 2010 that they somewhat inadequately named “augmented Zagreb index.” It is defined as follows [18]:

$$AZI(G) = \sum_{rs \in E(G)} \left(\frac{d_r d_s}{d_r + d_s - 2} \right)^3. \quad (14)$$

The invariant RR seems to be first encountered in a paper by Favaron, Mah'eo. The reciprocal Randić index is defined as follows:

$$RR(G) = \sum_{rs \in E(G)} \sqrt{d_r d_s}. \quad (15)$$

In the same manner, the reduced second Zagreb index (equation (13)), is related to the ordinary second Zagreb index (equation (12)). The reduced reciprocal Randić index might be viewed as the reduced analogue of the reciprocal Randić index (equation (15)):

$$RRR(G) = \sum_{rs \in E(G)} \sqrt{(d_r - 1)(d_s - 1)}. \quad (16)$$

Vukicevic et al. introduce the symmetric division deg index in 2010 [19, 20] as

$$\text{SDD}(G) = \sum_{rs \in E(G)} \frac{d_r^2 + d_s^2}{d_r d_s}. \quad (17)$$

Vukicevic and Gašperov in [20] initiated the study on the inverse sum indeg index of a network. The inverse sum indeg index is defined as follows [21]:

$$\text{SDD}(G) = \sum_{rs \in E(G)} \frac{d_r d_s}{d_r + d_s}. \quad (18)$$

Another index which belongs to the 4th class of ABC index was invented by Ghorbani and Hosseinzadeh in 2010 [22] as

$$\text{ABC}(G) = \sum_{rs \in E(G)} \sqrt{\frac{S_r + S_s - 2}{S_r S_s}}. \quad (19)$$

The fifth class of geometric-arithmetic index, denoted by GA_5 , was presented by Graovac et al. in 2011 [23] as

$$\text{GA}(G) = \sum_{rs \in E(G)} \frac{2\sqrt{S_r S_s}}{S_r + S_s}. \quad (20)$$

2. Main Results of Boron B_{12} Graph

In this paper, we deal with the topological properties of boron B_{12} . Boron B_{12} is a two-dimensional icosahedral network. A recent study of high-pressure solid boron affirmed that the icosahedral B_{12} -containing structures are quite universal [8]. On the other hand, previous experimental and theoretical studies of freestanding boron clusters have shown that the B_{12} structure is unstable in the gas phase [9, 10].

The molecular graph of Boron B_{12} is shown in Figure 1. There are $11mn + 11m + 11n + 9$ vertices and $24mn + 22m + 22n + 18$ edges.

Theorem 1. Let G be the boron B_{12} network with $m > 1$ and $n > 1$, then

$$\begin{aligned} M_\alpha &= 2(2m + 2n)2^\alpha + (3mn + m + 5)3^\alpha \\ &+ (3mn + 2m + 3n + 4)3^\alpha + (m + 2n + 1)4^\alpha \\ &+ (9mn + 7m + 6n + 5)4^\alpha + (9mn + 7m + 7n + 3)5^\alpha. \end{aligned} \quad (21)$$

Proof. In G , there are total $11mn + 11m + 11n + 9$ vertices. There are $2m + 2n$ vertices of degree 2, $2mn + m + n + 3$ vertices of degree 3, $3mn + 3m + 3n + 3$ vertices of degree 4, and $36mn + 5m + 5n + 3$ vertices of degree 5. Since M_α is expressed in equation (2),

$$M_\alpha(G) = \sum_{r \in V(G)} (d_r)^\alpha, \quad (22)$$

$$\begin{aligned} M_\alpha &= 2(2m + 2n)2^\alpha + (3mn + m + 5)3^\alpha \\ &+ (3mn + 2m + 3n + 4)3^\alpha \\ &+ (m + 2n + 1)4^\alpha + (9mn + 7m + 6n + 5)4^\alpha \\ &+ (9mn + 7m + 7n + 3)5^\alpha. \end{aligned} \quad (23)$$

In the following six theorems, we considered the Randic index, sum connectivity index, ABC index, GA index, harmonic index, reduced Randic index, forgotten index, symmetric division deg index, inverse sum indeg index, ABC_4 index, and GA_5 index. This is the edge partition of boron B_{12} on the basis of starting and ending vertices of each edge, and we proceed this edge division to compute the topological indices.

Theorem 2. Let G be the boron B_{12} network with $m > 1$ and $n > 1$, then

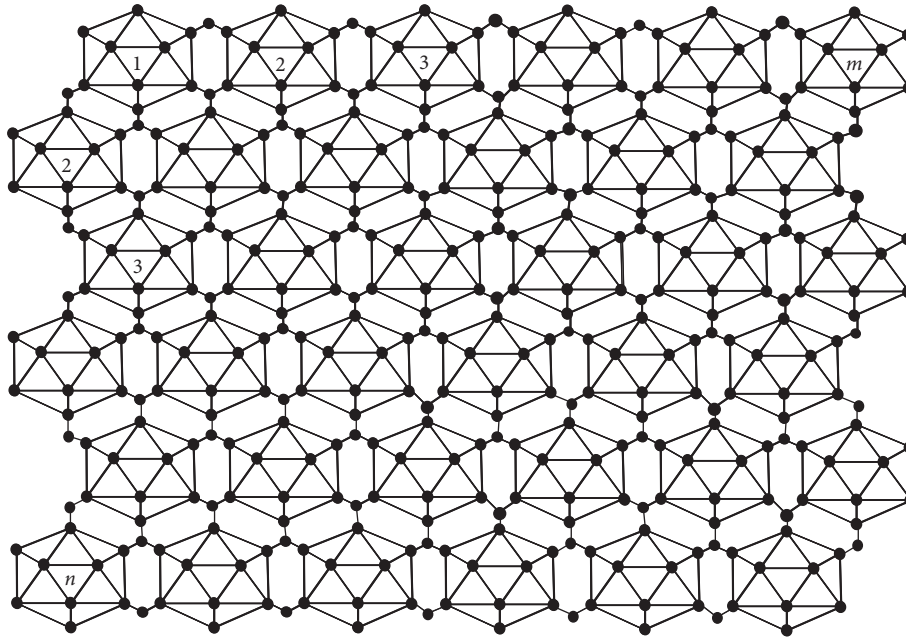
- (1) $R_\alpha(G) = (2m + 2n)8^\alpha + (2m + 2n)10^\alpha + (3mn + m + 5)12^\alpha + (m + 2n + 1)16^\alpha + (3mn + 2m + 3n + 4)15^\alpha + (9mn + 7m)20^\alpha + (9mn + 7m + 7n + 3)25^\alpha + (6n + 5)20^\alpha$
- (2) $\chi_\alpha(G) = (2m + 2n)6^\alpha + (2m + 2n)7^\alpha + (3mn + m + 5)7^\alpha + (m + 2n + 1)8^\alpha + (3mn + 2m + 3n + 4)8^\alpha + (9mn + 7m + 6n + 5)9^\alpha + (9mn + 7m + 7n + 3)10^\alpha$
- (3) $\text{ABC}(G) = (2m + 2n)\sqrt{2} + (1/6)(3mn + m + 5)\sqrt{15} + (1/5)(3mn + 2m + 3n + 4)\sqrt{10} + (1/4)(m + 2n + 1)\sqrt{6} + (1/10)(9mn + 7m)\sqrt{35} + (1/10)(6n + 5)\sqrt{35} + (2/5)(9mn + 7m + 7n + 3)\sqrt{2}$
- (4) $\text{GA}(G) = (2/3)(2m + 2n)\sqrt{2} + (2/7)(2m + 2n)\sqrt{10} + (4/7)(3mn + m + 5)\sqrt{3} + (1/4)(3mn + 2m + 3n + 4)\sqrt{15} + (4/9)(9mn + 7m + 6n + 5)\sqrt{5} + (9mn + 8m + 9n + 4)$

Proof. The network of boron B_{12} has $24mn + 22m + 22n + 18$ number of edges. There are seven disjoint edge sets of edge set $E(G)$ depending on the degrees of the end vertices, i.e., $E(G) = E_1(G) \cup E_2(G) \cup E_3(G) \cup E_4(G) \cup E_5(G) \cup E_6(G) \cup E_7(G)$. The edge partition $E_1(G)$ holds $2m + 2n$ edges rs , where $d_r = 2$ and $d_s = 4$, the edge partition $E_2(G)$ holds $2m + 2n$ edges rs , where $d_r = 2$ and $d_s = 5$, the edge partition $E_3(G)$ holds $3mn + m + 5$ edges rs , where $d_r = 3$ and $d_s = 4$, the edge partition $E_4(G)$ holds $3mn + 2m + 3n + 4$ edges rs , where $d_r = 3$ and $d_s = 5$, the edge partition $E_5(G)$ holds $m + 2n + 1$ edges rs , where $d_r = d_s = 4$, the edge partition $E_6(G)$ holds $9mn + 7m + 6n + 5$ edges rs , where $d_r = 4$ and $d_s = 5$, and the edge partition $E_7(G)$ holds $9mn + 7m + 7n + 3$ edges rs , where $d_r = d_s = 5$. From formulas (1) and (3)–(5), we get the desired results.

Theorem 3. Let G be the boron B_{12} network with $m > 1$ and $n > 1$, then

- (1) $HM(G) = 1678m + 1676n + 1968mn + 1270$
- (2) $PM_1(G) = 6^{2m+2n} \times 7^{2m+2n} \times 7^{3mn+m+5} \times 8^{3mn+2m+3n+4} \times 8^{m+2n+1} \times 9^{9mn+7m+6n+5} \times 10^{9mn+7m+7n+3}$
- (3) $PM_2(G) = 8^{2m+2n} \times 10^{2m+2n} \times 12^{3mn+m+5} \times 15^{3mn+2m+3n+4} \times 16^{m+2n+1} \times 20^{9mn+7m+6n+5} \times 25^{9mn+7m+7n+3}$

Proof. Let G be the network of boron B_{12} . The edge set $E(G)$ is distributed in seven categories which depend on the degrees of the end vertices. The first disjoint edge set $E_1(G)$

FIGURE 1: (n, m) unit of boron.

holds $2m + 2n$ edges rs , where $d_r = 2$ and $d_s = 4$, the second disjoint edge set $E_2(G)$ holds $2m + 2n$ edges rs , where $d_r = 2$ and $d_s = 5$, the third disjoint edge set $E_3(G)$ holds $3mn + m + 5$ edges rs , where $d_r = 3$ and $d_s = 4$, the fourth disjoint edge set $E_4(G)$ holds $3mn + 2m + 3n + 4$ edges rs , where $d_r = 3$ and $d_s = 5$, the fifth disjoint edge set $E_5(G)$ holds $m + 2n + 1$ edges rs , where $d_r = d_s = 4$, the sixth disjoint edge set $E_6(G)$ holds $9mn + 7m + 6n + 5$ edges rs , where $d_r = 4$ and $d_s = 5$, and the seventh disjoint edge set $E_7(G)$ holds $9mn + 7m + 7n + 3$ edges rs , where $d_r = d_s = 5$. Now, $|E_1(G)| = e_{2,4}$, $|E_2(G)| = e_{2,5}$, $|E_3(G)| = e_{3,4}$, $|E_4(G)| = e_{3,5}$, $|E_5(G)| = e_{4,4}$, $|E_6(G)| = e_{4,5}$, and $|E_7(G)| = e_{5,5}$. We obtained results by using formulas (6), (9), and (10).

Theorem 4. Let G be the boron B_{12} network with $m > 1$ and $n > 1$, then

- (1) $M_1(G, p) = (2m + 2n)p^6 + (2m + 2n)p^7 + (3mn + m + 5)p^7 + (m + 2n + 1)p^8 + ((3mn + 2m)p^8 + (3n + 4))p^8 + (9mn + 7m + 6n + 5)p^9 + (9mn + 7m + 7n + 3)p^{10}$
- (2) $M_1(G, p) = (2m + 2n)p^8 + (2m + 2n)p^{10} + (3mn + m + 5)p^{12} + ((3mn + 2m)p^{15} + (3n + 4))p^{15} + (m + 2n + 1)p^{16} + (9mn + 7m + 6n + 5)p^{20} + (9mn + 7m + 7n + 3)p^{25}$

Proof. Let G be the network of boron B_{12} . The edge set $E(G)$ is distributed in seven categories which depend on the degree of end vertices of each edge. The disjoint set is represented by $e_{r,s}$. The first disjoint set is $e_{2,4}$, the second disjoint set is $e_{2,5}$, the third disjoint set is $e_{3,4}$, the fourth disjoint set is $e_{3,5}$, the fifth disjoint set is $e_{4,4}$, the sixth disjoint set is $e_{4,5}$, and the seventh disjoint set is $e_{5,5}$. By using formulas (11) and (12), we obtained the required results.

Theorem 5. Let G be the boron B_{12} network with $m > 1$ and $n > 1$, then

- (1) $RM_2(G) = 241m + 240n + 294mn + 179$
- (2) $AZI(G) = (12576690219/21952000)mn + (40043532353/84672000)m + (2230300883/4741632)n + (42526959271/118540800)$

Proof. Let G be the network of boron B_{12} . The edge set $E(G)$ is distributed in seven categories which depend on the degree of end vertices of each edge. The disjoint set is represented by $e_{r,s}$. The first disjoint set is $e_{2,4}$, the second disjoint set is $e_{2,5}$, the third disjoint set is $e_{3,4}$, the fourth disjoint set is $e_{3,5}$, the fifth disjoint set is $e_{4,4}$, the sixth disjoint set is $e_{4,5}$, and the seventh disjoint set is $e_{5,5}$. We get the results by using formulas (13) and (14). \square

Theorem 6. Let G be the boron B_{12} network with $m > 1$ and $n > 1$, then

- (1) $H(G) = (6589/1260)m + (731/140)n + (757/140)mn + (5531/1260)$
- (2) $RR(G) = 2(2m + 2n)\sqrt{2} + (2m + 2n)\sqrt{10} + 2(3mn + m + 5)\sqrt{3} + ((3mn + 2m)\sqrt{15} + (3n + 4))\sqrt{15} + 2(9mn + 7m + 6n + 5)\sqrt{5} + 45mn + 39m + 43n + 19$
- (3) $RRR(G) = (2m + 2n)\sqrt{3} + 2(3mn + 2m)\sqrt{2} + 2(3n + 4)\sqrt{2} + 2(3mn + m + 5)\sqrt{6} + 2(9mn + 7m + 6n + 5)\sqrt{3} + 36mn + 35m + 38n + 15$

Proof. Let G be the network of boron B_{12} . The edge set $E(G)$ is distributed in seven categories which depend on the degree of end vertices of each edge. The disjoint set is represented by $e_{r,s}$. The first disjoint set is $e_{2,4}$, the second disjoint set is $e_{2,5}$, the third disjoint set is $e_{3,4}$, the fourth

disjoint set is $e_{3,5}$, the fifth disjoint set is $e_{4,4}$, the sixth disjoint set is $e_{4,5}$, and the seventh disjoint set is $e_{5,5}$. By using formulas (7), (15), and (16), we get the desired results.

Theorem 7. Let G be the boron B_{12} network with $m > 1$ and $n > 1$, then

- (1) $F(G) = 860m + 860n + 996mn + 648$
- (2) $SDD(G) = (1433/30)m + (479/10)n + (99/2)mn + (566/15)$
- (3) $ISI(G) = (11603/252)m + (2575/25562)n + (2983/56)mn + (2311/63)$

Proof. Let G be the network of boron B_{12} . The edge set $E(G)$ is distributed in seven categories which depend on the

degree of end vertices of each edge. The disjoint set is represented by $e_{r,s}$. The first disjoint set is $e_{2,4}$, the second disjoint set is $e_{2,5}$, the third disjoint set is $e_{3,4}$, the fourth disjoint set is $e_{3,5}$, the fifth disjoint set is $e_{4,4}$, the sixth disjoint set is $e_{4,5}$, and the seventh disjoint set is $e_{5,5}$. We obtained the required results by using formulas (8), (17), and (18).

In the following two theorems, we considered the fourth atom-bond connectivity index and the fifth geometric-arithmetic index. This is the edge partition of boron B_{12} on the basis of the degree sum of neighbors of end vertices of each edge. We proceed this edge division to compute $ABC_4(G)$ and $GA_5(G)$.

Theorem 8. Let G be the boron B_{12} network with $m > 1$ and $n > 1$, then

$$\begin{aligned}
 ABC_4(G) = & (1/2)\sqrt{2} + (4/221)\sqrt{1547} + (4/273)\sqrt{546} - (2/3) + (2/22)\sqrt{22} \\
 & + (1/22)\sqrt{42} + (1/10)(m-1)\sqrt{10} + (1/114)(m+2n+1)\sqrt{1330} + (1/68)(m-1)\sqrt{442} \\
 & + (1/391)(m+3)\sqrt{14858} + (1/374)(m+1)\sqrt{13838} + (1/34)(m-1)\sqrt{119} + (2/119)(m+1)\sqrt{357} \\
 & + (1/92)(m+2n+1)\sqrt{851} + (1/12)(m+2n+1)\sqrt{15} + (1/68)(m+3)\sqrt{527} + (2/115)(n-1)\sqrt{345} \\
 & + (4/285)(2n-2)\sqrt{570} + (1/238)(m+1)\sqrt{6902} + (1/266)(m+3)\sqrt{8246} + (1/154)(m+3)\sqrt{2618} \\
 & + (1/10)(m-1)\sqrt{14} + (1/8)(m+2n+1)\sqrt{11} + (1/68)(m-1)\sqrt{782} + (3/190)(m+2n+1)\sqrt{570} + (1/6)mn\sqrt{30} \\
 & + (1/35)mn\sqrt{1190} + (1/6)mn\sqrt{42} + (1/42)(3mn-2n-1)\sqrt{46} + (1/92)(m+4n-3)\sqrt{690} + (2/3)n\sqrt{11} + (1/6)(m+3)\sqrt{3} \\
 & + (1/506)(m+1)\sqrt{21758} + (1/84)(6mn-m-2n-1)\sqrt{602} + (1/23)(m+2n+3)\sqrt{46} + (1/20)(2m-2)\sqrt{35} \\
 & + (1/228)(m+2n+1)\sqrt{4674} + (2/437)(2n-2)\sqrt{4370} + (1/418)(m+3)\sqrt{16302} + (1/138)(2n-2)\sqrt{1794} \\
 & + (1/126)(6mn-2m-2n)\sqrt{1554} + (2/3)n.
 \end{aligned} \tag{24}$$

Proof. The network of boron B_{12} has $24mn + 22m + 22n + 18$ number of edges. There are 41 disjoint degree sum of neighbors of end vertices of each edge, i.e., $e_{8,16}$, $e_{8,17}$, $e_{10,19}$, $e_{10,20}$, $e_{12,18}$, \dots , $e_{24,24}$. By using formula (19), we get the desired result.

Theorem 9. Let G be the boron B_{12} network with $m > 1$ and $n > 1$, then

$$\begin{aligned}
 GA_5(G) = & (1/20)(m+3)\sqrt{391} + (1/19)(m+1)\sqrt{357} + (1/39)(m+1)\sqrt{374} + (1/19)(n-1)\sqrt{345} \\
 & + (1/17)(2n-2)\sqrt{285} + (2/29)(m+2n+1)\sqrt{190} + (2/31)(m+1)\sqrt{238} + (2/33)(m+3)\sqrt{266} \\
 & + (2/41)(m+3)\sqrt{418} + (1/21)(2n-2)\sqrt{437} + (1/22)(m+2n+3)\sqrt{483} + (2/45)(m+1)\sqrt{506} \\
 & + (2/15)\sqrt{273} + (2/13)(6mn-2m-2n)\sqrt{42} + (6/37)(m+2n+1)\sqrt{38} + (6/19)(m-1)\sqrt{10} + (4/41)(m-1)\sqrt{102} \\
 & + (8/37)(m+2n+1)\sqrt{21} + (4/37)(m-1)\sqrt{85} + (8/39)(m+2n+1)\sqrt{23} + (8/33)(m+3)\sqrt{17} + (12/17)(2n-2)\sqrt{2} \\
 & + (2/3)(m-1)\sqrt{2} + (1/9)(m+3)\sqrt{77} + (2/3)(m+2n+1)\sqrt{2} + (4/25)(m-1)\sqrt{34} + (12/7)mn\sqrt{3} + (1/2)mn\sqrt{35} \\
 & + (6/5)mn\sqrt{6} + (6/41)(2n-2)\sqrt{46} + (2/11)(2m-2)\sqrt{30} + (4/43)(m+2n+1)\sqrt{114} + (4/15)(6mn-m-2n-1)\sqrt{14} \\
 & + (4/23)(m+3)\sqrt{33} + (4/47)(m+4n-3)\sqrt{138} + (8/15)\sqrt{14} + (8/19)\sqrt{22} - n + 3mn.
 \end{aligned} \tag{25}$$

Proof. The network of boron B_{12} has $24mn + 22m + 22n + 18$ number of edges. There are 41 disjoint degree sum of neighbors of end vertices of each edge, i.e., $e_{8,16}$, $e_{8,17}$, $e_{10,19}$, $e_{10,20}$, $e_{12,18}$, \dots , $e_{24,24}$. By using formula (20), we get the desired result.

3. Conclusion

We have computed the following topological indices such as Zagreb index, the Randic index, sum connectivity index, ABC index, GA index, hyper-Zagreb index, multiple Zagreb indices, Zagreb polynomials, reduced second Zagreb index, augmented Zagreb index, harmonic index, reduced Randic index, reduced reciprocal Randic index, forgotten index, ABC_4 index, and GA_5 index for boron B_{12} structure.

In cheminformatics, Randic index is used to study the organic compounds. It is correlated with physicochemical properties of alkane such as boiling points, surface area, and enthalpy of formation. ABC index is based on some physicochemical properties like the stability of cyclo-alkane as well as strain energy. GA index has more predictive power than Randic and ABC index. Multiple Zagreb indices and Zagreb polynomials are applied to predict the bioactivity of graphs. The forgotten index is correlated with some chemical properties relating to energies of molecular graphs. AZI index is a valuable predictive index which is used in the study of the heat of formation. RRR index is used to study the normal boiling points of the graphs.

We have discussed the graph theoretically not experimentally. The results obtained in this paper provide a significant contribution to graph theory and correlate the chemical structure of boron B_{12} with the large amount of information about physicochemical properties.

Data Availability

No data were used to support this study.

Conflicts of Interest

The authors declare that they have no conflicts of interest.

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References

- [1] H. M. A. Siddiqui, "Computation of Zagreb indices and Zagreb polynomials of Sierpinski graphs," *Hacetatepe Journal of Mathematics and Statistics*, vol. 49, no. 2, pp. 754–765, 2020.
- [2] H. M. A. Siddiqui, S. Baby, M. K. Shafiq, and M. Faisal Nadeem, "Bounds of some degree based indices of lexicographic product of some connected graphs," *Polycyclic Aromatic Compounds*, 2020.
- [3] J.-B. Liu, B. Ali, M. Aslam Malik, H. M. A. Siddiqui, and M. Imran, "Reformulated Zagreb indices of some derived graphs," *Mathematics*, vol. 7, p. 283, 2019.
- [4] B. L. Jia, M. Imran, S. Baby, H. M. A. Siddiqui, and M. K. Shafiq, "Graph indices for Cartesian product of F-sum of connected graphs," *Combinatorial Chemistry & High Throughput Screening*, 2021.
- [5] J. Xu, J.-B. Liu, A. Bilal et al., "Distance degree index of some derived graphs," *Mathematics*, vol. 7, no. 3, p. 283, 2019.
- [6] M. Ghorbani and N. Azimi, "Note on multiple Zagreb indices," *Iranian Journal of Mathematical Chemistry*, vol. 3, no. 2, pp. 137–143, 2012.
- [7] I. Gutman, "Degree-based topological indices," *Croatica Chemica Acta*, vol. 86, no. 4, pp. 351–361, 2013.
- [8] A. R. Oganov, J. Chen, C. Gatti et al., "Ionic high-pressure form of elemental boron," *Nature*, vol. 457, no. 7231, pp. 863–867, 2009.
- [9] I. Boustani, "Systematic ab initio investigation of bare boron clusters: mDetermination of the geometry and electronic structures of B_n ($n = 2-14$)," *Physical Review B*, vol. 55, no. 24, p. 16426, 1997.
- [10] H. Li, N. Shao, B. Shang, L.-F. Yuan, J. Yang, and X. C. Zeng, "Icosahedral B_{12} -containing core-shell structures of B_{80} ," *Chemical Communications*, vol. 46, no. 22, pp. 3878–3880, 2010.
- [11] L. W. Beineke and R. J. Wilson, *Applications of Graph Theory*, Academic Press, London, UK, 1979.
- [12] B. Horoldagva, L. Buyantogtokh, K. C. Das, and S. G. Lee, "On general reduced second Zagreb index of graphs," *Hacetatepe Journal of Mathematics and Statistics*, vol. 48, no. 4, pp. 1040–1056, 2019.
- [13] K. C. Das, I. Gutman, and B. Furtula, "On atom-bond connectivity index," *Chemical Physics Letters*, vol. 511, no. 4–6, pp. 452–454, 2011.
- [14] K. C. Das, "On geometric-arithmetic index of graphs," *MATCH Communications in Mathematical and in Computer Chemistry*, vol. 64, no. 3, pp. 619–630, 2010.
- [15] D. Vukievi and B. Furtula, "Topological index based on the ratios of geometrical and arithmetical means of end-vertex degrees of edges," *Journal of Mathematical Chemistry*, vol. 46, no. 4, pp. 1369–1376, 2009.
- [16] S. Fajtlowicz, "Harmonic index," *Congressus Numerantium*, vol. 60, pp. 187–197, 1987.
- [17] Z. Shao, M. Siddiqui, and M. Muhammad, "Computing Zagreb indices and Zagreb polynomials for symmetrical nanotubes," *Symmetry*, vol. 10, no. 7, p. 244, 2018.
- [18] A. Ali, Z. Raza, and A. A. Bhatti, "On the augmented Zagreb index," 2014, <http://arxiv.org/abs/1402.3078>.
- [19] D. Vukievi, "Bond additive modeling 2. mathematical properties of max-min Rodeg index," *Croatica Chemica Acta*, vol. 83, no. 3, pp. 261–273, 2010.
- [20] D. Vukievi and M. Gašperov, "Bond additive modeling 1. adriatic indices," *Croatica Chemica Acta*, vol. 83, no. 3, pp. 243–260, 2010.
- [21] J. Sedlar, D. Stevanović, and A. Vasilyev, "On the inverse sum inddeg index," *Discrete Applied Mathematics*, vol. 184, pp. 202–212, 2015.
- [22] M. Ghorbani and M. A. Hosseinzadeh, "Computing ABC_4 index of nanostar dendrimers," *Optoelectronics and Advanced Materials-Rapid Communications*, vol. 4, no. 9, pp. 1419–1422, 2010.
- [23] A. Graovac, M. Ghorbani, and M. A. Hosseinzadeh, "Computing fifth geometric-arithmetic index for nanostar dendrimers," *Journal of Mathematical Nanoscience*, vol. 1, no. 1–2, pp. 33–42, 2011.