# Valency Based Topological Indices of Tri-Hexagonal Boron Nanotori

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**Abstract:** Topological indices receive a significance attention in the study of physicochemical properties of chemical compound. Among them, valency based topological indices have played a prominent role due to measure the chemical properties of nanostructure materials. Boron nanostructures acquire a number of interesting properties which are suitable for a diverse field of applications. In this paper, we study certain valency based topological indices of Tri-Hexagonal boron nanotorus and Tri-Hexagonal boron-$\alpha$(alpha) nanotorus.

**Keywords:** ABC index; GA index; Tri-Hexagonal boron nanotorus
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## 1. Introduction

Mathematical chemistry is a branch of theoretical chemistry in which we get information about the molecular structure by using mathematical techniques without assigning that structure to quantum mechanics [5, 27]. Chemical graph theory is such a branch of mathematical chemistry which implements graph theory to study mathematical modeling of chemical aspects [28]. This theory shows a prominent effect on the extension of the chemical sciences [15].

A molecular graph can be used to model the structure of molecules and molecular compounds by considering atoms as vertices and the chemical bonds between atoms as edges. By considering $V_G$ as vertex set and $E_G$ as edge set, let $G(V_G, E_G)$ or simply $G$ be a connected molecular graph. Consider the set $I_v$ having the edges of $G$ that are incident to a vertex $v \in V_G$ . Then the valency/degree of $v$ is represented by $d_v$ and is defined as $d_v = |I_v|$.

Molecular descriptors perform a prominent role in mathematical chemistry specifically in the QSAR/QSPR studies [8]. In QSAR/QSPR studies, topological indices are used to correlate the chemical structure of a molecular graph with its biological activities and chemical properties [9]. A topological descriptor or index (*TI*) is a numerical graph invariant which is built on several topological aspects of the corresponding molecular graph. There are two main categories of topological indices, one is distance based and the other is valency based topological indices. The first valency based topological index is the Randic connectivity index $\chi(G)$ which was presented by Milan Randic [25] and is defined as

$$\chi(G) = \sum_{uv \in E_G} \frac{1}{\sqrt{d_u . d_v}}$$

This index has been shown to reflect molecular branching and deeply examined by chemists and mathematicians [18]. Many physicochemical properties depend on such factors which are different rather than branching. With this motivation, Estrada et al. [10] presented the atom-bond connectivity index, defined as

$$ABC(G) = \sum_{uv \in E_G} \sqrt{\frac{d_u + d_v - 2}{d_u . d_v}}$$

It is reported in [10, 11, 16] that this index can be applied in modeling thermodynamic features of organic chemical compounds. In addition, Estrada [11] interpreted a new quantum theory which is presented that this index implements a model for consideration 1,2-, 1,3-, and 1,4-interactions in the carbon-atom skeleton of saturated hydrocarbons, and in this sense, it can be applied for rationalizing steric effects in such compounds.

Recently, Ghorbani et al. [13] presented the fourth atom-bond connectivity index $(ABC_4)$ which is defined as follows

$$ABC_4(G) = \sum_{uv \in E_G} \sqrt{\frac{\delta_u + \delta_v - 2}{\delta_u . \delta_v}}$$

where $\delta_u = \sum_{uv \in E_G} d_v$ and $\delta_v = \sum_{uv \in E_G} d_u$.

The sense for presenting a new index is to increase prediction of some property of molecules. One of the successor of Randic connectivity index, called geometric-arithmetic (*GA*) connectivity index which is presented by Vukicevic et al. [13] and is defined as

$$GA(G) = \sum_{uv \in E_G} \frac{2\sqrt{d_u . d_v}}{d_u + d_v}$$

It is recorded in [6, 29] that this index provides better prediction rate than the Randic index in various physicochemical properties such as entropy, enthalpy of formation, and standard enthalpy of vaporization. Furthermore, the enhancement in prediction accuracy rate of *GA* index comparing to Randic index is more than 9% for the standard enthalpy of vaporization. In this sense, *GA* index can be applied in the QSAR/QSPR studies. In [7], it also presents that there forms excellent correlation between heat of formation of benzenoid hydrocarbons and *GA* index (correlation coefficient is 0.972). The fifth *GA* index is presented by Graovac et al. [14] and is defined as

$$GA_5(G) = \sum_{uv \in E_G} \frac{2\sqrt{\delta_u . \delta_v}}{\delta_u + \delta_v}$$

Boron nanostructures have been considered as excellent nanomaterials for enhancing the characteristics of optoelectronic nano devices because of their broad elastic modulus, high melting-point, excessive conductivity, great emission uniformity and low turn-on field. Furthermore, these nanomaterials can carry excessive emission current, which recommends that they may have great prospective applications in field emission area [24]. Boron nanostructures materials also have some better properties compared to carbon nanostructure materials such as excessive resistance to oxidation at high temperatures, great chemical stability and are stable broad band-gap semiconductor. Due to these properties, boron nanomaterials may have great applications at high temperatures or in corrosive environments functioning as super capacitors, solid lubricants, fuel cells and batteries [4]. The stability, mechanical and electronic properties of boron nanostructure materials has been discussed in [23, 24].

The 3D nanostructure materials hold a remarkable morphology compared to 1D or 2D which are thought to produce a vast surface area and to promote the operation of reactants and products comprehensively, so that electrochemical capability can be tremendously enhanced [26].

Recently, *ABC*, $ABC_4$, *GA* and $GA_5$ indices are studied of an infinite class of tri-hexagonal boron nanotubes [22]. In this paper, we study these indices of certain tri-hexagonal boron nanotori. For further study of topological indices for certain molecular graphs, we refer the reader to consult the literature [1-3,12,17, 21, 30, 31].

**2. Tri-Hexagonal Boron Nanotorus**

Recently, Y. Liu et al. [30] predicted a new class of boron nanotube which is covered by hexagons and triangles. We call this nanotube as Tri-Hexagonal boron nanotube. A 3D perception of Tri-Hexagonal boron nanotube is shown in the Figure 1.

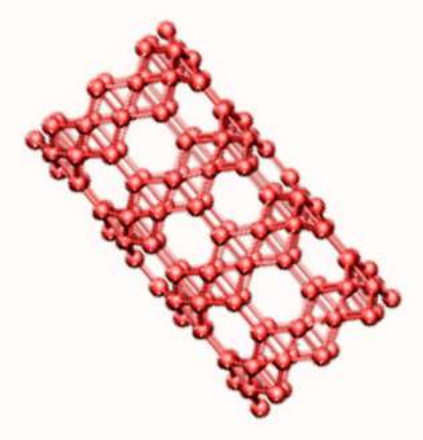

**Fig. 1**. Three-dimensional perception of Tri-Hexagonal boron nanotube.

We denote the corresponding Tri-hexagonal boron nanotorus by $G = THBC_3C_6[p,q]$, where $p$ denotes the number of hexagons in a row and $q$ denotes the number of hexagons in a column of the 2D graph of $G = THBC_3C_6[p,q]$ nanotorus. It is easy to see that $|V_G| = 8pq$ and $|E_G| = 18pq$. The molecular graph of $G = THBC_3C_6[p,q]$ nanotorus is shown in the Figure 2.

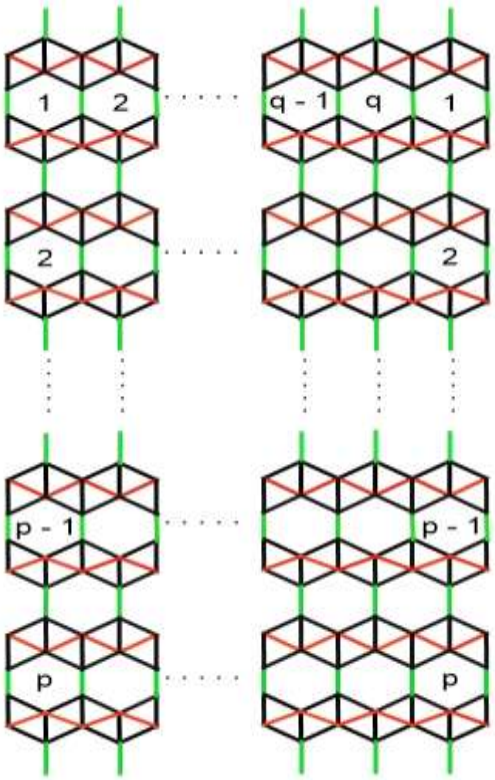


**Fig. 2**. A two-dimensional molecular graph of $G = THBC_3C_6[p,q]$ nanotorus.

In the following theorem, we present the *ABC* and $ABC_4$ indices of $THBC_3C_6[p,q]$ nanotorus.

**Theorem 2.1** Consider the Tri-Hexagonal boron nanotorus $THBC_3C_6[p, q]$ , then

$$ABC\left(THBC_3C_6[p,q]\right)=\left(\frac{\sqrt{6}}{2}+\frac{6\sqrt{7}}{\sqrt{5}}+\frac{8\sqrt{2}}{5}\right)pq$$

and

$$ABC_4\left(THBC_3C_6[p,q]\right)=\left(\frac{12}{19}+\frac{12\sqrt{39}}{\sqrt{418}}+\frac{2\sqrt{42}}{11}\right)pq$$

**Proof.** Consider the Tri-Hexagonal boron nanotube $G=THBC_3C_6[p,q]$ . There are three partite subsets of edge set correspond to their valency of end vertices which are presented as

$$E_{(4,4)}=\{uv\in E_G \mid d_u=d_v=4\}$$

$$E_{(4,5)}=\{uv\in E_G \mid d_u=4 \text{ and } d_v=5\}$$

$$E_{(5,5)}=\{uv\in E_G \mid d_u=d_v=5\}$$

The representatives of edges of these partite sets $E_{(4,4)}$ , $E_{(4,5)}$ and $E_{(5,5)}$ are assigned the colors green, black and red respectively as presented in Figure 2. The Table 1 presents the cardinality of each partite set of edges of *G* correspond to their valency of end vertices.

**Table 1.** The cardinalities of partite subsets of $E_G$ correspond to their valency of end vertices.

| $E_{(u,v)}$ | $\lvert E_{(u,v)}\rvert$ | Color |
|---|---|---|
| $E_{(4,4)}$ | $2pq$ | Green |
| $E_{(4,5)}$ | $12pq$ | Black |
| $E_{(5,5)}$ | $4pq$ | Red |

By using Table 1, the *ABC* index of *G* is computed as

$$ABC(G)=\sum_{uv\in E_G}\sqrt{\frac{d_u+d_v-2}{d_u.d_v}}$$

$$=\sum_{uv\in E_{(4,4)}}\sqrt{\frac{d_u+d_v-2}{d_u.d_v}}+\sum_{uv\in E_{(4,5)}}\sqrt{\frac{d_u+d_v-2}{d_u.d_v}}$$

$$+\sum_{uv\in E_{(5,5)}}\sqrt{\frac{d_u+d_v-2}{d_u.d_v}}$$

A

$$=\left|E_{(4,4)}\right|\sqrt{\frac{4+4-2}{4\times4}}+\left|E_{(4,5)}\right|\sqrt{\frac{4+5-2}{4\times5}}+$$

$$\left|E_{(5,5)}\right|\sqrt{\frac{5+5-2}{5\times5}}$$

$$=2pq\sqrt{\frac{4+4-2}{4\times4}}+12pq\sqrt{\frac{4+5-2}{4\times5}}+4pq\sqrt{\frac{5+5-2}{5\times5}}$$

fter simplification, we get

$$ABC(G)=\left(\frac{\sqrt{6}}{2}+\frac{6\sqrt{7}}{\sqrt{5}}+\frac{8\sqrt{2}}{5}\right)pq$$

The fourth *ABC* index of *G* is computed as follows.

There are also three partite subsets of the edge set of *G* correspond to their valency sum of neighbors of end vertices, given as

$$\delta_{(19,19)}=\{uv\in E_G \mid \delta_u=\delta_v=19\}$$

$$\delta_{(19,22)}=\{uv\in E_G \mid \delta_u=19 \text{ and } \delta_v=22\}$$

$$\delta_{(22,22)}=\{uv\in E_G \mid \delta_u=\delta_v=22\}$$

The representatives of partite sets $\delta_{(19,19)}$ , $\delta_{(19,22)}$ and $\delta_{(22,22)}$ corresponds to the colors green, black and red edges respectively as shown in Figure 2. The Table 2 presents the cardinality of each edge set of *G* corresponds to their valency sum of neighbors of end vertices.

**Table 2.** The cardinalities of partite subsets $E_G$ with respect to valency sum of neighbors of end vertices.

| $\delta_{(u,v)}$ | $\lvert\delta_{(u,v)}\rvert$ | Color |
|---|---|---|
| $\delta_{(19,19)}$ | $2pq$ | Green |
| $\delta_{(19,22)}$ | $12pq$ | Black |
| $\delta_{(22,22)}$ | $4pq$ | Red |

By using Table 2, the fourth *ABC* index of *G* is computed as

$$ABC_4(G)=\sum_{uv\in E_G}\sqrt{\frac{\delta_u+\delta_v-2}{\delta_u.\,\delta_v}}$$

$$=\left|\delta_{(19,19)}\right|.\sqrt{\frac{\delta_u+\delta_v-2}{\delta_u.\,\delta_v}}+\left|\delta_{(19,22)}\right|\sqrt{\frac{\delta_u+\delta_v-2}{\delta_u.\,\delta_v}}$$

$$+\left|\delta_{(22,22)}\right|.\sqrt{\frac{\delta_u+\delta_v-2}{\delta_u.\,\delta_v}}$$

$$=(2pq)\sqrt{\frac{19+19-2}{19\times 19}}+(12pq)\sqrt{\frac{19+22-2}{19\times 22}}$$

$$+(4pq)\sqrt{\frac{22+22-2}{22\times 22}}$$

After simplification, we get

$$ABC_4(G)=\left(\frac{12}{19}+\frac{12\sqrt{39}}{\sqrt{418}}+\frac{2\sqrt{42}}{11}\right)pq$$

The geometric-arithmetic (*GA*) index and the fifth *GA* index of $THBC_3C_6[p,q]$ nanotorus are computed in the following theorem.

**Theorem 2.2** Consider the Tri-Hexagonal boron nanotorus $THBC_3C_6\,[p,\,q]$ , then

$$GA\left(THBC_3C_6[p,q]\right)=\left(6+\frac{16\sqrt{5}}{3}\right)pq$$

and

$$GA_5\left(THBC_3C_6[p,q]\right)=\left(6+\frac{24\sqrt{418}}{41}\right)pq$$

**Proof.** Consider the Tri-Hexagonal boron nanotorus $G=THBC_3C_6[p,q]$. From Table 1, we have the cardinality of each partite subset of $E_G$ correspond to their valency of end vertices.

The *GA* index of *G* is computed as

$$GA(G)=\sum_{uv\in E_G}\frac{2\sqrt{d_u.\,d_v}}{d_u+d_v}$$

$$=\sum_{uv\in E_{(4,4)}}\frac{2\sqrt{d_u.\,d_v}}{d_u+d_v}+\sum_{uv\in E_{(4,5)}}\frac{2\sqrt{d_u.\,d_v}}{d_u+d_v}+\sum_{uv\in E_{(5,5)}}\frac{2\sqrt{d_u.\,d_v}}{d_u+d_v}$$

$$=\left|E_{(4,4)}\right|.\frac{2\sqrt{d_u.\,d_v}}{d_u+d_v}+\left|E_{(4,5)}\right|.\frac{2\sqrt{d_u.\,d_v}}{d_u+d_v}+\left|E_{(5,5)}\right|.\frac{2\sqrt{d_u.\,d_v}}{d_u+d_v}$$

$$=(2pq)\frac{2\sqrt{4\times 4}}{4+4}+(12pq)\frac{2\sqrt{4\times 5}}{4+5}+(4pq)\frac{2\sqrt{5\times 5}}{5+5}$$

After simplification, we get

$$GA(G)=\left(6+\frac{16\sqrt{5}}{3}\right)pq$$

Now we compute fifth *GA* index of *G*. From Table 2, we have the cardinality of each partite subset of $E_G$ correspond to their valency sum of neighbors of end vertices.

The fifth *GA* index is computed as

$$GA_5(G)=\sum_{uv\in E_G}\frac{2\sqrt{\delta_u.\,\delta_v}}{\delta_u+\delta_v}$$

$$=\left|\delta_{(19,19)}\right|.\frac{2\sqrt{\delta_u.\,\delta_v}}{\delta_u+\delta_v}+\left|\delta_{(19,22)}\right|.\frac{2\sqrt{\delta_u.\,\delta_v}}{\delta_u+\delta_v}$$

$$+\left|\delta_{(22,22)}\right|.\frac{2\sqrt{\delta_u.\,\delta_v}}{\delta_u+\delta_v}$$

$$=(2pq)\frac{2\sqrt{19\times 19}}{19+19}+(12pq)\frac{2\sqrt{19\times 22}}{19+22}$$

$$+(4pq)\frac{2\sqrt{22\times 22}}{22+22}$$

After simplification, we get

$$GA_5(G)=\left(6+\frac{24\sqrt{418}}{41}\right)pq$$

## 3. Tri-Hexagonal Boron-$\alpha$ Nanotorus

The boron-$\alpha$ sheet is acquired from carbon hexagonal sheet by inserting a new vertex to the center of certain hexagons of the hexagonal sheet [20, 31]. This boron-$\alpha$ sheet is designed by creating a combination of hexagons and triangles, called the Tri-Hexagonal boron-$\alpha$ sheet. A Tri-Hexagonal boron-$\alpha$ nanotorus is obtained from a Tri-Hexagonal boron-$\alpha$ sheet. We denote the molecular graph of boron-$\alpha$ nanotorus by $K=THBAC_3C_6[p,q]$ where $p=6m$ denotes the number of rows and $q=2n$ denotes the number of

columns in the 2D lattice of $K = THBAC_3C_6[p,q]$ nanotorus as presented in Figure 3. It is easy to check that $|V_K| = 4pq/3$ and $|E_K| = 7pq/2$.

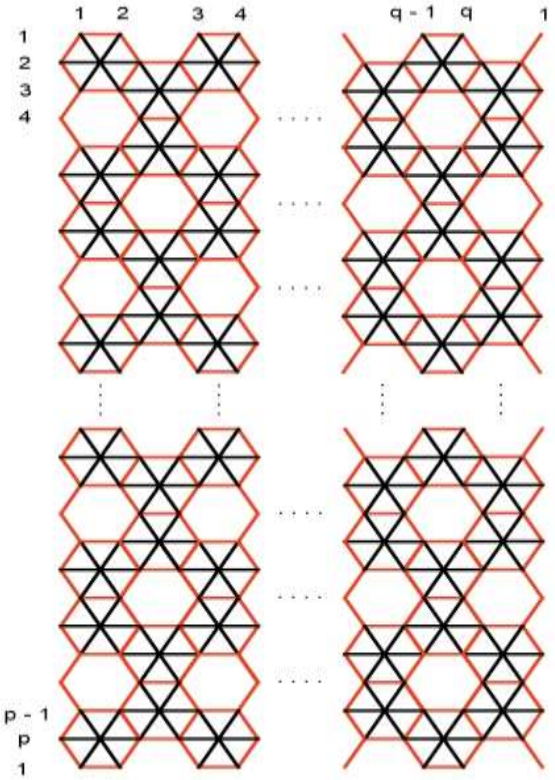


**Fig. 3**. A two-dimensional molecular graph of $K = THBAC_3C_6[p,q]$ nanotorus.

In the coming theorem, we compute *ABC* and the fourth *ABC* indices of *THBA* $C_3C_6[p,q]$ nanotorus.

**Theorem 3.1** Consider the Tri-Hexagonal boron-$\alpha$ nanotorus $THBAC_3C_6[p,q]$ , then

$$ABC\left(THBAC_3C_6[p,q]\right) = \left(\frac{3\sqrt{2}+\sqrt{30}}{5}\right)pq$$

and

$$ABC_4\left(THBAC_3C_6[p,q]\right) = \left(\frac{\sqrt{13}+\sqrt{22}}{9}\right)pq$$

**Proof.** Consider the Tri-Hexagonal boron nanotorus $K = THBAC_3C_6[p,q]$ . There are two disjoint partite subsets of $E_K$ correspond to their valency of end vertices, given by

$$E_{(5,5)} = \{uv \in E_G \mid d_u = d_v = 5\}$$

$$E_{(5,6)} = \{uv \in E_G \mid d_u = 5 \text{ and } d_v = 6\}$$

The representatives of these partite subsets $E_{(5,5)}$, $E_{(5,6)}$ correspond to the colors red and black edges respectively as presented in Figure 3. Table 3 presents the cardinality of each partite subset of $E_K$ corresponds to their valency of end vertices.

**Table 3.** The cardinalities of partite subsets of $E_K$ correspond to their valency of end vertices.

| $E_{(u,v)}$ | $\lvert E_{(u,v)}\rvert$ | Color |
|---|---|---|
| $E_{(5,5)}$ | $3pq/2$ | Red |
| $E_{(5,6)}$ | $2pq$ | Black |

The *ABC* index of *K* is computed as follows

$$ABC(K) = \sum_{uv\in E_G}\sqrt{\frac{d_u+d_v-2}{d_u.d_v}}$$

$$= \sum_{uv\in E_{(5,5)}}\sqrt{\frac{d_u+d_v-2}{d_u.d_v}} + \sum_{uv\in E_{(5,6)}}\sqrt{\frac{d_u+d_v-2}{d_u.d_v}}$$

$$= \left|E_{(5,5)}\right|.\sqrt{\frac{5+5-2}{5\times 5}} + \left|E_{(5,6)}\right|.\sqrt{\frac{5+6-2}{5\times 6}}$$

$$= \frac{3pq}{2}\sqrt{\frac{5+5-2}{5\times 5}} + (2pq)\sqrt{\frac{5+6-2}{5\times 6}}$$

After simplification, we get

$$ABC(K) = \left(\frac{3\sqrt{2}+\sqrt{30}}{5}\right)pq$$

Now we compute the fourth version of *ABC* index of *K*. There are also two disjoint partite subsets of $E_K$ correspond to their valency sum of neighbors of end vertices, given as

$$\delta_{(27,27)} = \{uv \in E_K \mid d_u = d_v = 27\}$$

$$\delta_{(27,30)} = \{uv \in E_K \mid d_u = 27 \text{ and } d_v = 30\}$$

The representatives of these partite subsets $\delta_{(27,27)}$ and $\delta_{(27,30)}$ correspond to the colors red and black respectively as presented in Figure 3. Table 4 presents the cardinality of each partite correspond to their valency sum of neighbors of end vertices.

**Table 4.** The cardinalities of partite sets with respect to valency sum of neighbors of end vertices.

| $\delta_{(u,v)}$ | $\lvert\delta_{(u,v)}\rvert$ | Color |
|---|---|---|
| $\delta_{(27,27)}$ | $3pq/2$ | Red |

| | | |
|---|---|---|
| $\delta_{(27,30)}$ | 2pq | Black |

The fourth *ABC* index of *K* is computed as

$$ABC_4(K)=\sum_{uv\in E_K}\sqrt{\frac{\delta_u+\delta_v-2}{\delta_u.\,\delta_v}}$$

$$=\left|\delta_{(27,27)}\right|.\sqrt{\frac{27+27-2}{27\times 27}}+\left|\delta_{(27,30)}\right|.\sqrt{\frac{27+30-2}{27\times 30}}$$

$$=\frac{3pq}{2}\sqrt{\frac{27+27-2}{27\times 27}}+2pq\sqrt{\frac{27+30-2}{27\times 30}}$$

After simplification, we get

$$ABC_4(K)=\left(\frac{\sqrt{13}+\sqrt{22}}{9}\right)pq$$

The *GA* index and fifth *GA* index of $THBAC_3C_6[p,q]$ nanotorus is computed in the coming theorem.

**Theorem 3.2** Consider the Tri-Hexagonal boron-$\alpha$ nanotorus $THBAC_3C_6[p,q]$, then

$$GA(THBAC_3C_6[p,q])=\left(\frac{4\sqrt{30}}{11}+\frac{3}{2}\right)pq \text{ and}$$

$$GA_5(THBAC_3C_6[p,q])=\left(\frac{36\sqrt{10}}{57}+\frac{3}{2}\right)pq$$

**Proof.** Consider the Tri-Hexagonal boron nanotorus $K=THBAC_3C_6[p,q]$. From Table 3, we have the cardinality of disjoint partite subsets of $E_K$ correspond to their valency of end vertices. The *GA* index of *K* is computed as

$$GA(K)=\sum_{uv\in E_K}\frac{2\sqrt{d_u.\,d_v}}{d_u.\,d_v}$$

$$=\left|E_{(5,5)}\right|.\frac{2\sqrt{5\times 5}}{5+5}+\left|E_{(5,6)}\right|.\frac{2\sqrt{5\times 6}}{5+6}$$

$$=\frac{3pq}{2}.\frac{2\sqrt{5\times 5}}{5+5}+2pq.\frac{2\sqrt{5\times 6}}{5+6}$$

After simplification, we get

$$GA(K)=\left(\frac{4\sqrt{30}}{11}+\frac{3}{2}\right)pq$$

Now we compute the fifth *GA* index of *K*. From Table 4, we have the cardinality of each disjoint partite subset of $E_K$ correspond to their valency sum of neighbors of end vertices. The fifth *GA* index of *K* is computed as follows

$$GA_5(K)=\sum_{uv\in E_K}\frac{2\sqrt{\delta_u.\,\delta_v}}{\delta_u+\delta_v}$$

$$=\left|\delta_{(27,27)}\right|.\frac{2\sqrt{27.\,27}}{27+27}+\left|\delta_{(27,30)}\right|.\frac{2\sqrt{27.\,30}}{27+30}$$

$$=\frac{3pq}{2}.\frac{2\sqrt{27.\,27}}{27+27}+2pq.\frac{2\sqrt{27.\,30}}{27+30}$$

After simplification, we get

$$GA_5(K)=\left(\frac{36\sqrt{10}}{57}+\frac{3}{2}\right)pq$$

## 4. Conclusions

The connectivity indices called *ABC*, $ABC_4$, *GA* and $GA_5$ are very useful tools in the characterization of topological properties of nanostructures. In this article, we study these indices for some 3D boron nanostructures. By using this study, we can find mathematical models of certain physicochemical properties for these nanostructures.

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