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# On Reverse Degree based Topological Descriptors of Boron Nanotubes

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**Abstract:** Chemical indices are very helpful to design the properties of biological, medical, chemical and pharmacological of chemical compounds. Boron triangular nanotubes are attained by replacing usual carbon nanotubes due to their excellent properties. These nanotubes are great interest materials due to the existence of multicenter bonds and have novel electronic properties. Also, these materials have some dominant issues in Nano device approaches like mechanical and thermal stability. Reverse valency based chemical indices play an important role for the calculation of molecular descriptor. Here, we find an explicit expression of the reverse degree based chemical indices of the boron triangular nanotube. A graphical comparison between the computed various types of the reverse valency based chemical indices is also shown.

**Keywords** Reverse degree, Reverse topological indices, Nanomaterials, Boron triangular nanotubes.

## 1. Introduction

Let $\Lambda((V(\Lambda), X(\Lambda))$ be an ordered pair of graphs, where $V(\Lambda)$ is a non-empty vertex set and $X(\Lambda)$ is an edge set. A molecular graph is a set of points denoting the atoms in the molecule and collection of lines denoting the covalent bonds. The topological descriptors are helpful in the forecast of physical, chemical properties and the bio activity of chemical compounds [2], [3]. Topological indices are obtained from the molecular structure. They are playing a very important role in the field of chemistry.

Topological indices are important tools for investigating many physio-chemical properties of molecules without performing any testing. They are also used to study Quantitative Structure Activity Relationship (QSAR) of pharmaceuticals to determine their molecular characteristics by numerical computation [19]. Various types of topological indices of graphs are classified into distance-based topological indices, degree-based topological indices and spectrum-based topological indices. Among these, degree-based topological indices play a vital role in

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theoretical chemistry and pharmacology. Some important degree-based indices are Randic index, Zagreb indices, Harmonic index and sum connectivity index etc. For example, Randic index is one of the excellent molecular descriptors in QSAR studies and desirable for measuring the extent of branching of the carbon-atom skeleton of saturated hydrocarbons [17]. Zagreb type indices relieved to differentiate some alkane isomers boiling points and have aided in the invention, along with other indices, of a few thousand topological graph indices accepted in the chemical data bases [18]. There is a number of researches on the Zagreb indices and their chemical applications [16].

In chemical graph theory, a topological index predicts the biological activity of the molecular graph of chemical compounds. [4] At first, Wiener gave the idea of topological indices during his work on boiling point of paraffin and mentioned it as Wiener index, a initial topological index. In literature, the most widely used topological indices are Zagreb and Randic [5, 6].

The degree of vertex $x$ in a graph is the total number of edges incident with vertex $x$, it is denoted by $\varphi(x)$. A graph can be explained by numerical value, matrix and by polynomial. The concept of reverse vertex degree $\bar{\Re}(x)=\Delta(\Lambda)-\varphi(x)+1$ was given by Kulli [7]. In a graph, the maximum vertex degree is denoted by $\Delta(\Lambda)$. Degree, distance, eccentric and spectrum based indices are special varieties of topological indices. The computation of topological indices has brought up a wide diversity of dormant uses for the evaluation of QSAR antiparasitic products. The reverse degree based topological indices of Remdesivir applied in the prevention of corona virus are discussed in [1].

Recently, the reverse degree based indices of polycyclic metal organic network was discussed by zhao et al [27]. In 2019, Jung et. al studied the reverse degree based indices of some nanotubes [28]. Some reversed degree-based topological indices for graphene is well presented in [29]. Nazeer et.al explained the new reversed topological invariants of nanotubes [30]. Reversed degree-based topological indices for Benzenoid systems are extensively studied in [26]. Recently, Rosary and J. B. Liu presented the reverse degree based topological analysis on the line graph and para line graph of Remdesivir used for the treatment of corona virus [25,24]. In this article, we discuss the reverse degree based topological indices of the boron triangular nanotube and compare the results graphically.

Milan Randic introduced the first degree-based index [6]. Wei et al. defined the reverse Randic index as [1]:

$$\bar{\Re}\Re_{\alpha}(\Lambda)=\sum_{xy\in X(\Lambda)}[\bar{\Re}\varphi(x)\times\bar{\Re}\varphi(y)]^{\alpha};\alpha=1,-1,\frac{1}{2},-\frac{1}{2}$$

Estrada et al. presented the atom bond connectivity index [11]. Wei et al. defined the reverse atom bond connectivity index as [1]:

$$\bar{\Re}ABC(\Lambda)=\sum_{xy\in X(\Lambda)}\sqrt{\frac{\bar{\Re}\varphi(x)+\bar{\Re}\varphi(y)-2}{\bar{\Re}\varphi(x)\times\bar{\Re}\varphi(y)}}$$

Vukicevic et al. proposed the geometric arithmetic index [12]. Wei et al. defined the reverse geometric arithmetic index as [1]:

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$$\bar{\Re}GA(\Lambda)=\sum_{xy\in X(\Lambda)}\frac{2\sqrt{\bar{\Re}\varphi(x)\times\bar{\Re}\varphi(y)}}{\bar{\Re}\varphi(x)+\bar{\Re}\varphi(y)}$$

In 1972, Gutman discussed the first and second Zagreb indices [5], [13]. Wei et al. defined the reverse first and reverse second Zagreb indices as [1]:

$$\bar{\Re}M_1(\Lambda)=\sum_{xy\in X(\Lambda)}(\bar{\Re}\varphi(x)+\bar{\Re}\varphi(y))$$

$$\bar{\Re}M_2(\Lambda)=\sum_{xy\in X(\Lambda)}(\bar{\Re}\varphi(x)\times\bar{\Re}\varphi(y))$$

In 2008, Doslic and Gutman et al [14, 15] presented the first and second Zagreb co-indices. Wei et al. defined the reverse first and reverse second Zagreb co-indices as [1]:

$$\bar{\Re}\bar{M}_1(\Lambda)=2|X(\Lambda)|(|V(\Lambda)|-1)-\bar{\Re}M_1(\Lambda)$$

$$\bar{\Re}\bar{M}_2(\Lambda)=2|X(\Lambda)|^2-\frac{1}{2}\bar{\Re}M_1(\Lambda)-\bar{\Re}M_2(\Lambda)$$

In 2013, Shirdel et al [8] discussed hyper Zagreb index. Wei et al. defined the reverse hyper Zagreb index as [1]:

$$\bar{\Re}HM(\Lambda)=\sum_{xy\in X(\Lambda)}[\bar{\Re}\varphi(x)+\bar{\Re}\varphi(y)]^2$$

Wei et al. defined the reverse first multiple and the reverse second multiple Zagreb indices as [1]:

$$\bar{\Re}PM_1(\Lambda)=\prod_{xy\in X(\Lambda)}[\bar{\Re}\varphi(x)+\bar{\Re}\varphi(y)]$$

$$\bar{\Re}PM_2(\Lambda)=\prod_{xy\in X(\Lambda)}[\bar{\Re}\varphi(x)\times\bar{\Re}\varphi(y)]$$

Furtula and Gutman [9] introduced Forgotten index. Wei et al. defined the reverse forgotten index as [1]:

$$\bar{\Re}F(\Lambda)=\sum_{xy\in X(\Lambda)}[\bar{\Re}\varphi(x)^2+\bar{\Re}\varphi(y)^2]$$

Rajini et al [10] explained redefined first, second and third Zagreb indices for a graph. Wei et al. defined the reverse redefined first, second and third Zagreb indices as [1]:

$$\bar{\Re}\Re eZG_1(\Lambda)=\sum_{xy\in X(\Lambda)}\frac{\bar{\Re}\varphi(x)+\bar{\Re}\varphi(y)}{\bar{\Re}\varphi(x)\times\bar{\Re}\varphi(y)}$$

$$\bar{\Re}\Re eZG_2(\Lambda)=\sum_{xy\in X(\Lambda)}\frac{\bar{\Re}\varphi(x)\times\bar{\Re}\varphi(y)}{\bar{\Re}\varphi(x)+\bar{\Re}\varphi(y)}$$

$$\bar{\Re}\Re eZG_3(\Lambda)=\sum_{xy\in X(\Lambda)}(\bar{\Re}\varphi(x)\times\bar{\Re}\varphi(y))(\bar{\Re}\varphi(x)+\bar{\Re}\varphi(y))$$

Furtula et al [19] presented augmented Zagreb index. Wei et al. defined the reverse augmented Zagreb index as [1]:

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$$\bar{\Re}AZI(\Lambda)=\sum_{xy\in X(\Lambda)}\left(\frac{\bar{\Re}\varphi(x)\times\bar{\Re}\varphi(y)}{\bar{\Re}\varphi(x)\times\bar{\Re}\varphi(y)-2}\right)^{3}$$

## 2. Boron Triangular Nanotube

The recent finding of pure boron triangular nanotubes disputes the monopoly of carbon. In 2004, the initial boron triangular nanotubes were created and are obtained from a triangular sheet [21-23]. A boron triangular sheet is formed from a hexagonal sheet by adding an extra atom to the centre of each hexagon. Researchers conclude that boron triangular nanotubes are better than carbon hexagonal nanotubes [23,20].

We consider the Boron triangular nanotubes $\Lambda = BNTt[x,y]$ of order $x\times y$, where $x$ are rows and $y$ are columns. It is noted that boron nanotubes have only an odd number of rows and an even number of columns. There are $\frac{3xy}{2}$ vertices and $\frac{3x(3y-2)}{2}$ edges in Boron triangular nanotubes. The 2-dimensional structure of the Boron triangular nanotubes is depicted in Fig 1.

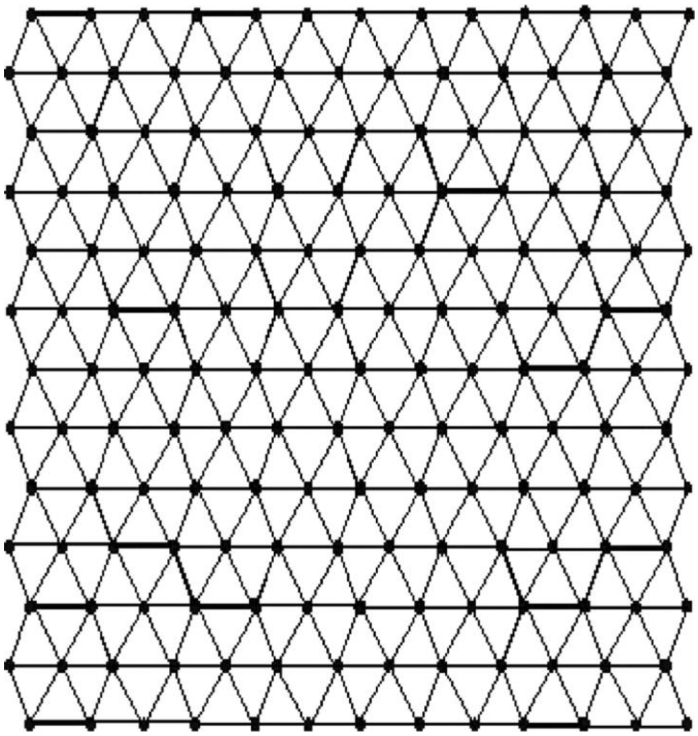

Fig 1: Boron triangular nanotube of the order 13 × 8.

| $(\varphi(x),\varphi(y))$ | Number of edges |
|---|---|
| $(4,4)$ | $3x$ |
| $(4,6)$ | $6x$ |
| $(6,6)$ | $\frac{9xy-24x}{2}$ |

Table 1. Edge partition of Boron triangular nanotube

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| $(\bar{\Re}\varphi(x),\bar{\Re}\varphi(y))$ | Number of edges |
|---|---|
| (3,3) | $3x$ |
| (3,1) | $6x$ |
| (1,1) | $\frac{9xy-24x}{2}$ |

Table 2. Reverse based edge partition of Boron triangular nanotube

The set of edges of Boron triangular nanotube is divided into three partition based on the degree of end vertices. The first edge partition includes of $3x$ edges $xy$, where $\varphi(x)=4$ and $\varphi(y)=4$. The second edge partition includes of $6x$ edges $xy$, where $\varphi(x)=4$ and $\varphi(y)=6$. The third edge partition includes of $\frac{9xy-24x}{2}$ edges $xy$, where $\varphi(x)=6$ and $\varphi(y)=6$.

Table 1 shows the edge partition of Boron triangular nanotube.

The maximum degree of the vertex of Boron triangular nanotube is 6. By using the definition of reverse vertex degree $\bar{\Re}(x)=\Delta(\Lambda)-\varphi(x)+1$, the reverse degree based edge partition of Boron triangular nanotube is given in Table 2.

Now we calculate the reverse degree based topological indices as:

- **Reverse General Randic index**

$$\bar{\Re}\Re_{\alpha}(\Lambda)=\sum_{xy\in X(\Lambda)}[\bar{\Re}\varphi(x)\times\bar{\Re}\varphi(y)]^{\alpha};\alpha=1,-1,\frac{1}{2},-\frac{1}{2}$$

For $\alpha=1$;

$$\bar{\Re}\Re_{1}(\Lambda)=\sum_{xy\in X(\Lambda)}[\bar{\Re}\varphi(x)\times\bar{\Re}\varphi(y)]^{1};$$

$$=(3x)(3\times3)+(6x)(3\times1)+\left(\frac{9xy-24x}{2}\right)(1\times1)$$

$$=27x+18x+\left(\frac{9xy-24x}{2}\right)$$

$$=45x+\left(\frac{9xy-24x}{2}\right)$$

$$=33x+\frac{9xy}{2}$$

For $\alpha=-1$,

$$\bar{\Re}\Re_{-1}(\Lambda)=\sum_{xy\in X(\Lambda)}[\bar{\Re}\varphi(x)\times\bar{\Re}\varphi(y)]^{-1};$$

$$=\frac{3x}{3\times3}+\frac{6x}{3\times1}+\frac{9xy-24x}{2(1\times1)}$$

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$$=\frac{3x}{9}+\frac{6x}{3}+\frac{9xy-24x}{2}$$
$$=\frac{9xy}{2}-\frac{29x}{3}$$

For $\alpha=\frac{1}{2}$,

$$\bar{\Re}\Re_{\frac{1}{2}}(\Lambda)=\sum_{xy\in X(\Lambda)}[\bar{\Re}\varphi(x)\times\bar{\Re}\varphi(y)]^{\frac{1}{2}};$$
$$=3x\times\sqrt{3\times3}+6x\times\sqrt{3\times1}+(9xy-24x)\times2\sqrt{1\times1}$$

$$=18xy+6\sqrt{3}x-39x$$

For $\alpha=-\frac{1}{2}$,

$$\bar{\Re}\Re_{-\frac{1}{2}}(\Lambda)=\sum_{xy\in X(\Lambda)}[\bar{\Re}\varphi(x)\times\bar{\Re}\varphi(y)]^{-\frac{1}{2}};$$
$$=\frac{3x}{\sqrt{3\times3}}+\frac{6x}{\sqrt{3\times1}}+\frac{9xy-24x}{2\sqrt{1\times1}}$$
$$=\frac{3x}{\sqrt{9}}+\frac{6x}{\sqrt{3}}+\frac{9xy-24x}{2\sqrt{1}}$$
$$=\frac{9xy}{2}+2\sqrt{3}x-11x$$

- **Reverse Atom Bond Connectivity index**

$$\bar{\Re}ABC(\Lambda)=\sum_{xy\in X(\Lambda)}\sqrt{\frac{\bar{\Re}\varphi(x)+\bar{\Re}\varphi(y)-2}{\bar{\Re}\varphi(x)\times\bar{\Re}\varphi(y)}}$$
$$=(3x)\sqrt{\frac{3+3-2}{3\times3}}+(6x)\sqrt{\frac{3+1-2}{3\times1}}+\left(\frac{9xy-24x}{2}\right)\sqrt{\frac{1+1-2}{1\times1}}$$
$$=(3x)\sqrt{\frac{4}{9}}+(6x)\sqrt{\frac{2}{3}}$$
$$=2\sqrt{6}x+2x$$

- **Reverse Geometric Arithmetic index**

$$\bar{\Re}GA(\Lambda)=\sum_{xy\in X(\Lambda)}\frac{2\sqrt{\bar{\Re}\varphi(x)\times\bar{\Re}\varphi(y)}}{\bar{\Re}\varphi(x)+\bar{\Re}\varphi(y)}$$
$$=(3x)\left[\frac{2\sqrt{3\times3}}{3+3}\right]+(6x)\left[\frac{2\sqrt{3\times1}}{3+1}\right]+\left(\frac{9xy-24x}{2}\right)\left[\frac{2\sqrt{1\times1}}{1+1}\right]$$
$$=(3x)\left[\frac{2\sqrt{9}}{6}\right]+(6x)\left[\frac{2\sqrt{3}}{4}\right]+\left(\frac{9xy-24x}{2}\right)\left[\frac{2\sqrt{1}}{2}\right]$$

$$=3x+3\sqrt{3}x+\left(\frac{9xy-24x}{2}\right)$$

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- **Reverse First Zagreb index**

$$\Re M_1(\Lambda) = \sum_{xy\in X(\Lambda)} (\Re\varphi(x) + \Re\varphi(y))$$

$$= (3x)(3+3) + (6x)(3+1) + \left(\frac{9xy-24x}{2}\right)(1+1)$$

$$= (3x)(6) + (6x)(4) + \left(\frac{9xy-24x}{2}\right)(2)$$

$$= 18x + 9xy$$

- **Reverse Second Zagreb index**

$$\Re M_2(\Lambda) = \sum_{xy\in X(\Lambda)} (\Re\varphi(x) \times \Re\varphi(y))$$

$$= (3x)(3\times 3) + (6x)(3\times 1) + \left(\frac{9xy-24x}{2}\right)(1\times 1)$$

$$= 27x + 18x + \left(\frac{9xy-24x}{2}\right)$$

$$= 45x + \left(\frac{9xy-24x}{2}\right)$$

$$= 33x + \frac{9xy}{2}$$

- **Reverse First Zagreb Co-index**

$$\Re \bar{M}_1(\Lambda) = 2|X(\Lambda)|(|V(\Lambda)|-1) - \Re M_1(\Lambda)$$

$$= 2\left[\frac{3x(3y-2)}{2}\right]\left(\frac{3xy}{2}-1\right) - (18x+9xy)$$

$$= \left[\frac{27x^2y^2}{2}\right] - 9x^2y - 18xy - 12x$$

- **Reverse Second Zagreb Co-index**

$$\Re \bar{M}_2(\Lambda) = 2|X(\Lambda)|^2 - \frac{1}{2}\Re M_1(\Lambda) - \Re M_2(\Lambda)$$

$$= 2\left[\frac{3x(3y-2)}{2}\right]^2 - \frac{1}{2}(18x+9xy) - \left(33x + \frac{9xy}{2}\right)$$

$$= \frac{81x^2y^2}{2} - 54x^2y + 18x^2 - 9xy - 42x$$

- **Reverse Hyper Zagreb index**

$$\Re HM(\Lambda) = \sum_{xy\in X(\Lambda)} [\Re\varphi(x) + \Re\varphi(y)]^2$$

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$$=(3x)(3+3)^2+(6x)(3+1)^2+\left(\frac{9xy-24x}{2}\right)(1+1)^2$$
$$=156x+18xy$$

- **Reverse Forgotten index**

$$\bar{\Re}F(\Lambda)=\sum_{xy\in X(\Lambda)}[\bar{\Re}\varphi(x)^2+\bar{\Re}\varphi(y)^2]$$
$$=(3x)(3^2+3^2)+(6x)(3^2+1^2)+\left(\frac{9xy-24x}{2}\right)(1^2+1^2)$$
$$=90x+9xy$$

- **Reverse First Multiple Zagreb index**

$$\bar{\Re}PM_1(\Lambda)=\prod_{xy\in X(\Lambda)}[\bar{\Re}\varphi(x)+\bar{\Re}\varphi(y)]$$
$$=(3x)(3+3)\times(6x)(3+1)\times\left(\frac{9xy-24x}{2}\right)(1+1)$$
$$=(3888y-10368)x^3$$

- **Reverse Second Multiple Zagreb index**

$$\bar{\Re}PM_2(\Lambda)=\prod_{xy\in X(\Lambda)}[\bar{\Re}\varphi(x)\times\bar{\Re}\varphi(y)]$$
$$=(3x)(3\times3)\times(6x)(3\times1)\times\left(\frac{9xy-24x}{2}\right)(1\times1)$$
$$=(1458y-3888)x^3$$

- **Reverse First Redefined Zagreb index**

$$\bar{\Re}\Re eZG_1(\Lambda)=\sum_{xy\in X(\Lambda)}\frac{\bar{\Re}\varphi(x)+\bar{\Re}\varphi(y)}{\bar{\Re}\varphi(x)\times\bar{\Re}\varphi(y)}$$
$$=(3x)\frac{3+3}{3\times3}+(6x)\frac{3+1}{3\times1}+\left(\frac{9xy-24x}{2}\right)\frac{1+1}{1\times1}$$
$$=-14x+9xy$$

- **Reverse Second Redefined Zagreb index**

$$\bar{\Re}\Re eZG_2(\Lambda)=\sum_{xy\in X(\Lambda)}\frac{\bar{\Re}\varphi(x)\times\bar{\Re}\varphi(y)}{\bar{\Re}\varphi(x)+\bar{\Re}\varphi(y)}$$
$$=(3x)\frac{3\times3}{3+3}+(6x)\frac{3\times1}{3+1}+\left(\frac{9xy-24x}{2}\right)\frac{1\times1}{1+1}$$
$$=\frac{12x+9xy}{4}$$

- **Reverse Third Redefined Zagreb index**

$$\bar{\Re}\Re eZG_3(\Lambda)=\sum_{xy\in X(\Lambda)}(\bar{\Re}\varphi(x)\times\bar{\Re}\varphi(y))(\bar{\Re}\varphi(x)+\bar{\Re}\varphi(y))$$

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$$= (3x)(3\times3)(3+3)+(6x)(3\times1)(3+1)+\left(\frac{9xy-24x}{2}\right)(1\times1)(1+1)$$
$$= 210x+9xy$$

- **Reverse Augmented Zagreb index**

$$\bar{\Re}AZI(\Lambda)=\sum_{xy\in X(\Lambda)}\left(\frac{\bar{\Re}\varphi(x)\times\bar{\Re}\varphi(y)}{\bar{\Re}\varphi(x)+\bar{\Re}\varphi(y)-2}\right)^3$$
$$=(3x)\left(\frac{3\times3}{3+3-2}\right)^3+(6x)\left(\frac{3\times1}{3+1-2}\right)^3+\left(\frac{9xy-24x}{2}\right)\left(\frac{1\times1}{1+1-2}\right)^3$$
$$=54.4218x$$

The graphical comparison of the different types of chemical indices of boron triangular nanotube are as follows.

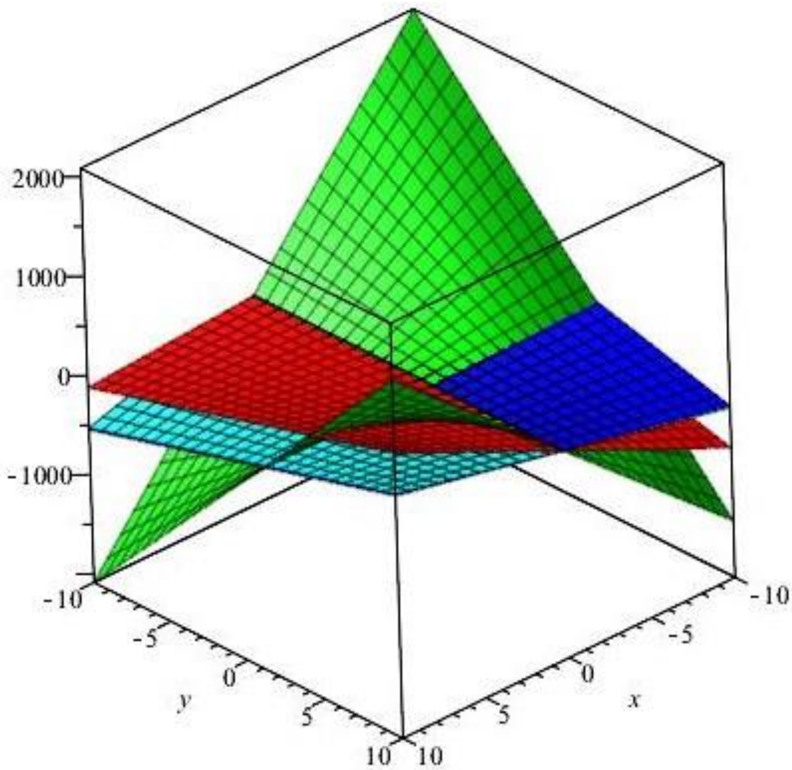


Fig 2. Comparison of the reverse Randic index of boron triangular nanotube for $\alpha=1,-1,\frac{1}{2},-\frac{1}{2}$ where red, blue, green and cyan denotes the reverse Randic index for $\alpha=1,-1,\frac{1}{2},-\frac{1}{2}$ respectively

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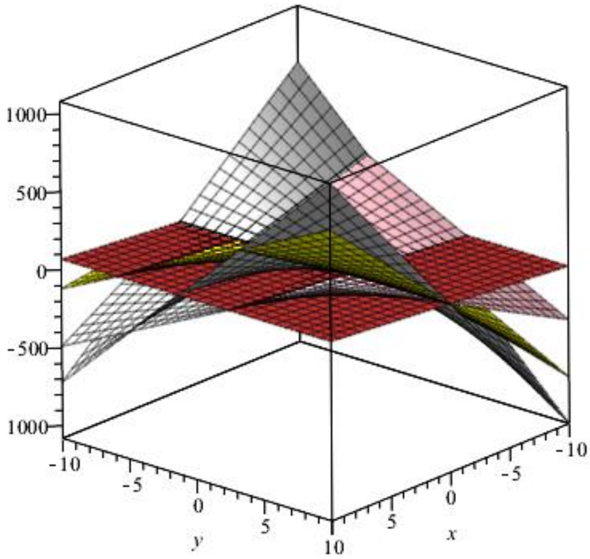


Fig 3. Comparison of the reverse Atom bond connectivity index $\bar{\Re}ABC(\Lambda)$, the reverse geometric arithmetic index $\bar{\Re}GA(\Lambda)$, the reverse first Zagreb index $\bar{\Re}M_1(\Lambda)$ and the reverse second Zagreb index $\bar{\Re}M_2(\Lambda)$ where brown, pink, grey and yellow denotes the reverse $\bar{\Re}ABC(\Lambda)$, $\bar{\Re}GA(\Lambda)$, $\bar{\Re}M_1(\Lambda)$ and $\bar{\Re}M_2(\Lambda)$ respectively.

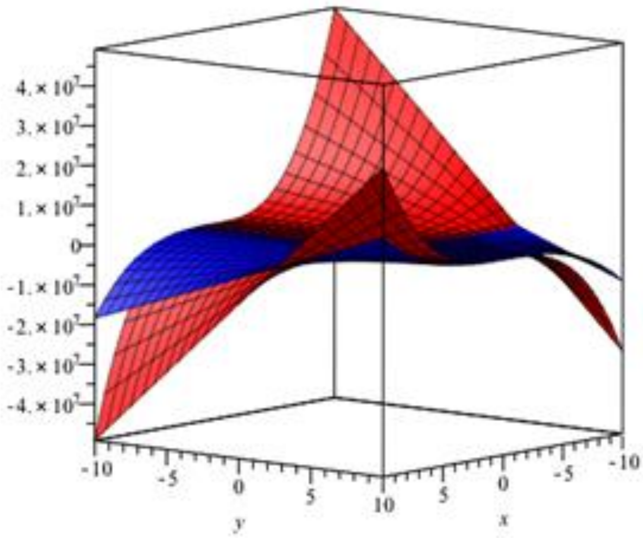


Fig 4. Comparison of the reverse first multiple Zagreb index $\bar{\Re}PM_1(\Lambda)$ and the reverse second multiple Zagreb index $\bar{\Re}PM_2(\Lambda)$ where red and blue denotes the reverse $\bar{\Re}PM_1(\Lambda)$ and $\bar{\Re}M_2(\Lambda)$ respectively

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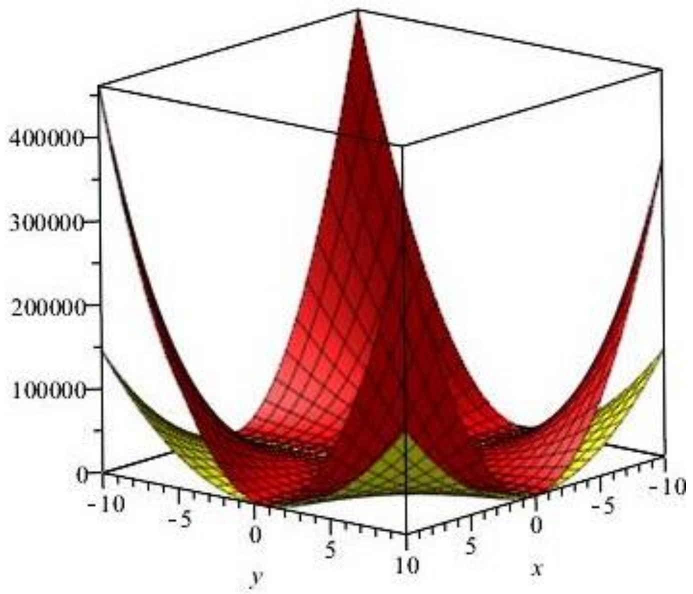


Fig. 5. Comparison of the reverse first Zagreb coindex $\Re\bar{M}_1(\Lambda)$ and the reverse second Zagreb coindex $\Re\bar{M}_2(\Lambda)$ where yellow and red denotes the reverse $\Re\bar{M}_1(\Lambda)$ and $\Re\bar{M}_2(\Lambda)$ respectively.

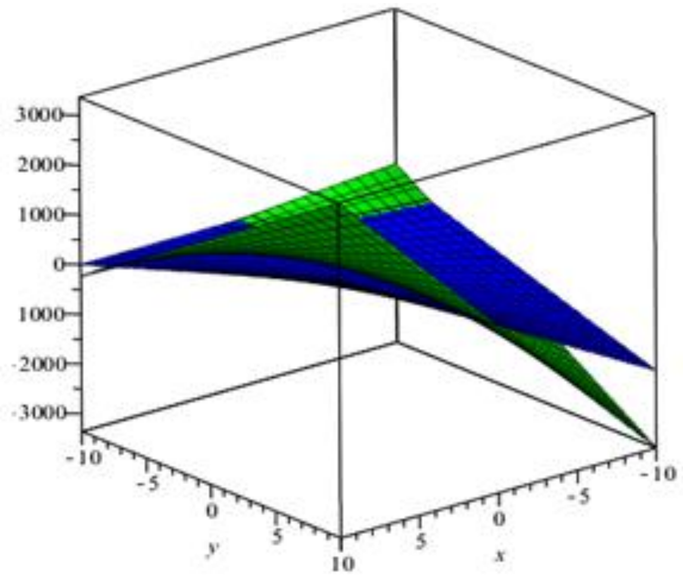


Fig 6. Comparison of the reverse hyper Zagreb $\Re HM(\Lambda)$ and the reverse forgotten index $\Re F(\Lambda)$ where green and blue denotes the reverse $\Re HM(\Lambda)$ and $\Re F(\Lambda)$ respectively.

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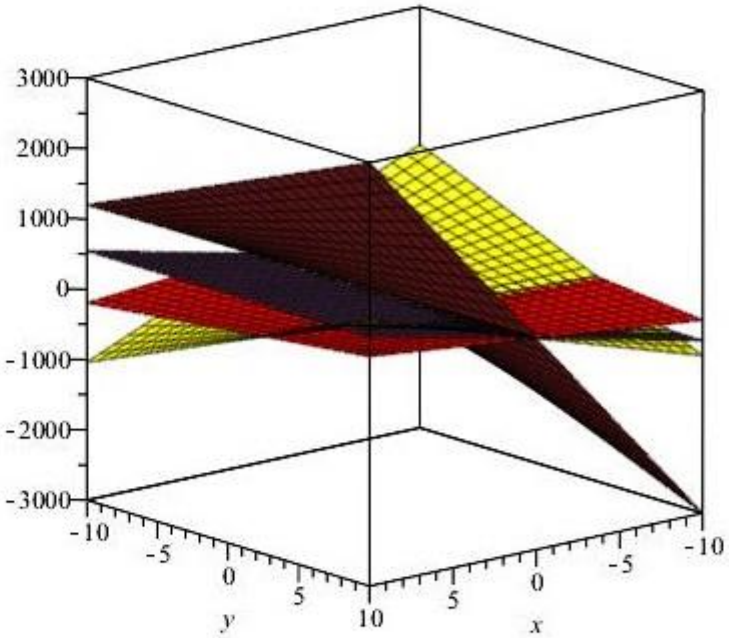


Fig. 7. Comparison of the reverse redefined first Zagreb index $\bar{\Re}\mathrm{Re}ZG_1(\Lambda)$, the reverse redefined second Zagreb index $\bar{\Re}\mathrm{Re}ZG_2(\Lambda)$, the reverse redefined third Zagreb index $\bar{\Re}\mathrm{Re}ZG_3(\Lambda)$ and the reverse augmented Zagreb index $\bar{\Re}AZI(\Lambda)$ where yellow, red, brown and violet denotes the reverse $\bar{\Re}\mathrm{Re}ZG_1(\Lambda)$, $\bar{\Re}\mathrm{Re}ZG_2(\Lambda)$, $\bar{\Re}\mathrm{Re}ZG_3(\Lambda)$ and $\bar{\Re}AZI(\Lambda)$ respectively.

## 3. Conclusion

In the analysis of the quantitative structure property relationships (QSPRs) and (QSARs), chemical indices are important tools to approximate the characteristics of the bioactivity, physical, biomedicine and chemical compounds. In this paper, we have provided the results on reverse chemical indices as depicted in Figures 2-7 for Boron triangular nanotube, besides indices showed increased values for Boron triangular nanotube. The computational results which we get will aid the investigators to recognise the preferred structure more easily and would inspire the others to concentrate on the Boron triangular nanotube. The methodology discussed here are very helpful to evaluate the physico chemical properties, biological properties of stated chemical structures, and are economical and sensible.

**Data Availability Statement:** All data required for this research work are within the manuscript.

**Conflicts of Interest:** The authors declare no conflict of interest.

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