Quantitative Structural Edge-version Topological Descriptors for Boric Acid Graphite Structure

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Abstract

A quantitative structural analysis was carried out to predict the physical properties of boric acid structure. A topological descriptor of chemical molecule structure is a numerical value that distinguishes between a base structure and its branching pattern in the knowledge of chemical, physical, and biological aspects of molecular structure. In modern chemistry, theoretical chemistry, pharmacology, toxicology, and environmental chemistry, a large number of numerical graph invariants (topological indices) have been established and used for correlation analysis. In this paper, edge-version of distance based topological descriptors like edge Wiener, edge Szeged, edge PI and vertex-edge Wiener are computed for the structure of boric acid graphite sheet and Theta, Omega, Sd and PI polynomials and their subsequent topological indices for boric acid graphite structure are quantified. Further, using Theta and Omega polynomials, we devise a new approach for calculating the PI and Sd indices.

Keywords: Edge-version of distance based topological descriptors, boric acid graphite structure, cut method, four polynomials.

1 Introduction

Chemical graph theory is an interdisciplinary field in which the molecular structures of chemical molecules and biomolecules are considered as a graph where the molecules are called vertices and the chemical bonds connecting them are called edges and it is related mathematical questions are explored using graph theoretical techniques and computational tools. The molecular structure of boric acid that we have taken in this study is more significant in biological and chemical fields.

Boric acid is a weak monobasic Lewis acid of boron that is an inorganic material that belongs to the discipline of modern science. Boric acid, often known as H_3BO_3, is a weak acid that exists as an uncharged small molecule at physiological pH. Boric acid, first noted by the Arab chemist Geber

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around 700 AD. Boric acid is a soluble neutron absorber, soluble poison or chemical shim that is dissolved in the reactor coolant to control neutron reactivity in the core [1]. Other soluble neutron absorbers, such as gadolinium or cadmium nitrate have also been studied. Because such materials have large neutron capture cross-sections, they may be effective even at low concentrations. However there are possible drawbacks in terms of solubility and hydrolysis reactions and the current standard of care is to use boric acid exclusively. The use of boric acid has the advantages of being sufficiently soluble in water to yield the required concentrations having sufficient chemical and physical stability over the required temperature range and having a low proclivity for incorporation into oxide films which could result in local neutron poison and acidity [1] established the equilibrium constants and showed that the initial reaction of H_3BO_3 was the key predictor of pH in the primary coolant in a study of boric acid dissociation over temperatures relevant to a PWR [2]. This is because polyborates lose their relevance at high temperatures, low boron concentrations and low hydroxide concentrations. Through electron donor-acceptor interactions, it forms complexes with amino- and hydroxy acids, carbohydrates, nucleotides and vitamins. Human health may benefit from these relationships. As a result, nutritional and/or medicinal applications for synthetic bis-chelate complexes of boric acid with organic bimolecular are being studied [2]. Anionic diesters, anionic monoesters and Boric acid interact with bio molecules containing cis-hydroxy groups (aryl, acyl, R=H, alkyl) and these interactions are pH-dependent with diol binding preferable at basic pH and esterification with hydroxy-carboxylic acids preferable at acidic pH [3–8].

In this paper, we have converted the boric acid molecular structure into mathematical structure. Mathematical structures or the study of graphs is known as graph theory in mathematics. In the field of graph theory, a graph can be identified by a sequence of numbers, matrix, polynomial or numeric number that represents the entire graph and these description are intended to be particularly defined for that graph [9–11]. Chemical graph theory is one of the important field in graph theory and the topic topological indices plays an important role in it.

One of the important idea in chemical graph theory is the search for techniques that can convert a structure of molecule to a single numerical number or a set of quantifiers known as topological descriptors. A topological descriptor also known as a connectivity index in the fields of chemical graph theory, molecular topology, and mathematical chemistry are a type of molecular descriptor calculated based on a molecular structures of chemical compounds. Topological indices can also help in the creation of new molecules in the field of cell press family and chemistry. Hybrid degree-distances, vertex degrees, topological distances and other connectivity-based values are used to calculate various topological descriptors [12]. Topological indices are useful tools for analyzing the physico-chemical properties of chemical compound structures [13].

Modeling with the Quantitative Structure-Activity Relationship (QSAR) and Quantitative Structure-Property Relationship (QSPR) investigations are mathematical quantification techniques that are widely employed in pharmaceutical and agricultural chemistry to screen compounds for specific activity [14-17]. Regression models have been created to link an empirically determined attribute or biological activity to molecule structure [18-19]. Ethical, theoretical, physicochemical properties [20] and quantum mechanically computed parameters are the descriptors employed in QSAR models. It is possible to predict the activity/property of any number of structurally related compounds, including those that have yet to be synthesized and tested, once a correlation between structure and biological activity or a physicochemical characteristic has been established. Appropriate molecular descriptors must be used to create QSAR models with strong prediction capacity. A molecular descriptor attempts to fully characterize a molecule structure or a specific feature of the structure using mathematics. In this paper, we also cover QSPR analysis of the following distance based topological descriptors like edge-Wiener, edge-Szeged, edge-PI and vertex-edge-Wiener indices. The mentioned descriptors was noticed by observing a correlation between a molecular structure and its boiling point [21]. The distance of edge can then be specified in a variety of ways. The distance between two edges is defined as the minimal distance between the edges and end vertices as shown in [22,23]. Liu J, et.al. [15] and Rauf A, et.al. [16] as shown more interested in the analytical computation technique to help us to find the physico-chemical and biological properties of boric acid graphite sheet.

Some topological indices are derived by pilfering integrals or derivatives in counting polynomials and assigning specific values to the variable. Counting polynomials are well-known approach of expressing molecular invariants in polynomial form in a chemical graph. Chemical graph features like matching sets, independent sets, chromatic numbers and equidistant edges influence these polynomials. Wiener polynomial, Hosoya polynomial, PI polynomials, Matching polynomial, Omega polynomials and Sadhana polynomials are some well-known polynomials. Polynomials can be used to produce a variety of significant topological indices, either directly or after taking derivatives or integrals. These polynomials are crucial in predicting a physiochemical properties of molecule since they count equidistant and non equidistant edges in a graph.

Early Hückel theory calculates the levels of S-electron energy of the molecular orbitals in conjugated hydrocarbons as roots of the characteristic polynomial in Quantum Chemistry [25-27]. That is,

$$P(G, y) = det[yI - B(G)] \tag{1}$$

where, I is the unit matrix of a pertinent order, and B is the adjacency matrix of the graph G in equation (1). The characteristic polynomial is used to calculate topological resonance energy (TRE), topological impact on molecular orbital (TEMO), aromatic sextet theory and the Kekulé structure count, among other things [28-29].

The coefficients $m(G,t)$ in the polynomial expression

$$P\left(G,y\right)=\sum_{t}m\left(G,k\right)y^{t} \tag{2}$$

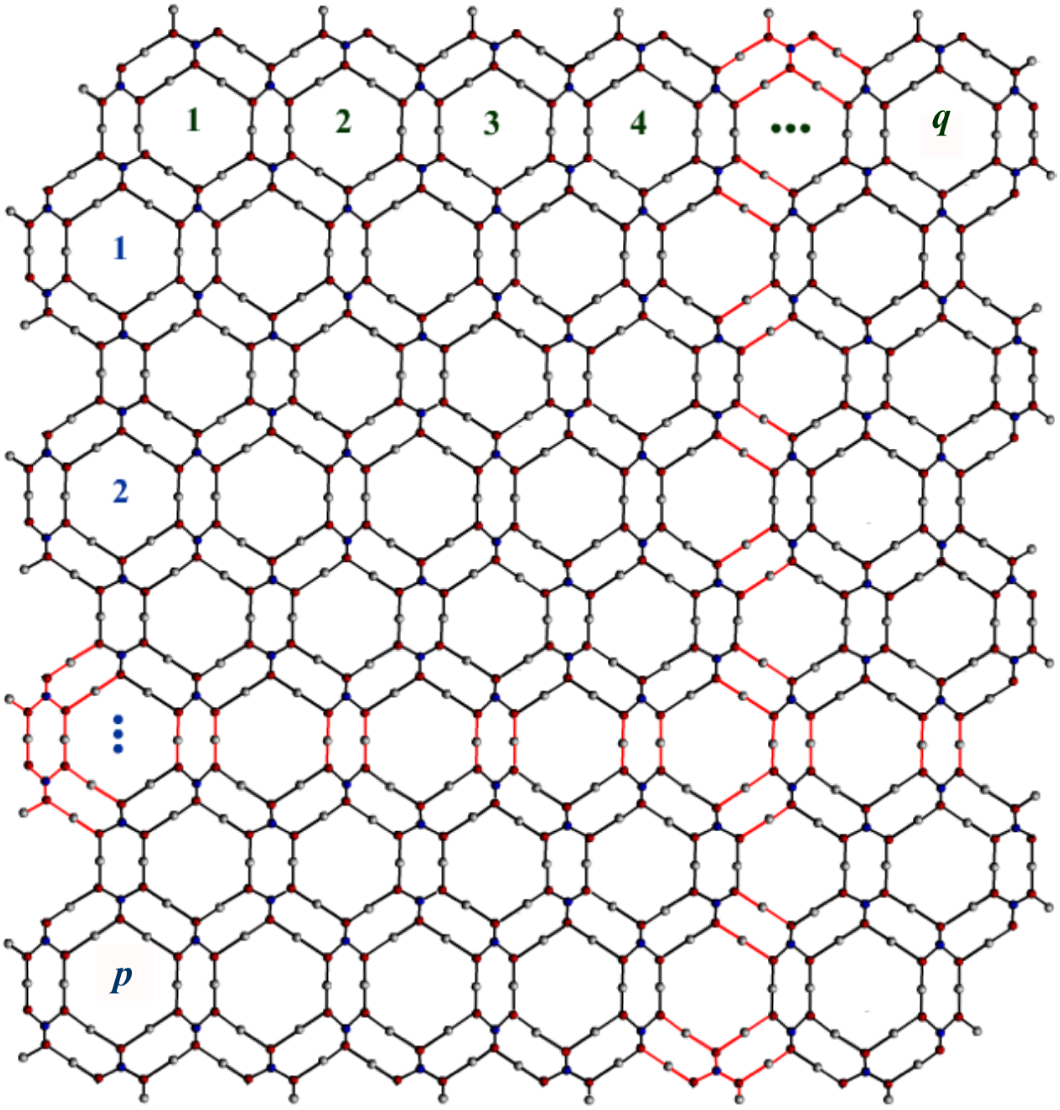
are deduced from the graph G using a method that employs Sachs graphs, which are G's subgraphs. Sachs, Harary, Miliü, Spialter, Hosoya, and others discovered Relation (2) separately [25].

In the Mathematical Chemistry literature, counting polynomials is associated with the name Hosoya [30,31] and independent edge sets are calculated by $Z\left(G,y\right)$ and distances are tallied by $H\left(G,y\right)$ (originally termed Wiener and then Hosoya) [32,33] polynomials. The characterization of the topological of hydrocarbons is based on their roots and coefficients. For counting the resonant rings in a chemical molecules, Hosoya suggested the sextet polynomial [34-37]. The sextet polynomial is significant in relation to the Clar aromatic sextets, which are believed to stabilise aromatic compounds [38]. In this work, further using the Omega polynomial, new relations have been developed to determine Theta, PI, and Sadhana indices. A fascinating set of results is produced by derivative of these four polynomials. The Some following indices like PI index PI(G), and Sd index Sd(G) were generated using the first derivatives of Omega, Theta polynomials. In QSPR/QSAR investigations, a topological index known as the PI index was associated with the Szeged and Wiener indices and used as a well qualified parameter [39-44].

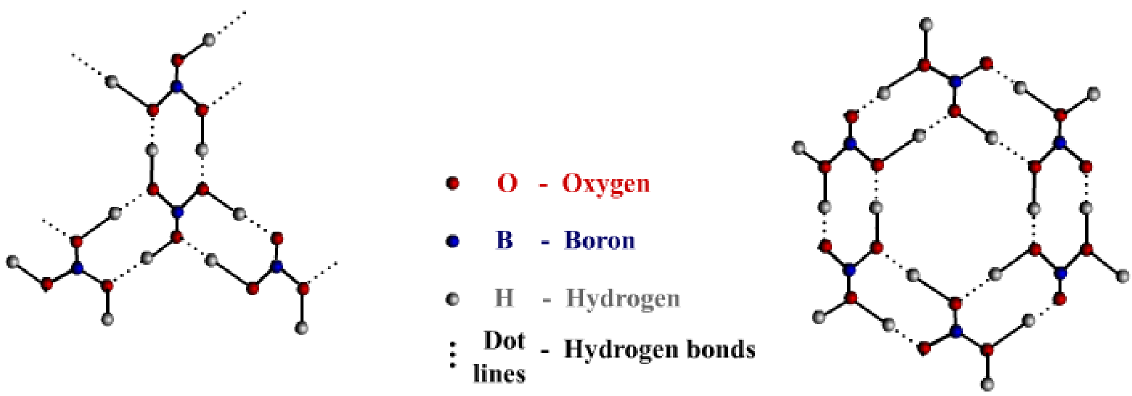
Farahani, et.al. calculated the circumcorone's Omega [45], Theta, PI polynomial [46] and Sadhana polynomials [47]. They also discovered the Sadhana polynomial [48] and the (G,y) polynomial [49], both of which are connected with an infinite class of linear parallelograms $P(p,q)$. For each $c,d\in N$ and $c\geq d$, which consists of $c-d+1$ rows, the Theta, PI polynomials [50], Omega and Sadhana polynomials [51] of the hexagonal trapezoid system $T_{c,d}$ were computed. In this study, we generalized the results of edge-Wiener, edge-Szeged, edge-PI and vertex-edge-Wiener indices for boric acid graphene sheet as well as the four polynomials and subsequent indices.

2 Boric acid graphite sheet

Boric acid is also known as orthoboric acid, boracic acid and hydrogen borate is a weak, monobasic Lewis acid of boron. Hydrogen bonding in boric acid creates a layered structure by joining BO_3^{3-}(See Figure.1b) units with unsymmetrical hydrogen bonds. Weak forces of attraction hold the adjacent layers of a boric acid crystal together. Boric acid is a planar solid with intermolecular hydrogen bonding generating a near hexagonal layered structure (Hydrogen bonded solid boric acid 2D sheet($BA-2D$)(See Figure.1c) comparable to graphite $BAG(p,q)$.(See Figure.1a)



(a) $BAG(p, q)$



(b) BA (c) $BA - 2D$

Figure 1: Boric acid structures

3 Preliminaries

In this paper, we consider a molecular graph without loops and multiple edges as $G = (V(G), E(G))$, where $V(G)$ is the set of vertices of G and $E(G)$ is the set of edges of G and let $P = |V(G)|$ and $R = |E(G)|$. The length of the shortest u_1u_2-path is called the distance $d_G(u_1, u_2)$ between two vertices $u_1, u_2 \in V(G)$. If $e_1 = f_1g_1 \in E(G)$ and $u_1 \in V(G)$, then the distance $d_G(u_1, e_1)$ between them is defined a $min\{d_G(u_1, f_1), d_G(u_1, g_1)\}$. The distance $D_G(e_1, e_2)$ between edges $e_1 = f_1g_1$ and $e_2 = u_1u_2$ is the minimum number of edges along a shortest e_1, u_1-path or a shortest e_1, u_2-path [22, 52]. The following topological indices are given in Table.1 are computed in this study.

Table 1: **Edge distance based topological indices (TI's)**

TI's	**Formula**
$W_e(G)$[52]	$W_e(G) = \sum_{\{e_1,e_2\}\subseteq E(G)} D(e_1, e_2)$
$Sz_e(G)$[53]	$Sz_e(G) = \sum_{e\in E(G)} m_u(e)m_v(e)$
$PI_e(G)$[54]	$PI_e(G) = \sum_{e\in E(G)} m_u(e) + m_v(e)$
$W_{ve}(G)$[52]	$W_{ve}(G) = \frac{1}{2} \sum_{u\in V(G)} \sum_{e_2\in E(G)} d(u, e_2)$

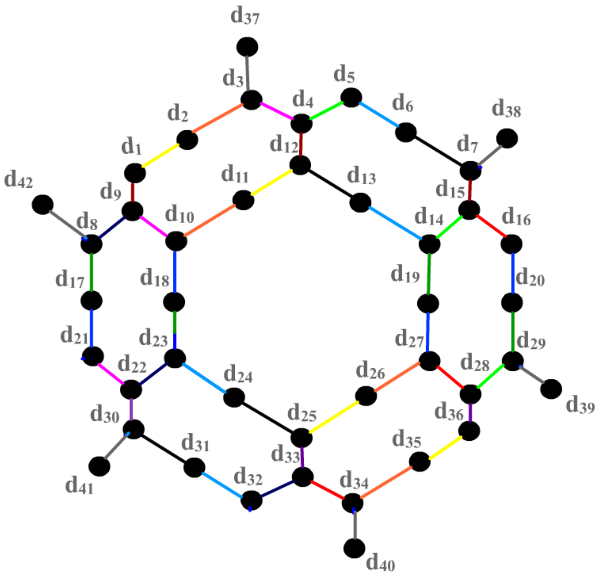
Let G be a graph and K is the subgraph of G. Then K is said to be isometric if $d_K(u_1, u_2) = d_G(u_1, u_2)$ for any $u_1, u_2 \in V(K)$. A function $f : V(K) \to V(G)$ is isometric embedding of K into G if $f(K) \subseteq G$. If an isometric embedding into the p-dimensional hypercube (Q_p) is allowed by a graph K, then we tells that a graph K is a partial cube.

Let $e_1 = fg \in E(G)$ and $e_2 = uv \in E(G)$, then $e_1 \Theta e_2$ if $d_G(f, u)+d_G(g, v) \neq d_G(f, v)+d_G(g, u)$ is called Djković Winkler relation Θ [55, 56] and the two edges e_1 and e_2, then co-distant (e_1 co e_2) said to be co relation (r) iff $d_G(g, u) = d_G(g, v) + 1 = d_G(f, u) + 1 = d_G(f, v)$ which play a key role in our analytical computation. The relation Θ and co are not transitive but it is reflexive and symmetric.

The relation Θ is also transitive and hence an equivalence relation if molecular graph G is a partial cube. In general, the transitive closure Θ^* of Θ forms an equivalence on any connected graph G and thus partitions $E(G)$ into Θ^*-classes $\mathcal{F}(G)$. If $\mathcal{F}(G) = \{F_1, F_2, ..., F_r\}$, then each graph $G - F_i$ divides into two connected components $A^i_1, A^i_2, ..., A^i_s$. The quotient graph G/F_i of $\mathcal{F}(G)$ is a graph with $V(G/F_i) = \{A^i_j|1 \leq j \leq s_i\}$ and $E(G/F_i) = \{A^i_jA^i_k|\exists u_1 \in V(A^i_j)$ and $u_2 \in V(A^i_k) \ni u_1u_2 \in F_i\}$. Finally, if every section E_i is collection of one or more Θ^* of G, then a partition $\mathcal{E}(G) = \{E_1, E_2, ..., E_s\}$ of $E(G)$ is coarser, then the partition of $\mathcal{F}(G)$. The idea of strength weighted (G_{sw}) graph was derived in [57] and the generalization of results were given in [12] and also for example, basic definitions of (G_{sw}) for edge Wiener and vertex-edge Wiener indices were derived in [12].

Theorem 3.1 (12)**.** *Let* $G_{sw} = (G, (w_v, s_v), s_e)$ *be a strength weighted graph. Then a partition* $\mathcal{E}(G_{sw}) = \{E_1, E_2, ..., E_t\}$ *of* $E(G)$ *coarser than* $\mathcal{F}'(G_{sw})$*. If* $X \in \{W_e, Sz_e, PI_e, W_{ve}\}$*, then* $X(G_{sw}) = \sum_{i=1}^{t} X(G/E_i, (w_v^i, s_v^i), s_e^i)$*.*

Let $A(y) = \{e_2 \in E(G) | e_1 \ co \ e_2\}$. Now $A(y)$ is called an orthogonal cut oc for G. Now $E(G) = A_1 \cup A_2 \cup ... \cup A_k, A_i \cap A_j \neq \phi, i \neq j$ and $i, j = 1, 2, ..., k$ can be divided into orthogonal cut. If $A(y)$ is not satisfy the condition of transitive then it is derived as quasi-orthogonal cut (qoc). Then $\Omega(G, y)$ polynomial said by Diudea [58] with opposite edge strip (ops) and ops is equal to qoc in plane graph. The below is a molecular graph ops defined on faces and relation co defined in the graph.



(a) $BA - 2D$

Figure 2: **The *co*-relation in hydrogen bonded solid boric acid $2D$ sheet**

Now qoc are calculated for the hydrogen bonded solid boric acid $2D$ structure. The same color edges are co-distinct in Figure $2a$. For the two edges $a = d_9 d_{10}, b = d_{21} d_{22}$ from the above Figure $2a$ be $a \ co \ b$. Now we define the Omega, Theta, PI and Sadhana polynomial are denoted as $\Omega(G, y)$, $\Theta(G, y)$, $Sd(G, y)$ and $PI(G, y)$ (From Table.2) which are called four polynomials ($4p$) and $4p$ are defined as follows,

Here

$$m(G, t) = n(qoc) \tag{3}$$

where t is the length of qoc and $n(qoc)$ is said to number of qoc.

Table 2: **4 polynomials**

4p	**Formula**
$\Omega(G,y)$[r]	$\sum_t m(G,t)y^t$
$\Theta(G,y)$[r]	$\sum_t m(G,t)ty^t$
$PI(G,y)$[r]	$\sum_t m(G,t)ty^{e-t}$
$Sd(G,y)$[r]	$\sum_t m(G,t)y^{e-t}$

First derivative of $4p$ at $y = 1$ gives Theta, PI and Sadhana indices are denoted by $\Theta(G)$, $PI(G)$ and $Sd(G)$ which are defined as follows,

$$\Omega^{'}(G,1) = R \tag{4}$$

$$\Theta^{'}(G,1) = \Theta(G) \tag{5}$$

$$PI^{'}(G,1) = PI(G) \tag{6}$$

$$Sd^{'}(G,1) = Sd(G) \tag{7}$$

Applying Theorem 3.2 the derivatives at $y = 1$, *4p* are obtained.

Theorem 3.2 (59)**.** *Let g and h be two functions which are differentiable such that*

$$\lim_{y\to b} g(y) = \lim_{y\to b} h(y) = 0$$

at $y = b$, where y is some finite point. Then LHôspitals rule defined as

$$\lim_{y\to b} \frac{g(y)}{h(y)} = \lim_{y\to b} \frac{g^{'}(y)}{h^{'}(y)}$$

If both $g^{'}(y)$ and $h^{'}(y)$ approach 0 as $y \to b$ then LHôspitals rule could be apply again and then assuming that both functions are sufficiently differentiable.

By Nadeem [60], Sd and PI descriptors are computed by using the below rule,

$$PI(G) = \{\Omega^{'}(G,y)_{y=1}\}^2 - \{\Theta^{'}(G,y)_{y=1}\} = \{\Theta(G,y)_{y=1}\}^2 - \{\Theta^{'}(G,y)_{y=1}\} \tag{8}$$

$$Sd(G) = \{\Omega^{'}(G,y)_{y=1}\}\{\Omega(G,y)_{y=1} - 1\} \tag{9}$$

Theorem 3.3 (24)**.**

Let G be a graph with Θ^*-classes F_i where $1 \leq i \leq k$. F_i can split into two Θ^*-subclasses F_{1i} and F_{1i}. Then $G - F_{1i}$ has exactly two components A and B and $G - F_{2i}$ has more than two components A, B and set of other components C which have only isolated vertices are convex. Let $n_1(A)$ and $n_2(B)$ are number of vertices of two components A and B respectively. And let $m_1(A)$ and $m_2(B)$ are number of edges of two components A and B respectively. The length of shortest path between two isolated vertices a and b of G is denoted by $d(a,b) = 0$. Then

For $G - F_{1i}$,

(i) $W_e(G) = \sum_{i=1}^{k} m_1(F_{1i})m_2(F_{1i})$,

(ii) $Sz_e(G) = \sum_{i=1}^{k} |F_{1i}| m_1(F_{1i})m_2(F_{1i})$,

(iii) $PI_v(G) = \sum_{i=1}^{k} |F_{1i}|(m_1(F_{1i}) + m_2(F_{1i}))$,

(iv) $W_{ve}(G) = \frac{1}{2}\sum_{i=1}^{k} [n_1(F_{1i})m_2(F_{1i}) + n_2(F_{1i})m_1(F_{1i})]$

and

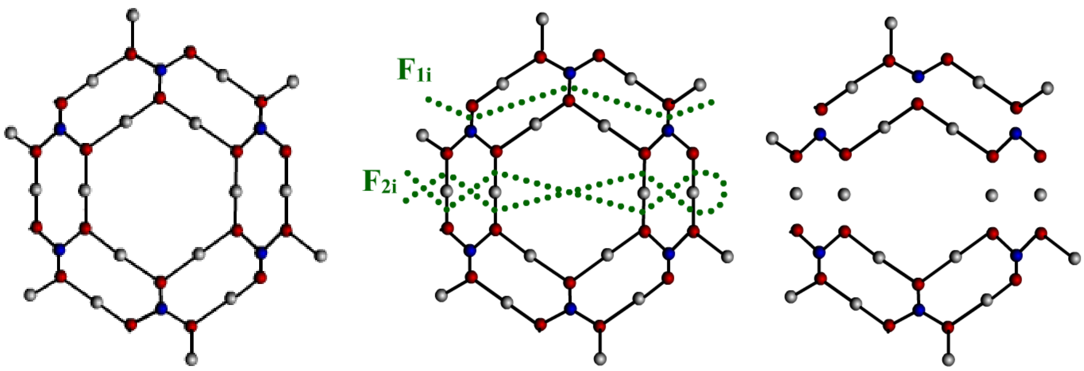
For $G - F_{2i}$,

(i) $W_e(G) = \sum_{i=1}^{k} 2m_1(F_{2i})m_2(F_{2i})$,

(ii) $Sz_e(G) = \sum_{i=1}^{k} |F_{2i}| m_1(F_{2i})m_2(F_{2i})$,

(iii) $PI_e(G) = \sum_{i=1}^{k} |F_{2i}|(m_1(F_{2i}) + m_2(F_{2i}))$,

(iv) $W_{ve}(G) = \frac{1}{2}\sum_{i=1}^{k} [n_1(F_{2i})m_2(F_{2i}) + n_2(F_{2i})m_1(F_{2i})]$.



(a) G (b) F_{1i} and F_{2i} (c) $G - F_{1i}$ and $G - F_{2i}$

Figure 3: **Illustration for Θ^*-relation of G**

4 Edge-version of distance based topological descriptors

In this part, we derived some edge-version of distance based topological descriptors for boric acid graphite sheet. Table 3 gives the notations for F_i depicted in Figure 3.

Table 3: **Notations of Types of cuts**

Types of cuts(F_i)	**Notations**		**Directions**	
Horizontal	H_{1i}, H_{2i}	H_{-1i}, H_{-2i}	North	South
Obtuse	O_{1i}, O_{2i}	O_{-1i}, O_{-2i}	North-east	South-west
Acute	A_{1i}, A_{2i}	A_{-1i}, A_{-2i}	North-west	South-east

Theorem 4.1. *Let G be a graphene like boric acid structure $BAG(p,q)$.*
a.If $p<q$, then

$$W_e(G)=\frac{-1}{5}(648p^5-3240p^4q-1440p^4-6480p^3q^2-17280p^3q-5940p^3-6480p^2q^3-20520p^2q^2-17340p^2q+2430p^2-5760pq^3-5670pq^2-3200pq-318p-1280q^3+1035q^2-630q+210)$$

$$Sz_e(G)=\frac{2}{15}(3024p^5-2520p^4q-4070p^4+58320p^3q^3+136080p^3q^2+123740p^3q+25700p^3+74520p^2q^3+90360p^2q^2+36540p^2q-12235p^2+32370pq^3+8070pq^2+4420pq+5551p+4575q^3-4050q^2+1785q-510)$$

$$PI_e(G)=\frac{4}{3}(40p^3+972p^2q^2+1500p^2q+660p^2+780pq^2+330pq-205p+165q^2-99q+21)$$

$$W_{ve}(G)=\frac{1}{30}(11088p^5-30240p^4q-7210p^4+30240p^3q^2+9660p^3q-18200p^3+40320p^2q^3+154560p^2q^2+170940p^2q+34900p^2+10080pq^4+61460pq^3+65160pq^2+30880pq-4858p-3024q^5-5950q^4+6420q^3-4295q^2-1431q-600).$$

b. If $p=q$, then

$$W_e(G)=\frac{-1}{15}(3564p^5-14580p^4q-2880p^4-19440p^3q^2-63720p^3q-17200p^3-16200p^2q^3-54000p^2q^2-55560p^2q+8310p^2-14400pq^3-14730pq^2-10140pq-1574p-3200q^3+2625q^2-1270q+435)$$

$$Sz_e(G)=\frac{-2}{15}(3240p^6-9720p^5q+1476p^5-26100p^4q+6750p^4-51840p^3q^3-120960p^3q^2-142700p^3q-23040p^3-65520p^2q^3-78240p^2q^2-41160p^2q+13365p^2-28210pq^3-6750pq^2-4800pq-5751p-3935q^3+3570q^2-1645q+390)$$

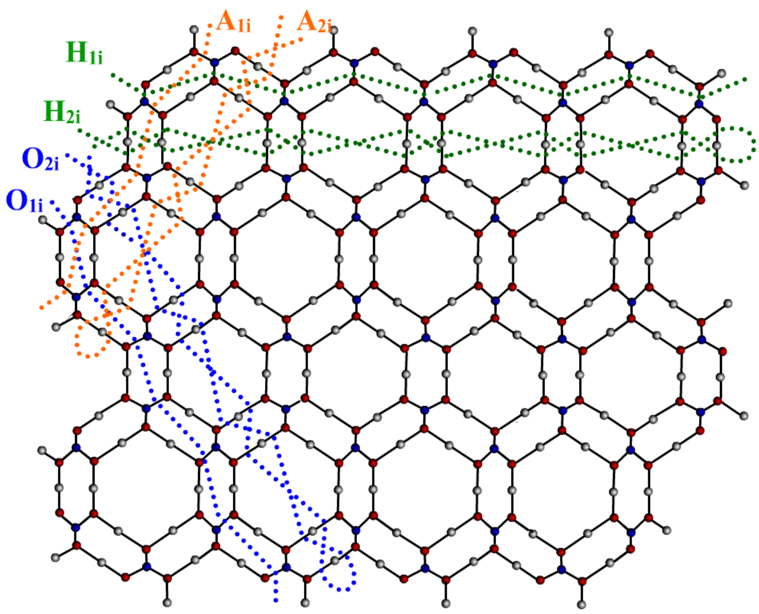
$$PI_e(G)=\frac{2}{3}(216p^3q+248p^3+1728p^2q^2+3036p^2q+1380p^2+1356pq^2+648pq-422p+282q^2-186q+39)$$

$$W_{ve}(G)=\frac{1}{30}(6552p^5-12600p^4q-7560p^4+30240p^3q^2+53620p^3q-6280p^3+35280p^2q^3+141120p^2q^2+184740p^2q+25425p^2+10080pq^4+56700pq^3+59700pq^2+36260pq-5927p-3024q^5-5950q^4+5300q^3-3875q^2-161q-300).$$

Proof. Let G be graphene like boric acid structure $BAG(p,q)$. Let $P=|V(G)|=28p+14q+28pq$

and $R = |E(G)| = 32p + 16q + 36pq - 2$. The collections of two Θ^*-classes F_{1i} and F_{2i} are the parts of F_i (See Figure.4). The Θ^*-classes F_{1i} and F_{2i} in the directions of North-west, North-east and East are also called Obtuse (O), Acute (A) and Horizontal (H) respectively. The collections of Θ^*-classes F_{1i} are $\{O_{1i}|1 \leq i \leq p+q+1\}$, $\{A_{1i}|1 \leq i \leq p+q\}$, $\{H_{1i}|1 \leq i \leq 2p+1\}$, $\{P_i|1 \leq i \leq 4p+2q+2\}$ and the collections of Θ^*-classes F_{2i} are $\{O_{2i}|1 \leq i \leq p+q\}$, $\{A_{2i}|1 \leq i \leq p+q\}$, $\{H_{2i}|1 \leq i \leq 2p\}$ (See Table.4).

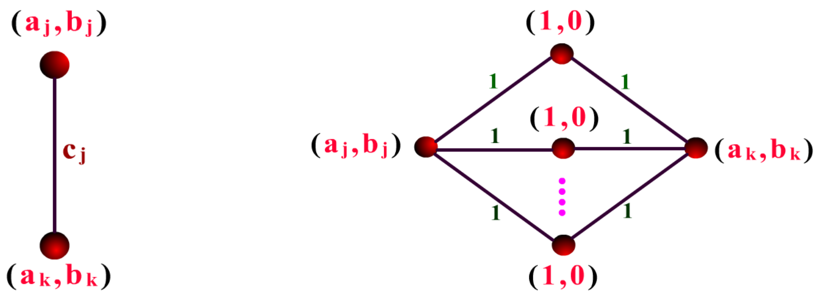
Let $|F_{1i}| = |F_{2i}| = c_j = m(G,t)$ (from Equation (3)) and number of c_j be $n(c_j)$.



(a) Types of cuts F_i

Figure 4

Applying Θ^*-classes F_{1i} on G, we get the quotient graph $Q_1 = (G/F_{1i}, (w_v^{1i}, s_v^{1i}), s_e^{1i})$ (See Figure.5a), which is a complete bipartite graph K_2. The values of vertex-weighted and strength-weighted functions (a_j, b_j), (a_k, b_k) and c_j are given in the Table.5.



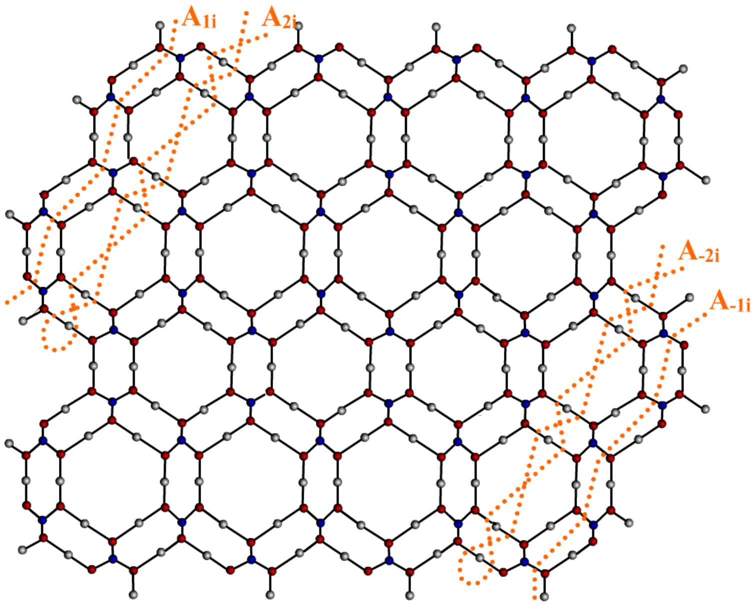
(a) Q_1 (b) Q_2

Figure 5: **a)** G/F_{1i}, **b)** G/F_{2i}

Table 4: **Size of Θ^*-classes of F_{1i} and F_{2i}**

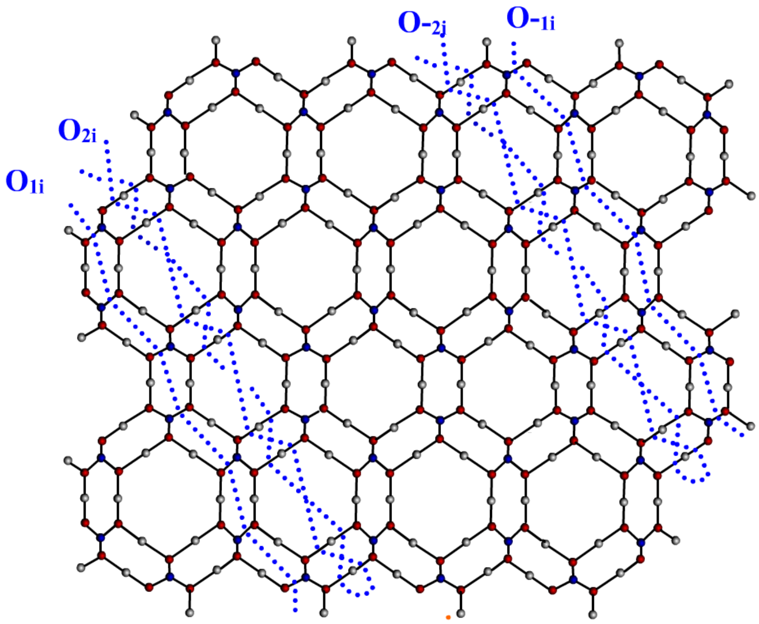
F_{1i} and F_{2i}	Range	c_j	c_j	Cases
O_{1i}	$1 \leq i \leq p$	$c_1 = 4i - 1$	$n(c_1) = 4i - 1$	if $p < q$
	$p+1 \leq i \leq p+1$	$c_2 = 4p + 1$	$n(c_2) = 4p + 1$	
	$p+2 \leq i \leq q$	$c_3 = 4p + 2$	$n(c_3) = 4p + 2$	
O_{1i}	$1 \leq i \leq p$	$c_4 = 4i - 1$	$n(c_4) = 4i - 1$	if $p = q$
	$p+1 \leq i \leq p+1$	$c_5 = 4p$	$n(c_5) = 4p$	
A_{1i}	$1 \leq i \leq p$	$c_6 = 4i + 1$	$n(c_6) = 4i + 1$	if $p \leq q$
	$p+1 \leq i \leq q$	$c_7 = 4p + 2$	$n(c_7) = 4p + 2$	
H_{1i}	$1 \leq i \leq 1$	$c_8 = 2q + 1$	$n(c_8) = 2q + 1$	if $p \leq q$
	$2 \leq i \leq 2p$	$c_9 = 2q + 2$	$n(c_9) = 2q + 2$	
P_i	$1 \leq i \leq 4p + 2q + 2$	$c_{10} = 1$	$n(c_{10}) = 1$	if $p \leq q$
O_{2i}	$1 \leq i \leq p$	$c_{11} = 1$	$n(c_{11}) = 8i$	if $p \leq q$
	$p+1 \leq i \leq q$	$c_{12} = 1$	$n(c_{12}) = 8p + 4$	
A_{2i}	$1 \leq i \leq p - 1$	$c_{13} = 1$	$n(c_{13}) = 8i + 4$	if $p \leq q$
	$p \leq i \leq q$	$c_{14} = 1$	$n(c_{14}) = 8p + 4$	
H_{2i}	$1 \leq i \leq 2p$	$c_{15} = 1$	$n(c_{15}) = 8q + 4$	if $p \leq q$

Applying Θ^*-classes F_{2i} on G, we get the quotient graph $Q_2 = (G/F_{2i}, (w_v^{2i}, s_v^{2i}), s_e^{2i})$ (See Figure 5b), which is complete bipartite graph $K_{2,t}$ where $t = n(c_j)$, where $11 \leq j \leq 15$. The values of vertex-weighted and strength-weighted functions (a_j, b_j), (a_k, b_k), $(1, 0)$ and 1 are depicted in the Table.5.



(a) Acute cuts

Figure 6



(a) Obtuse cuts

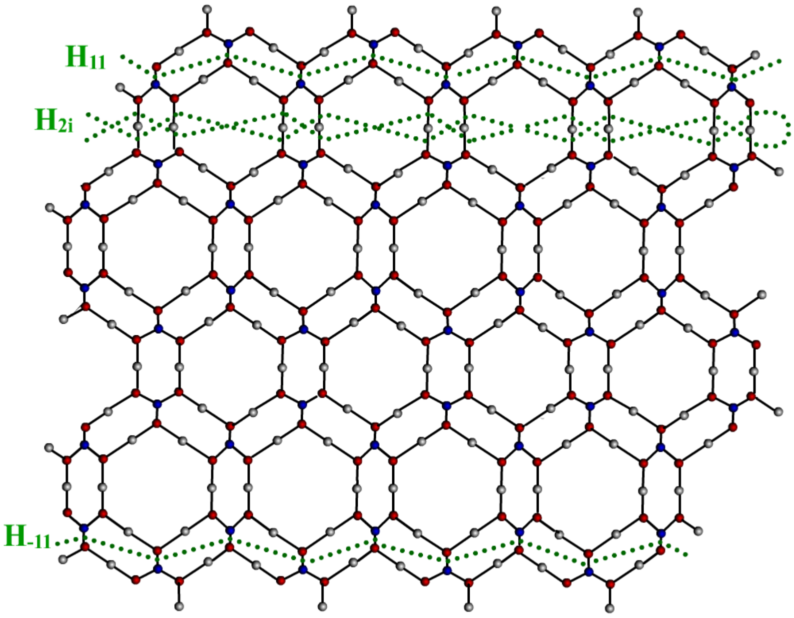
Figure 7

Table 5: **Vertex weighted and strength-weighted values for Q_1 and Q_2 of G**

Quotient graphs	Range	w_v	s_v	c_j	Cases
G/O_{1i}	$1 \leq i \leq p$	$a_1 = 14i^2 - 7i + 2$	$b_1 = 18i^2 - 14i + 4$	$c_1 = 4i - 1$	if $p < q$
	$p+1 \leq i \leq p+1$	$a_3 = 14p^2 + 21p + 2$	$b_3 = 18p^2 + 22p + 1$	$c_2 = 4p + 2$	
	$p+2 \leq i \leq q$	$a_5 = 14i + 28ip - 12$	$b_5 = i(36p+16) - 18p^2 - 30p - 18$	$c_3 = 4i + 2$	
G/O_{1i}	$1 \leq i \leq p$	$a_7 = 14i^2 - 7i + 2$	$b_7 = 18i^2 - 14i + 4$	$c_4 = 4i - 1$	if $p = q$
	$p+1 \leq i \leq p+1$	$a_9 = 14p^2 + 21p$	$b_9 = 18p^2 + 22p - 1$	$c_5 = 4p$	
G/A_{1i}	$1 \leq i \leq p$	$a_{11} = 14i^2 + 7i - 5$	$b_{11} = 18i^2 + 4i - 7$	$c_6 = 4i + 1$	if $p \leq q$
	$p+1 \leq i \leq q$	$a_{13} = (28p+14)i - 14p^2 - 7p - 7$	$b_{13} = i(36p+16) - 18p^2 - 12p - 10$	$c_7 = 4p$	
	$1 \leq i \leq 1$	$a_{15} = 7q + 2$	$b_{15} = 7q + 1$	$c_8 = 2q + 1$	if $p \leq q$
G/H_{1i}	$2 \leq i \leq 2p$	$a_{17} = 14i + (14i-7)q - 14$	$b_{17} = (18i-11)q + 16i - 18$	$c_9 = 2q + 2$	
G/P_i	$1 \leq i \leq 4p + 2q + 2$	$a_{19} = 4p + 2q + 2$	$b_{19} = 0$	$c_{10} = 1$	if $p \leq q$
G/O_{2i}	$1 \leq i \leq p$	$a_{21} = 14i^2 + 5i$	$b_{21} = 18i^2 + 2i$	$c_{11} = 1$	if $p \leq q$
	$p+1 \leq i \leq q$	$a_{23} = i(28p+14)i - 14p^2 - 9p - 8$	$b_{23} = i(36p+16) - 18p^2 - 14p - 11$	$c_{12} = 1$	
G/A_{2i}	$1 \leq i \leq p-1$	$a_{25} = 14i^2 + 19i - 1$	$b_{25} = 18i^2 + 20i–3$	$c_{13} = 1$	if $p \leq q$
	$p \leq i \leq q$	$a_{27} = (28p+14)i - 14p^2 + 5p - 1$	$b_{27} = 4p - 18p^2 + i(36p+16) - 3$	$c_{14} = 1$	
G/H_{2i}	$1 \leq i \leq 2p$	$a_{29} = 14i - q + 14iq - 8$	$b_{29} = 16i + (18i-3)q - 11$	$c_{15} = 1$	if $p \leq q$

$a_{2s} = P - a_{2s-1}$ and $b_{2s} = R - b_{2s-1} - c_j$, where $1 \leq s = j \leq 10$.

$a_{2s} = P - a_{2s-1} - \frac{n(c_j)}{2}$ and $b_{2s} = R - b_{2s-1} - n(c_j)$, where $11 \leq s = j \leq 15$.



(a) Horizontal cuts

Figure 8

By symmetry, we have $(A_{1i}) = (A_{-1i})$, $(O_{1i}) = (O_{-1i})$, for $1 \leq i \leq p$ and $H_{11} = H_{-11}$ and $(O_{2i}) = (O_{-2i})$ for $1 \leq i \leq p$ and $(A_{2i}) = (A_{-2i})$ for $1 \leq i \leq p-1$.(See Figures 6, 7 and 8)

If $p < q$ then,

$$(X(O_{1i}), \circ) = \sum_{i=1}^{p}(b_1 \circ b_2)c_1 + \sum_{i=p+1}^{p+1}(b_3 \circ b_4)c_2 + \sum_{i=p+2}^{q}(b_5 \circ b_6)c_3$$

$$(X(A_{1i}), \circ) = 2\sum_{i=1}^{p}(b_{11} \circ b_{12})c_6 + \sum_{i=p+1}^{q}(b_{13} \circ b_{14})c_7$$

$$(X(H_{1i}), \circ) = 2\sum_{i=1}^{1}(b_{15} \circ b_{16})c_8 + \sum_{i=2}^{2p}(b_{17} \circ b_{18})c_9$$

$$(X(P_i), \circ) = \sum_{i=1}^{4p+2q+2}(b_{19} \circ b_{20})c_{10}$$

And

$$(X(O_{2i}), \circ) = 2\sum_{i=1}^{p}2(b_{21} \circ b_{22})n(c_{11}) + \sum_{i=p+1}^{q}2(b_{23} \circ b_{24})n(c_{12})$$

$$(X(A_{2i}), \circ) = 2\sum_{i=1}^{p-1}2(b_{25} \circ b_{26})n(c_{13}) + \sum_{i=p}^{q}2(b_{27} \circ b_{28})n(c_{14})$$

$$(X(H_{2i}), \circ) = \sum_{i=1}^{2p}2(b_{29} \circ b_{30})n(c_{15}),$$

And also,

$$Y(O_{1i}) = \frac{1}{2}[\sum_{i=1}^{p} a_1b_2 + b_1a_2 + \sum_{i=p+1}^{p+1} a_3b_4 + b_3a_4 + \sum_{i=p+2}^{q} a_5b_6 + b_5a_6]$$
$$Y(A_{1i}) = \frac{1}{2}[2\sum_{i=1}^{p} a_{11}b_{12} + b_{11}a_{12} + \sum_{i=p+1}^{q} a_{13}b_{14} + b_{13}a_{14}]$$
$$Y(H_{1i}) = \frac{1}{2}[2\sum_{i=1}^{1} a_{15}b_{16} + b_{15}a_{16} + \sum_{i=2}^{2p} a_{17}b_{18} + b_{17}a_{18}]$$
$$Y(P_i) = \frac{1}{2}[\sum_{i=1}^{4p+2q+2} a_{19}b_{20} + b_{19}a_{20}]$$

And

$$Y(O_{2i}) = \frac{1}{2}[2\sum_{i=1}^{p} 2(a_{21}b_{22} + b_{21}a_{22}) + \sum_{i=1}^{p} \frac{n(c_{11})}{2}(b_{21}b_{22}) + \sum_{i=1}^{p} 2(a_{23}b_{24} + b_{23}a_{24})$$
$$+ \textstyle\sum_{i=p+1}^{p} \frac{n(c_{12})}{2}(b_{23}b_{24})]$$
$$Y(A_{2i}) = \frac{1}{2}[2\sum_{i=1}^{p-1} 2(a_{25}b_{26} + b_{25}a_{26}) + \sum_{i=1}^{p-1} \frac{n(c_{13})}{2}(b_{25}b_{26}) + \sum_{i=p}^{q} 2(a_{27}b_{28} + b_{28}a_{27})$$
$$+ \textstyle\sum_{i=p}^{q} \frac{n(c_{14})}{2}(b_{27}b_{28})]$$
$$Y(H_{2i}) = \frac{1}{2}[2\sum_{i=1}^{2p} 2(a_{29}b_{30} + b_{29}a_{30}) + \sum_{i=1}^{2p} \frac{n(c_{15})}{2}(b_{29}b_{30})].$$

Here $(X(G), \circ) = (X(O_{1i}), \circ) + (X(A_{1i}), \circ) + (X(H_{1i}), \circ) + (X(P_{1i}), \circ) + (X(O_{2i}), \circ) + (X(A_{2i}), \circ) + (X(H_{2i}), \circ)$ and $Y(G) = Y(O_{1i}) + Y(A_{1i}) + Y(H_{1i}) + Y(P_{1i}) + Y(O_{2i}) + Y(A_{2i}) + Y(H_{2i})$, where $(X, \circ)$=$(W_e, \times)$, $(Sz_e, \times)$, $(PI_e, +)$ and Y=W_{ve}, for $(X(G), \circ) = (W_e, \times)$ substitute $c_j = n(c_j) = 1$, where $1 \leq j \leq 15$.

Further, an analytical computation of $(X(G), \circ)$ and $Y(G)$ give the result of the Theorem 4.1(a).

If $p = q$ then,

$$(X(O_{1i}), \circ) = 2\sum_{i=1}^{p}(b_7 \circ b_8)c_4 + \sum_{i=p+1}^{q} (b_9 \circ b_{10})c_5$$
$$(X(A_{1i}), \circ) = 2\sum_{i=1}^{p}(b_{11} \circ b_{12})c_6 + \sum_{i=p+1}^{q} (b_{13} \circ b_{14})c_7$$
$$(X(H_{1i}), \circ) = 2\sum_{i=1}^{1}(b_{15} \circ b_{16})c_8 + \sum_{i=2}^{2p}(b_{17} \circ b_{18})c_9$$
$$(X(P_i), \circ) = \sum_{i=1}^{4p+2q+2} (b_{19} \circ b_{20})c_{10}$$

And

$$(X(O_{2i}), \circ) = 2\sum_{i=1}^{p} 2(b_{21} \circ b_{22})n(c_{11}) + \sum_{i=p+1}^{q} 2(b_{23} \circ b_{24})n(c_{12})$$
$$(X(A_{2i}), \circ) = 2\sum_{i=1}^{p-1} 2(b_{25} \circ b_{26})n(c_{13}) + \sum_{i=p}^{q} 2(b_{27} \circ b_{28})n(c_{14})$$
$$(X(H_{2i}), \circ) = \sum_{i=1}^{2p} 2(b_{29} \circ b_{30})n(c_{15}),$$

Hence,

$$Y(O_{1i}) = \frac{1}{2}[2\sum_{i=1}^{p} a_7b_8 + b_7a_8 + \sum_{i=p+1}^{q} a_9b_{10} + b_9a_{10}]$$

$$Y(A_{1i}) = \frac{1}{2}[2\sum_{i=1}^{p} a_{11}b_{12} + b_{11}a_{12} + \sum_{i=p+1}^{q} a_{13}b_{14} + b_{13}a_{14}]$$

$$Y(H_{1i}) = \frac{1}{2}[2\sum_{i=1}^{1} a_{15}b_{16} + b_{15}a_{16} + \sum_{i=2}^{2p} a_{17}b_{18} + b_{17}a_{18}]$$

$$Y(P_i) = \frac{1}{2}[\sum_{i=1}^{4p+2q+2} a_{19}b_{20} + b_{19}a_{20}]$$

And

$$Y(O_{2i}) = \frac{1}{2}[2\sum_{i=1}^{p} 2(a_{21}b_{22} + b_{21}a_{22}) + \sum_{i=1}^{p} \frac{n(c_{11})}{2}(b_{21}b_{22}) + \sum_{i=1}^{p} 2(a_{23}b_{24} + b_{23}a_{24}) + \sum_{i=p+1}^{p} \frac{n(c_{12})}{2}(b_{23}b_{24})]$$

$$Y(A_{2i}) = \frac{1}{2}[2\sum_{i=1}^{p-1} 2(a_{25}b_{26} + b_{25}a_{26}) + \sum_{i=1}^{p-1} \frac{n(c_{13})}{2}(b_{25}b_{26}) + \sum_{i=p}^{q} 2(a_{27}b_{28} + b_{28}a_{27}) + \sum_{i=p}^{q} \frac{n(c_{14})}{2}(b_{27}b_{28})]$$

$$Y(H_{2i}) = \frac{1}{2}[2\sum_{i=1}^{2p} 2(a_{29}b_{30} + b_{29}a_{30}) + \sum_{i=1}^{2p} \frac{n(c_{15})}{2}(b_{29}b_{30})].$$

Here $(X(G), \circ) = (X(O_{1i}), \circ) + (X(A_{1i}), \circ) + (X(H_{1i}), \circ) + (X(P_{1i}), \circ) + (X(O_{2i}), \circ) + (X(A_{2i}), \circ) + (X(H_{2i}), \circ)$ and $Y(G) = Y(O_{1i}) + Y(A_{1i}) + Y(H_{1i}) + Y(P_{1i}) + Y(O_{2i}) + Y(A_{2i}) + Y(H_{2i})$, where $(X, \circ)$=$(W_e, \times)$, $(Sz_e, \times)$, $(PI_e, +)$ and Y=W_{ve}, for $(X(G), \circ) = (W_e, \times)$ substitute $c_j = n(c_j) = 1$, where $1 \leq j \leq 15$.

Further, an analytical computation of $(X(G), \circ)$ and $Y(G)$ give the result of the Theorem 4.1(b). □

Theorem 4.2. *Let G is graphene like boric acid structure $BAG(p, q)$. If $p > q$, then*

$$\begin{aligned}
We(G) = {} & \frac{1}{5}(12960p^3q^2 + 23040p^3q + 10240p^3 + 11880p^2q^2 + 4440p^2q - 5440p^2 + 3235pq^4 + 11550pq^3 \\
& + 18505pq^2 + 9280pq + 3190p - 643q^5 - 1470q^4 - 2955q^3 - 4105q^2 - 2242q - 795) \\
Sze(G) = {} & \frac{-2}{15}(3240p^5q + 3240p^5 - 9720p^4q^2 - 13680p^4q - 3960p^4 - 51840p^3q^3 - 146160p^3q^2 - 138120p^3q \\
& - 43640p^3 + 6480p^2q^4 - 9720p^2q^3 + 11760p^2q^2 + 54000p^2q + 27720p^2 - 9690pq^5 - 66030pq^4 \\
& - 161140pq^3 - 133320pq^2 - 43220pq - 9460p - 3270q^6 - 1866q^5 + 26920q^4 + 49695q^3 + 34925q^2 \\
& + 5886q + 2460) \\
PI_e(G) = {} & \frac{2}{3}(1944p^2q^2 + 3240p^2q + 1344p^2 + 1320pq^2 + 612pq - 432p + 108q^4 + 332q^3 + 516q^2 - 158q + 51) \\
W_{ve}(G) = {} & \frac{-1}{60}(5040p^4q + 5040p^4 - 141120p^3q^2 - 263760p^3q - 122640p^3 + 30240p^2q^3 - 70560p^2q^2 \\
& - 52080p^2q + 38640p^2 - 40320pq^4 - 134540pq^3 - 201780pq^2 - 76720pq - 13080p + 2016q^5
\end{aligned}$$

$$+ 2030q^4 + 13360q^3 + 22585q^2 + 14579q + 3960).$$

Proof. Let G be graphene like boric acid structure $BAG(p, q)$. Let $P = |V(G)| = 28p + 14q + 28pq$ and $R = |E(G)| = 32p + 16q + 36pq - 2$. The collections of two Θ^*-classes F_{1i} and F_{2i} are the parts of F_i. The Θ^*-classes F_{1i} and F_{2i} in the directions of North-west, North-east and East are also called Obtuse (O), Acute (A) and Horizontal (H) respectively. These collections of Θ^*-classes F_{1i} are $\{O_{1i}|1 \leq i \leq p+q+1\}$, $\{A_{1i}|1 \leq i \leq p+q\}$, $\{H_{1i}|1 \leq i \leq 2p+1\}$, $\{P_i|1 \leq i \leq 4p+2q+2\}$ and the collections of Θ^*-classes F_{2i} are $\{O_{2i}|1 \leq i \leq p+q\}$, $\{A_{2i}|1 \leq i \leq p+q\}$, $\{H_{2i}|1 \leq i \leq 2p\}$ (See Table.6).

Let $|F_{1i}| = |F_{2i}| = c_j = m(G, t)$ (from equation (3)) and number of c_j be $n(c_j)$.

Applying Θ^*-classes F_{1i} on G, we get the quotient graph $Q_1 = (G/F_{1i}, (w_v^{1i}, s_v^{1i}), s_e^{1i})$ (See Figure $5a$), which is a complete bipartite graph K_2. The values of vertex weighted and strength weighted functions (a_j, b_j), (a_k, b_k) and c_j are shown in the Table.7.

Table 6: **Size of Θ^*-classes of F_{1i} and F_{2i}**

F_{1i} and F_{2i}	Range	c_j	c_j	Cases
O_{1i}	$1 \leq i \leq q$	$c_1 = 4i - 1$	$n(c_1) = 4i - 1$	if $p > q$
	$q+1 \leq i \leq q+1$	$c_2 = 4q + 2$	$n(c_2) = 4q + 2$	
	$q+2 \leq i \leq p$	$c_3 = 4q + 4$	$n(c_3) = 4q + 4$	
A_{1i}	$1 \leq i \leq q$	$c_4 = 4i + 1$	$n(c_4) = 4i + 1$	if $p > q$
	$q+1 \leq i \leq p$	$c_5 = 4q + 4$	$n(c_5) = 4q + 4$	
H_{1i}	$1 \leq i \leq 1$	$c_6 = 2q + 1$	$n(c_6) = 2q + 1$	if $p \leq q$
	$2 \leq i \leq 2p$	$c_7 = 2q + 2$	$n(c_7) = 2q + 2$	
P_i	$1 \leq i \leq 4p + 2q + 2$	$c_8 = 1$	$n(c_8) = 1$	if $p \leq q$
O_{2i}	$1 \leq i \leq q$	$c_9 = 1$	$n(c_9) = 8i$	if $p \leq q$
	$q+1 \leq i \leq p$	$c_{10} = 1$	$n(c_{10}) = 8q + 4$	
A_{2i}	$1 \leq i \leq q - 1$	$c_{11} = 1$	$n(c_{11}) = 8i + 4$	if $p \leq q$
	$q \leq i \leq p$	$c_{12} = 1$	$n(c_{12}) = 8q + 4$	
H_{2i}	$1 \leq i \leq 2p$	$c_{13} = 1$	$n(c_{13}) = 4q + 4$	if $p \leq q$

Applying Θ^*-classes F_{2i} on G, we get the quotient graph $Q_2 = (G/F_{2i}, (w_v^{2i}, s_v^{2i}), s_e^{2i})$ (Figure $5b$), which is complete bipartite graph $K_{2,t}$, where $t = n(c_j)$, where $9 \leq j \leq 13$. The values of vertex-weighted and strength-weighted functions (a_j, b_j), (a_k, b_k), $(0, 1)$ and 1 are depicted in the Table 7.

Table 7: **Vertex-weighted and strength-weighted values for Q_1 and Q_2 of G**

Quotient graphs	Range	w_v	s_v	c_j	Cases
G/O_{1i}	$1 \leq i \leq q$	$a_1 = 14i^2 - 7i + 2$	$b_1 = 18i^2 - 14i + 4$	$c_1 = 4i - 1$	if $p > q$
	$q+1 \leq i \leq q+1$	$a_3 = 14q^2 + 21q + 7$	$b_3 = 18q^2 + 22q + 6$	$c_2 = 4q + 2$	
	$q+2 \leq i \leq p$	$a_5 = i(28q+28) - 14q^2 - 35q - 28$	$b_5 = (36p+32)i - 18p^2 - 46p - 35$	$c_3 = 4q + 4$	
G/A_{1i}	$1 \leq i \leq q$	$a_7 = 14i^2 + 7i - 5$	$b_7 = 18i^2 + 4i - 7$	$c_4 = 4i + 1$	if $p > q$
	$q+1 \leq i \leq p$	$a_9 = i(28q+28) - 14q^2 - 35q - 28$	$b_9 = i(36q+32) - 19q^2 - 25q - 21$	$c_5 = 4q + 4$	
H_{1i}	$1 \leq i \leq 1$	$a_{11} = 7q + 2$	$b_{11} = 7q + 1$	$c_6 = 2q + 1$	
	$2 \leq i \leq 2p$	$a_{13} = 14i + (14i-7)q - 14$	$b_{13} = (18i-11)q + 16i - 18$	$c_7 = 2q + 2$	if $p > q$
P_i	$1 \leq i \leq 4p + 2q + 2$	$a_{15} = 4p + 2q + 2$	$b_{15} = 0$	$c_8 = 1$	if $p > q$
G/O_{2i}	$1 \leq i \leq q$	$a_{17} = 14i^2 + 5i$	$b_{17} = 18i^2 + 2i$	$c_9 = 1$	if $p > q$
	$q+1 \leq i \leq p$	$a_{19} = i(28q+28) - 14q^2 - 9q - 1)$	$b_{19} = i(36q+32) - 18q^2 - 30q - 19$	$c_{10} = 1$	
G/A_{2i}	$1 \leq i \leq q-1$	$a_{21} = 14i^2 + 19i - 1$	$b_{21} = 18i^2 + 20i - 3$	$c_{11} = 1$	if $p > q$
	$q \leq i \leq p$	$a_{23} = (28q+28)i - 14q^2 - 9q - 1$	$b_{23} = i(36q+32) - 18q^2 - 12q - 3$	$c_{12} = 1$	
G/H_{2i}	$1 \leq i \leq 2p$	$a_{25} = 14i - q + 14iq - 8$	$b_{25} = 16i + q(18i-3) - 11$	$c_{13} = 1$	if $p > q$

$a_{2s} = P - a_{2s-1}$ and $b_{2s} = R - b_{2s-1} - c_j$, where $1 \le s = j \le 8$

$a_{2s} = P - a_{2s-1} - \frac{n(c_j)}{2}$ and $b_{2s} = R - b_{2s-1} - n(c_j)$, where $9 \le s = j \le 13$

By symmetry, we have $(A_{1i}) = (A_{-1i})$, $(O_{1i}) = (O_{-1i})$, for $1 \le i \le p$ and $H_{11} = H_{-11}$ and $(O_{2i}) = (O_{-2i})$ for $1 \le i \le p$ and $(A_{2i}) = (A_{-2i})$ for $1 \le i \le p-1$.

Hence, If $p > q$ then,

$$(X(O_{1i}), \circ) = \sum_{i=1}^{q} (b_1 \circ b_2)c_1 + \sum_{i=q+1}^{q+1} (b_3 \circ b_4)c_2 + \sum_{i=q+2}^{p} (b_5 \circ b_6)c_3$$

$$(X(A_{1i}), \circ) = 2\sum_{i=1}^{q} (b_7 \circ b_8)c_4 + \sum_{i=q+1}^{p} (b_9 \circ b_{10})c_5$$

$$(X(H_{1i}), \circ) = 2\sum_{i=1}^{1} (b_{11} \circ b_{12})c_6 + \sum_{i=2}^{2p} (b_{13} \circ b_{14})c_7$$

$$(X(P_i, \circ)) = \sum_{i=1}^{4p+2q+2} (b_{15} \circ b_{16})c_8$$

And

$$(X(O_{2i}), \circ) = 2\sum_{i=1}^{q} 2(b_{17} \circ b_{18})n(c_9) + \sum_{i=q+1}^{p} (b_{19} \circ b_{20})n(c_{10})$$

$$(X(A_{2i}), \circ) = 2\sum_{i=1}^{q-1} 2(b_{21} \circ b_{22})n(c_{11}) + \sum_{i=q}^{p} (b_{23} \circ b_{24})n(c_{12})$$

$$(X(H_{2i}), \circ) = \sum_{i=1}^{2p} 2(b_{25} \circ b_{26})n(c_{13}),$$

$$Y(O_{1i}) = \frac{1}{2}[\sum_{i=1}^{q} a_1b_2 + b_1a_2 + \sum_{i=q+1}^{q+1} a_3b_4 + b_3a_4 + \sum_{i=q+2}^{p} a_5b_6 + b_5a_6]$$

$$Y(A_{1i}) = \frac{1}{2}[2\sum_{i=1}^{q} a_7b_8 + b_7a_8 + \sum_{i=q+1}^{p} a_9b_{10} + b_9a_{10}]$$

$$Y(H_{1i}) = \frac{1}{2}[2\sum_{i=1}^{1} a_{11}b_{12} + b_{11}a_{12} + \sum_{i=2}^{2p} a_{13}b_{14} + b_{13}a_{14}]$$

$$Y(P_i) = \frac{1}{2}[\sum_{i=1}^{4p+2q+2} a_{15}b_{16} + b_{15}a_{16}]$$

And

$$Y(O_{2i}) = \frac{1}{2}[2\sum_{i=1}^{q} 2(a_{17}b_{18} + b_{17}a_{18}) + \sum_{i=1}^{q} \frac{n(c_9)}{2}(b_{17}b_{18}) + \sum_{i=1}^{p} 2(a_{19}b_{20} + b_{19}a_{20}) + \sum_{i=q+1}^{p} \frac{n(c_{10})}{2}(b_{19} + b_{20})]$$

$$Y(A_{2i}) = \frac{1}{2}[2\sum_{i=1}^{q-1} 2(a_{21}b_{22} + b_{21}a_{22}) + \sum_{i=1}^{q-1} \frac{n(c_{11})}{2}(b_{21}b_{22}) + \sum_{i=q}^{p} 2(a_{23}b_{24} + b_{23}a_{24}) + \sum_{i=q}^{p} \frac{n(c_{12})}{2}(b_{23} + b_{24})]$$

$$Y(H_{2i}) = \frac{1}{2}[2\sum_{i=1}^{2p} 2(a_{25}b_{26} + b_{25}a_{26}) + \sum_{i=1}^{2p} \frac{n(c_{13})}{2}(b_{25} + b_{26})].$$

Here $(X(G),\circ) = (X(O_{1i}),\circ) + (X(A_{1i}),\circ) + (X(H_{1i}),\circ) + (X(P_{1i}),\circ) + (X(O_{2i}),\circ) + (X(A_{2i}),\circ) + (X(H_{2i}),\circ)$ and $Y(G) = Y(O_{1i}) + Y(A_{1i}) + Y(H_{1i}) + Y(P_i) + Y(O_{2i}) + Y(A_{2i}) + Y(H_{2i})$, where $(X,\circ)$=$(W_e,\times)$, $(Sz_e,\times)$, $(PI_e,+)$ and Y=W_{ve}, for $(X(G),\circ) = (W_e,\times)$ substitute $c_j = n(c_j) = 1$, where $1 \le j \le 13$.

Further, an analytical computation of $(X(G),\circ)$ and $Y(G)$ gives the result of the Theorem 4.2. $\square$

5 Four polynomials and Subsequent indices

5.1 Four polynomials

In this section, we have done the results of four counting polynomials using the aforementioned preliminary results (from Section3).

Theorem 5.1. *Let G be a $BAG(p,q)$. Then Ω-polynomial of $BAG(p,q)$ is generalized as follows;*

a. $\Omega(G,y) = \frac{1}{y^4-1}[y^3(y^{4p}-1) + y^{4p+1}(y^4-1) - y^{4p+2}(p-q+1)(y^4-1) + 2y^5(y^{4p}-1) - y^{4p+2}(p-q)(y^4-1) + 2y^{2q+1}(y^4-1) + y^{(2q+2)(2p-1)}(y^4-1) + 2y(3p+2q+1)(y^4-1)]$, *(if $p<q$).*

b. $\Omega(G,y) = \frac{1}{y^4-1}[y^3(y^{4p}-1) + y^{4p}(y^4-1) + 2y^5(y^{4p}-1) - y^{4p+2}(p-q)(y^4-1) + 2y^{2q+1}(y^4-1) + y^{(2q+2)(2p-1)}(y^4-1) + 2y(3p+2q+1)(y^4-1)]$, *(if $p=q$).*

Proof. Let G be a $BAG(p,q)$. Now $m(G,t) = n(qoc)$ which is included F_{1i} and F_{2i}. Now c_j denotes the number of edges in each qoc. Using the definition of Omega polynomial, we obtain the following equation.

$$a.\ \Omega(G,y) = \sum_{i=1}^{p} y^{4i-1} + \sum_{i=p+1}^{p+1} y^{4p+1} + \sum_{i=p+2}^{q} y^{4p+2} + 2\sum_{i=1}^{p} y^{4i+1} + \sum_{i=p+1}^{q} y^{4p+2} + 2\sum_{i=1}^{1} y^{2q+1} + \sum_{i=2}^{2p} y^{2q+2} + \sum_{i=1}^{4p+2q+2} y + 2\sum_{i=1}^{p} y + \sum_{i=p+1}^{q} y + 2\sum_{i=1}^{p-1} y + \sum_{i=p}^{q} y + \sum_{i=1}^{2p} y. \quad (10)$$

Further more, an analytical computation obtain the result of Theorem 5.1(a)

b. For $p=q$ case, instead of $\sum_{i=p+1}^{p+1} y^{4p+1} + \sum_{p+2}^{q} y^{4p+2}$, substitute $\sum_{i=p+1}^{p+1} y^{4p}$ in equation (10) then further more, an analytical computation obtain the result of Theorem 5.1(b) $\square$

Theorem 5.2. *Let G be a $BAG(p,q)$. Then the Θ-polynomial of $BAG(p,q)$ is generalized as follows;*

a. $\Theta(G,y) = \frac{1}{(y^4-1)^2}[-y^3(4py^{4p} + 3y^{4p} - y^4 + y^{4p+4} - 4py^{4p+4} - 3) + y^{4p+1}(4p+1)(y^4-1)^2 - y^{(4p+2)}(4p+2)(p-q+1)(y^4-1)^2 - 2y^5(4py^{4p} + 5y^{4p} + y^4 - y^{4p+4} - 4py^{4p+4} - 5) - y^{(4p+2)}(4p+2)(p-q)(y^4-1)^2 + 2y^{2q+1}(2q+1)(y^4-1)^2 + y^{2q+2}(2p-1)(2q+2)(y^4-1)^2 + 2y(3p+2q+1)(y^4-1)^2]$, *(if $p<q$).*

$$b.\ \Theta(G,y) = \frac{1}{(y^4-1)^2}[-y^3(4py^{4p}+3y^{4p}-y^4+y^{4p+4}-4py^{4p+4}-3)+4py^{4p}(y^4-1)^2 - 2y^5(4py^{4p}+5y^{4p}+y^4-y^{4p+4}-4py^{4p+4}-5)-y^{4p+2}(4p+2)(p-q)(y^4-1)^2+2y^{2q+1} (2q+1)(y^4-1)^2+y^{2q+2}(2p-1)(2q+2)(y^4-1)^2+(y^4-1)^2(2y(3p+2q+1))], (if\, p{=}q).$$

Proof. Let G be a $BAG(p,q)$. Each summation is computed by MATLAB software. By using the definition of Theta polynomial, we obtain the following equation.

$$\begin{aligned}\Theta(G,y) = {} & \sum_{i=1}^{p}(4i-1)y^{4i-1} + \sum_{i=p+1}^{p+1}(4p+1)y^{4p+1} + \sum_{i=p+2}^{q}(4p+2)y^{4p+2} + 2\sum_{i=1}^{p}(4i+1)y^{4i+1} + \\ & \sum_{i=p+1}^{q}(4p+2)y^{4p+2} + \sum_{i=1}^{1}(2q+1)y^{2q+1} + \sum_{i=2}^{2p}(2q+2)y^{2q+2} + \sum_{i=1}^{4p+2q+2} y + 2\sum_{i=1}^{p} y + \\ & \sum_{i=p+1}^{q} y + 2\sum_{i=1}^{p-1} y + \sum_{i=p}^{q} y + \sum_{i=1}^{2p} y. \end{aligned} \tag{11}$$

Further, an analytical computation obtain the result of Theorem 5.2(a)

b. For case $p=q$, instead of $\sum_{i=p+1}^{p+1}(4p+1)y^{4p+1}+\sum_{p+2}^{q}(4p+2)y^{4p+2}$, we substitute $\sum_{i=p+1}^{p+1} 4py^{4p}$ in equation (11) then further, an analytical computation obtain the result of Theorem 5.2(b) $\square$

Theorem 5.3. *Let G be a $BAG(p,q)$. Then the PI-polynomial of $BAG(p,q)$ is generalized as follows;*

$$a.\ PI(G,y) = \frac{y^{32p+16q+36pq-2}}{(y^4-1)^2}[y^{-4p+1}(4p-4py^4+y^{4p}-3y^4+3y^{4p+4})+(4p+1)y^{-4p-1}(y^4-1)^2 - y^{-4p-2}(4p+2)(p-q+1)(y^4-1)^2+2y^{-4p-1}(4p-4py^4-y^{4p}-5y^4+5y^{4p+4}+1) - y^{-4p-2}(4p+2)(p-q)(y^4-1)^2+2(2q+1)y^{-2q-1}(y^4-1)^2+2y^{-2q-2}(2p-1)(2q+2)(y^4-1)^2 + (y^4-1)^2((4p+2q+2)y^{-1}+2py^{-1}-(p-q)y^{-1}+2(p-1)y^{-1}+(q-p+1)y^{-1}+2py^{-1})],$$

(if $p<q$).

$$b.\ PI(G,y) = \frac{y^{32p+16q+36pq-2}}{(y^4-1)^2}[y^{-4p+1}(4p-4py^4+y^{4p}-3y^4+3y^{4p+4})+4py^{-4p}+2y^{-4p-1} (4p-4py^4-y^{4p}-5y^4+5y^{4p+4}+1)-y^{-4p-2}(4p+2)(p-q)(y^4-1)^2+2(2q+1)y^{-2q-1}(y^4-1)^2 + 2y^{-2q-2}(2p-1)(2q+2)(y^4-1)^2+(y^4-1)^2((4p+2q+2)y^{-1}+2py^{-1}-(p-q)y^{-1} + 2(p-1)y^{-1}+(q-p+1)y^{-1}+2py^{-1})],$$

(if $p=q$).

Proof. Let G be a $BAG(p,q)$. After computing equation (12) by using definition of PI polynomial and applying $e=R=32p+16q+36pq-2$ in it then we obtain the PI polynomials.

$$\begin{aligned}PI(G,y) = {} & \sum_{i=1}^{p}(4i-1)y^{e-(4i-1)} + \sum_{i=p+1}^{p+1}(4p+1)y^{e-(4p+1)} + \sum_{i=p+2}^{q}(4p+2)y^{e-(4p+2)} \\ & + 2\sum_{i=1}^{p}(4i+1)y^{e-(4i+1)} + \sum_{i=p+1}^{q}(4p+2)y^{e-(4p+2)} + 2\sum_{i=1}^{1}(2q+1)y^{e-(2q+1)}\end{aligned}$$

$$+\sum_{i=2}^{2p}(2q+2)y^{e-(2q+2)}+\sum_{i=1}^{4p+2q+2}y^{e-1}+2\sum_{i=1}^{p}y^{e-1}+\sum_{i=p+1}^{q}y^{e-1}+2\sum_{i=1}^{p-1}y^{e-1}+\sum_{i=p}^{q}y^{e-1}$$
$$+\sum_{i=1}^{2p}y^{e-1}. \tag{12}$$

Further, an analytical computation obtain the result of Theorem 5.3(a)

b. For case $p=q$, instead of substituting $\sum_{i=p+1}^{p+1}(4p+1)y^{e-(4p+1)}+\sum_{p+2}^{q}(4p+2)y^{e-(4p+2)}$, we substitute $\sum_{i=p+1}^{p+1}4py^{e-4p}$ in equation (12) then further, an analytical computation obtain the result of theorem 5.3(b) □

Theorem 5.4. *Let G be a $BAG(p,q)$. Then the Sd-polynomial of $BAG(p,q)$ is generalized as follows;*

a. $Sd(G,y)=\frac{y^{32p+16q+36pq-2}}{y^4-1}[y^{-4p+1}(y^{4p}-1)+y^{-4p-1}(y^4-1)-y^{-4p-2}(p-q+1)(y^4-1)$
$+2y^{-4p-1}(y^{4p}-1)-y^{-4p-2}(p-q)(y^4-1)+y^{-2q-1}(y^4-1)+(y^{4p}-1)(y^{-2q-2}(2p-1)$
$+(4p+2q+2)y^{-1}+py^{-1}-(p-q)y^{-1}+(p-1)y^{-1}+(p-q+1)y^{-1}+2py^{-1})$, *(if $p<q$).*

b. $Sd(G,y)=\frac{y^{32p+16q+36pq-2}}{y^4-1}[y^{-4p+1}(y^{4p}-1)+y^{-4p}(y^{4p}-1)+2y^{-4p-1}(y^{4p}-1)-y^{-4p-2}(p-q)(y^4-1)$
$+y^{-2q-1}(y^4-1)+(y^{4p}-1)(y^{-2q-2}(2p-1)+(4p+2q+2)y^{-1}+py^{-1}-(p-q)y^{-1}+(p-1)y^{-1}$
$+(p-q+1)y^{-1}+2py^{-1})]$, *(if $p=q$).*

Proof. Let G be a $BAG(p,q)$. Apply $e=R=32p+16q+36pq-2$ in Equation (13) then we obtain the Sadhana polynomial.

$$Sd(G,y)=\sum_{i=1}^{p}y^{e-(4i-1)}+\sum_{i=p+1}^{p+1}y^{e-(4p+1)}+\sum_{i=p+2}^{q}y^{e-(4p+2)}+2\sum_{i=1}^{p}y^{e-(4i+1)}+\sum_{i=p+1}^{q}y^{e-(4p+2)}$$
$$+2\sum_{i=1}^{1}y^{e-(2q+1)}+\sum_{i=2}^{2p}y^{e-(2q+2)}+\sum_{i=1}^{4p+2q+2}y^{e-1}+2\sum_{i=1}^{p}y^{e-1}+\sum_{i=p+1}^{q}y^{e-1}+2\sum_{i=1}^{p-1}y^{e-1}$$
$$+\sum_{i=p}^{q}y^{e-1}+\sum_{i=1}^{2p}y^{e-1}. \tag{13}$$

Further, an analytical computation obtain the result of theorem 5.4(a)

b. For case $p=q$, instead of substituting $\sum_{i=p+1}^{p+1}y^{e-(4p+1)}+\sum_{p+2}^{q}y^{e-(4p+2)}$, we substitute $\sum_{i=p+1}^{p+1}y^{e-4p}$ in equation (13), then further, an analytical computation obtain the result of Theorem 5.4(b) □

Theorem 5.5. *Let G be a $BAG(p,q)$. Then Ω-polynomial of $BAG(p,q)$ is generalized as follows,*

$\Omega(G,y)=\frac{1}{y^4-1}[y^3(y^{4q}-1)+(y^{4q+2})(y^4-1)-y^{4q+4}(q-p+1)(y^4-1)+2y^5(y^{4q}-1)+(y^{4q+4}(p-q)$
$+2y^{2q+1}+y^{(2q+2)}(2p-1)+y(4p+2q+2)+2qy-y(q-p)+2y(q-1)+y(p-q+1)+2py)$

Proof. Let G be the $BAG(p,q)$. Now c_j denotes the number of edges in each qoc. Using the definition of Omega polynomial, we obtain the following equation.

$$\Omega(G,y) = \sum_{i=1}^{q} y^{4i-1} + \sum_{i=q+1} y^{4q+2} + \sum_{i=q+2}^{p} y^{4q+4} + 2\sum_{i=1}^{q} y^{4i+1} + \sum_{i=q+1}^{p} y^{4q+4} + \sum_{i=1}^{1} y^{2p+1} + \sum_{i=2}^{2p} y^{2p+2}$$
$$+ \sum_{i=1}^{4p+2q+2} y + 2\sum_{i=1}^{q} y + \sum_{i=q+1}^{p} y + 2\sum_{i=1}^{q-1} y + \sum_{i=q}^{p} y + \sum_{i=1}^{2p} y. \quad (14)$$

Further, an analytical computation obtain the result of Theorem 5.5. □

Theorem 5.6. *Let G be a $BAG(p,q)$. Then the Θ-polynomial of $BAG(p,q)$ is generalized as follows,*

$$\Theta(G,y) = \frac{1}{(y^4-1)^2}[-y^3(4qy^{4q} + 3y^{4q} - y^4 + y^{4q+4} - 4qy^{4q+4} - 3) + (4q+4)(y^{4q+2})(y^4-1)^2$$
$$-(4q+4)y^{4q+4}(q-p+1)(y^4-1)^2 - 2y^5(4qy^{4q} + 5y^{4q} + y^4 - y^{4q+4} - 4qy^{4q+4} - 5) + ((y^4-1)^2)$$
$$((4q+4)y^{4q+4}(p-q) + (2q+1)y^{2q+1} + (2p-1)(2q+2)y^{2q+2} + (4p+2q+2)y + 2qy - y(q-p)$$
$$+ 2y(q-1) + y(p-q+1) + 2py)]$$

Proof. Let G be a $BAG(p,q)$. Each summation is computed by MATLAB software. By using the definition of Theta polynomial, we obtain the following equation.

$$\Theta(G,y) = \sum_{i=1}^{q}(4i-1)y^{4i-1} + \sum_{i=q+1}(4q+2)y^{4q+2} + \sum_{i=q+2}^{p}(4q+4)y^{4q+4} + 2\sum_{i=1}^{q}(4i+1)y^{4i+1}$$
$$+ \sum_{i=q+1}^{p}(4q+4)y^{4q+4} + \sum_{i=1}^{1}(2p+1)y^{2p+1} + \sum_{i=2}^{2p}(2p+2)y^{2p+2} + \sum_{i=1}^{4p+2q+2} y + 2\sum_{i=1}^{q} y$$
$$+ \sum_{i=q+1}^{p} y + 2\sum_{i=1}^{q-1} y + \sum_{i=q}^{p} y + \sum_{i=1}^{2p} y \quad (15)$$

Further, an analytical computation obtain the result of Theorem 5.6. □

Theorem 5.7. *Let G be a $BAG(p,q)$. Then the PI-polynomial of $BAG(p,q)$ is generalized as follows,*

$$PI(G,y) = \frac{1}{(y^4-1)^2}[y^{e-4q+1}(4q - 4qy^4 + y^{4q} - 3y^4 + 3y^{4q+4} - 1) + (4q+2)(y^{e-4q-2})(y^4-1)^2$$
$$-(4q+4)y^{e-4q-4}(q-p+1)(y^4-1)^2 + 2y^{e-4q-1}(4q - 4qy^4 - y^{4q} - 5y^4 + 5y^{4q+4} + 1)$$
$$+(y^4-1)^2((4q+4)y^{e-4q-4}(p-q) + (2p+1)y^{e-2q-1} + (2p-1)(2q+2)y^{e-2q-2} +$$
$$+(4p+2q+2)y^{e-1} + 2qy^{e-1} - (q-p)y^{e-1} + 2y^{e-1}(q-1) + y^{e-1}(p-q+1) + 2py^{e-1})].$$

Proof. Let G be a $BAG(p,q)$. After computing equation (16) by using definition of PI polynomial and applying $e = R = 32p + 16q + 36pq - 2$ then we obtain the PI polynomials.

$$PI(G,y) = \sum_{i=1}^{q}(4i-1)y^{e-4i+1} + \sum_{i=q+1}(4q+2)y^{e-4q-2} + \sum_{i=q+2}^{p}(4q+4)y^{e-4q-4} + 2\sum_{i=1}^{q}(4i+1)y^{e-4i-1}$$
$$+ \sum_{i=q+1}^{p}(4q+4)y^{e-4q-4} + \sum_{i=1}^{1}(2q+1)y^{e-2q-1} + \sum_{i=2}^{2p}(2q+2)y^{e-2q-2} + \sum_{i=1}^{4p+2q+2} y^{e-1} + 2\sum_{i=1}^{q} y^{e-1}$$
$$+ \sum_{i=q+1}^{p} y^{e-1} + 2\sum_{i=1}^{q-1} y^{e-1} + \sum_{i=q}^{p} y^{e-1} + \sum_{i=1}^{2p} y^{e-1}. \quad (16)$$

Further, an analytical computation obtain the result of Theorem 5.7. □

Theorem 5.8. *Let G be a $BAG(p,q)$. Then the Sd-polynomial of $BAG(p,q)$ is generalized as follows,*

$$Sd(G,y) = \frac{1}{y^4-1}[y^{e-4q+1}(y^{4q}-1) + (y^4-1)y^{e-4q-2} - (y^4-1)y^{e-4q-4}(q-p+1) + 2y^{e-4q-1}(y^{4q}-1)$$
$$+ (y^4-1)(y^{e-4q-4}(p-q) + y^{e-2q-1} + y^{e-2q-2} + (4p+2q+2)y^{e-1} + 2qy^{e-1} - (q-p)y^{e-1}$$
$$+ 2y^{e-1}(q-1) + y^{e-1}(p-q+1) + 2py^{e-1})]$$

Proof. Let G be a $BAG(p,q)$. Apply $e = R = 32p + 16q + 36pq - 2$ in equation (17) then we obtain the Sadhana polynomial.

$$Sd(G,y) = \sum_{i=1}^{q} y^{e-4i+1} + \sum_{i=q+1} y^{e-4q-2} + \sum_{i=q+2}^{p} y^{e-4q-4} + 2\sum_{i=1}^{q} y^{e-4i-1} + \sum_{i=q+1}^{p} y^{e-4q-4} + \sum_{i=1}^{1} y^{e-2q-1}$$
$$+ \sum_{i=2}^{2p} y^{e-2q-2} + \sum_{i=1}^{4p+2q+2} y^{e-1} + 2\sum_{i=1}^{q} y^{e-1} + \sum_{i=q+1}^{p} y^{e-1} + 2\sum_{i=1}^{q-1} y^{e-1} + \sum_{i=q}^{p} y^{e-1} + \sum_{i=1}^{2p} y^{e-1} \quad (17)$$

Further, an analytical computation obtain the result of Theorem 5.8.

5.2 Subsequent indices

Theorem 5.9.

Let G be a $BAG(p,q)$. For three cases $p < q$, $p = q$ and $p > q$ of G, we can obtain the results of subsequent indices $\Theta(G)$, $PI(G)$ and $Sd(G)$ from Theorems$(5.1 - 5.8)$ by using equations $(4 - 9)$.

6 Conclusion

In this article, we have computed the exact results for edge-version of distance based descriptors for boric acid graphite structure. In material science, organic and inorganic fields, boric acid structure have a variety of applications like a wood fire retardant, as an antimicrobial. Analytical computation is done for the edge-version distance based descriptors of vertex weighted and strength weighted quotient graphs. There is a method behind this computation is to divide the original molecular structure into smaller vertex weighted and strength weighted quotient graphs. When the Sadhana and PI polynomials calculate the nonequidistant edges of the graph, the Omega and Theta polynomials count the equidistant edges of the graph. These polynomials allow scientists to talk about and predict molecule structure without the use of quantum mechanics. □

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