Article

Some Computational Aspects of Triangular Boron Nanotubes

Mobeen Munir [1], Waqas Nazeer [1], Shazia Rafique [2], Abdul Rauf Nizami [1] and Shin Min Kang [3,4,*]

[1] Division of Science and Technology, University of Education, Lahore 54000, Pakistan; mmunir@ue.edu.pk (M.M.); nazeer.waqas@ue.edu.pk (W.N.); arnizami@ue.edu.pk (A.R.N.)
[2] Center for Excellence in Molecular Biology, Punjab University Lahore, Lahore 53700, Pakistan, shahziarafique@gmail.com
[3] Department of Mathematics and RINS, Gyeongsang National University, Jinju 52828, Korea
[4] Center for General Education, China Medical University, Taichung 40402, Taiwan
* Correspondence: smkang@gnu.ac.kr; Tel.: +82-55-772-1420

Abstract: Recent discovery of triangular boron Nanotubes makes it a competitor of carbon in many respects. Closed forms of M-polynomial of nanotubes produce closed forms of many degree-based topological indices which are numerical parameters of the structure and, in combination, determine properties of the concerned nanotubes. In this report, we give M-polynomials of triangular boron nanotubes and recover many important topological degree-based indices of these nanotubes. We also plot surfaces associated to these nanotubes.

Keywords: M-polynomial; degree-based index; boron nanotubes

1. Introduction

Nanoscience has become the flavor of the modern era because of its increasing applications and uses. Amongst the nanomaterials, nanocrystals, nanowires and nanotubes, constitute three major categories, the last two being one-dimensional. Since the discovery of the carbon nanotubes in 1991, interest in one-dimensional nanomaterials has grown remarkable and a phenomenal number of research articles have been published on nanotubes as well as on nanowires.

The numerical tendencies of a certain property depend on the molecular structure which is, in fact, a graph where vertices represent atoms of nanomaterials and edges correspond to chemical bonds. Chemical graph theory is contributing a lion's share in predicting chemical properties of a nanomaterial without going into wet labs. Cheminformatics is another emerging field in which quantitative structure-activity (QSAR) and Structure-property (QSPR) relationships predict the biological activities and properties of nanomaterial see [2-5]. In these studies, some physio-chemical properties and topological indices are used to predict bioactivity of the chemical compounds see [13, 14, 15].

Boron nanotubes are coming increasingly interesting because of their remarkable properties, like: structural stability, work function, transport properties, and electronic structure [30]. Two structural classes of boron nanotubes are extremely important. First one is a nanotube derived from triangular sheet and the second one is derived from $\alpha-$ sheet. Regardless of their structure and chiralities, both boron nanotubes are more conductive than carbon nanotubes.

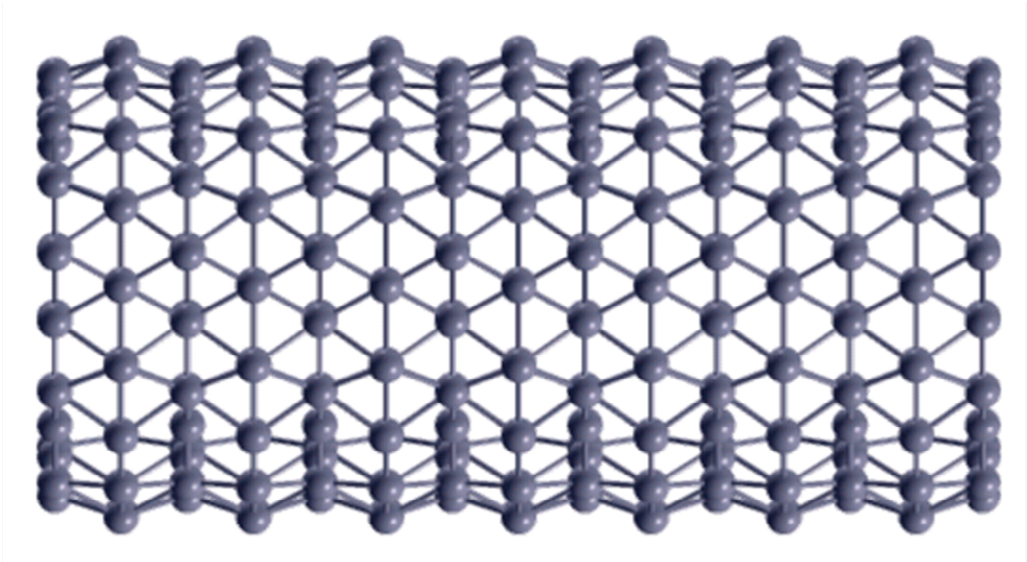

Figure 1. Triangular Boron nanotube

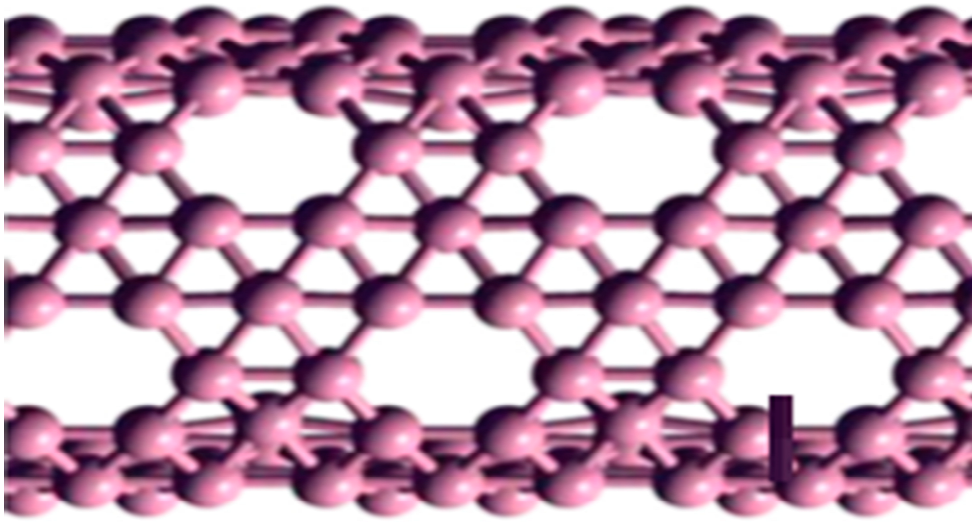

Figure 2. α-Boron nanotubes

In terms of chemical graph theory and mathematical chemistry, we associate a graph with the molecular structure where vertices correspond to atoms and edges to bonds. Following the same lines, we represent a boron triangular nanotube, by a planar graph, $BNT_t[m,n]$ of order n $\times$ m, as the in figure 3 demonstrates. This kind of boron nanotube appeared in 2004 [31,32]. Clearly, there are $\frac{3nm}{2}$ a number of vertices and $\frac{3m(3n-2)}{2}$ edges in 2D graph model of triangular boron nanotubes.

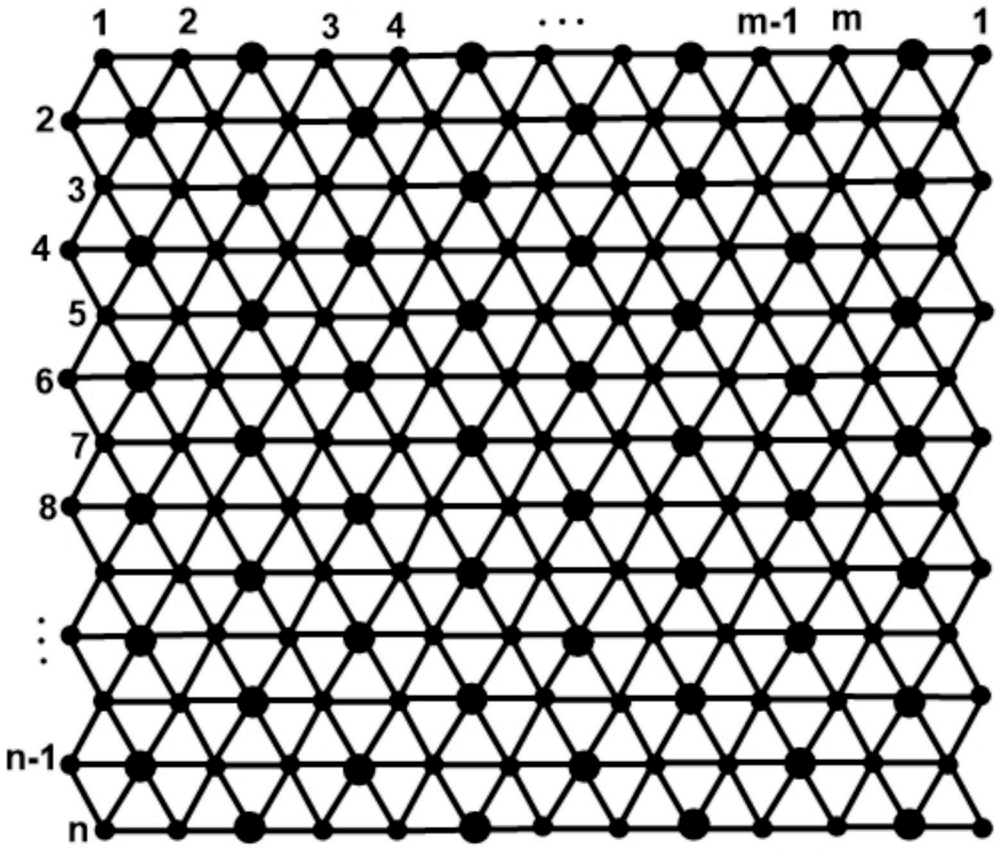

Figure 3. 2D structure of triangular boron nanotube

We refer the readers [27,28,29] for further study about nanomaterials.

Several algebraic polynomials have useful applications in chemistry such as Hosoya Polynomial (also called Wiener polynomial) [25] that plays a vital role in determining distance-based topological indices. Among Other algebraic polynomials, M-polynomial introduced recently in [26], plays the same role in determing many degree-based topological indices. These indices are actually score functions that capture the overall structure of the compound and predict chemical properties such as strain energy, the heat of formation, and boiling points etc.

The branch of chemistry which deals with the chemical structures with the help of mathematical tools is called mathematical chemistry. Chemical graph theory is that branch of mathematical chemistry which applies graph theory to mathematical modeling of chemical phenomena. In chemical graph theory, a molecular graph is a simple graph (having no loops and multiple edges) in which atoms and chemical bonds between them are represented by vertices and edges respectively. A graph $G(V,E)$ with vertex set V(G) and edge set E(G) is connected if there

exist a connection between any pair of vertices in G. A network is simply a connected graph having no multiple edges and loops. The degree of a vertex is the number of vertices which are connected to that fixed vertex by the edges. In a chemical graph, the degree of any vertex is at most 4. The distance between two vertices u and v is denoted as $d(u,v)=d_G(u,v)$ and is the length of shortest path between u and v in graph G. The number of vertices of G, adjacent to a given vertex v, is the "degree" of this vertex, and will be denoted by $d_v(G)$ or, if misunderstanding is not possible, simply by d_v. The concept of degree is some what closely related to the concept of valence in chemistry. For details on basics of graph theory, any standard text such as [4] can be of great help.

In this article, we calculated different degree-based topological indices of Boron nanotubes by using M-polynomial. Before this, we need to recall a few concepts from chemical graph theory. M-polynomial is recently introduced in [26]. Throughout this paper we fixed following notations:

d_v = the degree of a vertex v,

$V_{\{k\}} = \{v \in V(G) \mid d_v = k\}$,

$E_{\{i,j\}} = \{uv \in E(G) \mid d_u = j \text{ and } d_v = i\}$,

$|E|$ is no. of elements in the set E,

$\delta = \text{Min}\{d_v \mid v \in \text{V (G)}\}$,

$\Delta = \text{Max}\{d_v \mid v \in \text{V (G)}\}$,

$m_{ij}(G)$ is no of edges of G such that $\{d_v, d_u\} = \{i, j\}$.

The M-polynomial of G is defined as:

$$M(G,x,y) = \sum_{\delta \le i \le j \le \Delta} m_{ij}(G) x^i y^j .$$

This polynomial has been one of the key areas of interest in computational aspects of materials. From this M-polynomial, we can calculate many topological indices. The topological index of a molecule structure can be considered as a non-empirical numerical quantity which quantifies the molecular structure and its branching pattern in many ways. In this point of view, the topological index can be regarded as a score function which maps each molecular structure to a real number and is used as a descriptor of the molecule under testing [6, 7, 9, 10, 11]. Topological indices predict the variety of physico-chemical properties of the underlying structure like vapor pressure,

boiling point, the heat of evaporation, chromatographic retention times, heat of formation, and surface tension.

Weiner, in 1947, approximated the boiling point of alkanes as $\alpha W(G)+\beta P_3+\gamma$ where α, β and γ are empirical constants, $W(G)$ is the Weiner index and P_3 is the number of paths of length 3 in G [18]. Thus Weiner laid the foundation of Topological index which is also known as connectivity index. A lot of chemical experiments require determining the chemical properties of emerging nanotubes and nanomaterials. Chemical based experiments reveal that out of more than 140 topological indices no single index in strong enough to determine many physio-chemical properties, although, in combination, these topological indices can do this to some extent. The Wiener index is originally the first and most studied topological index and is $\sum_{i<j} d(v_i,v_j)$, for more details see [16]. Zagreb indices have been introduced by I. Gutman and N. Trinajstic [21].

First Zagreb index is $M_1(G)=\sum_{v\in V(G)}(\mathrm{d}_v)^2$ and the second Zagreb i $M_2(G)=\sum_{uv\in E(G)}\mathrm{d}_u\,\mathrm{d}_v$,

ndex[22, 23]. Second modified Zagreb index is defined by ${}^{m}M_2(G)=\sum_{uv\in E(G)}\frac{1}{d_u d_v}$. General Randic

index of G is defined as $\sum_{uv\in E(G)}(d_u d_v)^{\alpha}$, where α is an arbitrary real number see [24]. Symmetric

division index is defined by $SDD(G)=\sum_{uv\in E(G)}\left\{\frac{\min(d_u,d_v)}{\max(d_u,d_v)}+\frac{\max(d_u,d_v)}{\min(d_u,d_v)}\right\}$. The harmonic

index H(G) is another variant of Randic index defined as $H(G)=\sum_{vu\in E(G)}\frac{2}{d_u+d_v}$ [33-34]. The

inverse sum topological index ISI is defined as $ISI(G)=\sum_{vu\in E(G)}\frac{d_u d_v}{d_u+d_v}$. Augmented Zagreb

Index of G is defined as $AZI(G)=\sum_{vu\in E(G)}\left\{\frac{d_u d_v}{d_u+d_v-2}\right\}^3$ and it is useful for computing heat of

formation of alkanes [33,34]. These indices can help to characterize the chemical and physical properties of molecules see [6-10, 18-22,24–26]. Most recently M. Munir et al. computed M-polynomials and related topological indices for Nanostar dendrimers [1] and Titania Nanotubes in [19]. Some degree-based topological indices are derived from M-polynomial l [5]. The following table-1 relates these derivations.

Table 1. Derivation of some degree-based topological indices from M-polynomial

Topological Index	Derivation from $M(G;x,y)$
First Zagreb	$(D_x+D_y)\left(M(G;x,y)\right)\|_{x=y=1}$
Second Zagreb	$(D_xD_y)\left(M(G;x,y)\right)\|_{x=y=1}$
Second Modified Zagreb	$(S_xS_y)\left(M(G;x,y)\right)\|_{x=y=1}$
General Randić $\alpha \in \mathbb{N}$	$(D_x^{\alpha}D_y^{\alpha})\left(M(G;x,y)\right)\|_{x=y=1}$
General Randić $\alpha \in \mathbb{N}$	$(S_x^{\alpha}S_y^{\alpha})\left(M(G;x,y)\right)\|_{x=y=1}$
Symmetric Division Index	$(D_xS_y+S_xD_y)\left(M(G;x,y)\right)\|_{x=y=1}$
Harmonic Index	$2\,S_x\,J\,(M(G\,;x,y))_{x=1}$
Inverse sum Index	$S_x\,J\,D_x\,D_y(M(G\,;x,y))_{x=1}$
Augmented Zagreb Index	$S_x^3\,Q_{-2}\,J\,D_x^3D_y^3(M(G\,;x\,,y))_{x=1}$

Where, $D_xf=x\frac{\partial(f(x,y)}{\partial x}, D_yf=y\frac{\partial(f(x,y)}{\partial y}, S_x=\int_0^x\frac{f(t,y)}{t}dt, S_y=\int_0^y\frac{f(x,t)}{t}dt\, J(f(x,y))=f(x,x), Q_{\alpha}(f(x,y))=x^{\alpha}f(x,y)$ for non zero α, $J(f(x,y))=f(x,x)$, for more details see[25a].

In the present article, we compute the closed forms of M-polynomials triangular boron nanotubes and represent them graphically using Maple. As consequences, we derive as many as nine different topological degree-based indices. We start by defining M-polynomial of a general graph, see [25]. Recently a lot of research is in progress to find closed forms of certain topological indices. M-polynomial, introduced in 2015 [25], is an approach to obtain closed forms of many degree-based topological indices.

RESULTS AND DISCUSSION

In this section, we use symmetric structures of Boron triangular Nanotubes to determine closed parametric form of M-polynomials many topological indices for these tubes.

Theorem 1. Let $BNT_t[m,n]$ is boron triangular Nanotubes.then

$$M\left(BNT_t[m,n]?\mathfrak{R}\ y\right)=3mx^4y^4+6mx^4y^6+\frac{m}{2}m(9n-24)x^6y^6.$$

Proof. Let $BNT_t[m,n]$ be triangular boron nanotubes , where m is the number of columns and n is the number of rows. The graph has $\frac{3nm}{2}$ number of vertices and $\frac{3m(3n-2)}{2}$ edges.

Following are the tables for edge partitions of $BNT_t[m,n]$ nanotubes.

Table 2. Edge partition of edge set of $BNT_t[m,n]$

$(d_u,\ d_v)$	$(4\ ,\ 4)$	$(4\ ,\ 6)$	$(6\ ,\ 6)$
Number of edges	$3m$	$6m$	$\frac{m}{2}(9n-24)$

There are two partitions, $V_{\{2\}}=\{v\epsilon BNT_t[m,n]\,|\,d_v=4\}$, and $V_{\{6\}}=\{v\epsilon BNT_t[m,n]\,|\,d_v=6\}$ for the vertex set $V\left(BNT_t[m,n]\right)$ from table 1. Now the edge set of $BNT_t[m,n]$ can is written as

$$E_{\{4,4\}}=\left\{e=uv\in E\left(BNT_t[m,n]\right)|d_u=4?\mathfrak{A}_v=\ \right\}\rightarrow\left|E_{\{4,4\}}\right|=3m,$$

$$E_{\{4,6\}}=\left\{e=uv\in E\left(BNT_t[m,n]\right)|d_u=4,\mathfrak{A}_v=\ \right\}\rightarrow\left|E_{\{4,6\}}\right|=6m,\text{ and}$$

$$\mathfrak{E}_{\{6,6\}}=\left\{e=uv\in E\left(BNT_t[m\ \ n]\right)|d_u=6?\mathfrak{A}_v=\ \right\}\rightarrow\left|E_{\{6,6\}}\right|=\frac{m}{2}(9n-24).$$

Thus the M-polynomial of $BNT_t[m,n]$ is equal to:

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$$
\begin{aligned}
M\left(BNT_t[m,n],\text{賤},y\right) &= \sum_{i\le j} m_{ij}\left(BNT_t[m,n]\right)x^i y^j \\
&= \sum_{4\le 4} m_{44}\left(BNT_t[m,n]\right)x^4y^4 + \sum_{4\le 6} m_{46}\left(BNT_t[m,n]\right)x^4y^6 \\
&\quad + \sum_{6\le 6} m_{66}\left(BNT_t[m,n]\right)x^6y^6 \\
&= \sum_{uv\in E_{\{4,4\}}} m_{44}\left(BNT_t[m,n]\right)x^4y^4 + \sum_{uv\in E_{\{4,6\}}} m_{46}\left(BNT_t[m,n]\right)x^4y^6 \\
&\quad + \sum_{uv\in E_{\{6,6\}}} m_{66}\left(BNT_t[m,n]\right)x^6y^6 \\
&= \left|E_{\{4,4\}}\right|x^2y^4 + \left|E_{\{4,6\}}\right|x^4y^6 + \left|E_{\{6,6\}}\right|x^6y^6 \\
&= 3mx^4y^4 + 6mx^4y^6 + \frac{m}{2}(9n-24)x^6y^6.
\end{aligned}
$$

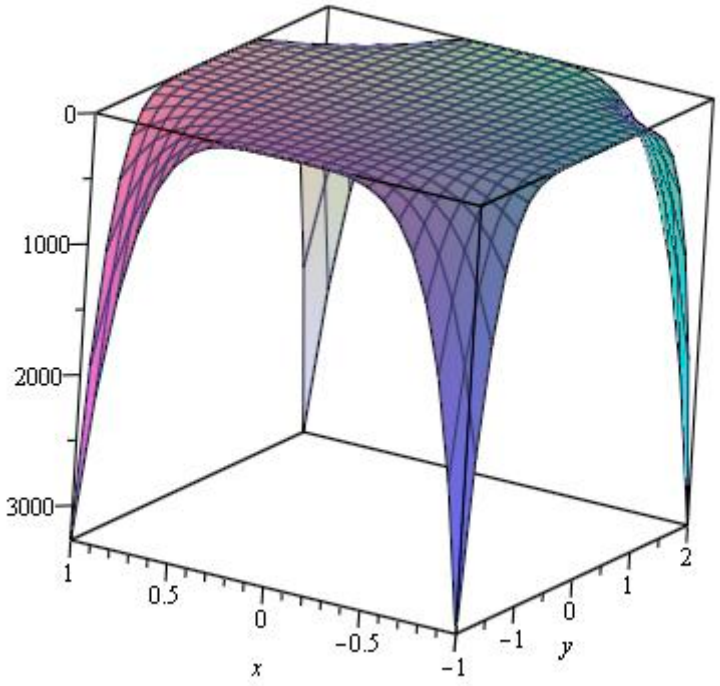

Figure 4. Plot of M-polynomial of $BNT_t[m,n]$

Above figure presents the Maple 13 plot of the M-polynomial of triangular Boron Nanotubes. Clearly, Values drastically decrease as $X \to \pm 1, Y \to \pm 2$ For the most part of [-1,1] × [-2,2], values remain stable.

Proposition 1. Let $BNT_t[m,n]$ is the boron triangular nanotube, then

1. $M_1(BNT_t[m,n]) = 6m(9n-10),$
2. $M_2(BNT_t[m,n] = m^2(729n^2 - 1620n + 864),$
3. ${}^m M_2(BNT_t[m,n]) = \frac{m^2}{16}(9n^2 - 1),$
4. $R_a(G) = (m^2(729n^2 - 1620n + 864))^{\alpha},$
5. $R_a(G) = (\frac{m^2}{16}(9n^2 - 1))^{\alpha},$
6. $SDD(G) = \frac{m^2}{4}(162n^2 - 180n + 12).$

Proof. Let $f(x,y)$ be the M-polynomial of $BNT_t[m,n]$. Then

$$f(BNT_t[m,n]?\, x,y) = 3mx^4y^4 + 6mx^4y^6 + \frac{m}{2}(9n-24)x^6y^6,$$

$$D_x(f(x,y)) = x\{12mx^3y^4 + 24mx^3y^6 + 3m(9n-24)x^5y^6\},$$

$$D_y(f(x,y)) = y\{12mx^4y^3 + 36mx^4y^5 + 3m(9n-24)x^6y^5\},$$

$$S_x(f(x,y)) = \tfrac{3}{4}mx^4y^4 + \tfrac{3}{4}mx^4y^6 + \tfrac{m}{2}(9n-24)x^6y^6,$$

$$S_y(f(x,y)) = \tfrac{3}{4}mx^4y^4 + mx^4y^6 + \tfrac{m}{12}(9n-12)x^6y^6,$$

$$D_x(f(BNT_t[m,n]?\, x,y))|_{x=y=1} = 9m(3n-4),$$

$$D_y(f(BNT_t[m,n]?\, x,y))|_{x=y=1} = 3m(9n-8),$$

$$S_x(f(BNT_t[m,n]?\, x,y))|_{x=y=1} = \tfrac{m}{4}(3n+1),$$

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$$S_y\left(f\left(BNT_t[m,n]?\,x,y\right)\right)|_{x=y=1}=m/4\,(3n-1),$$

1. $M_1\left(BNT_t[m,n]\right)?=(D_x+D_y)\left(M\left(G;x,y\right)\right)|_{x=y=1}=6m(9n-10),$
2. $M_2(BNT_t[m,n])=(D_xD_y)(M(G;x,y))|_{(x=y=1)}=m^2(729n^2-1620n+864),$
3. $^{m}M_2\left(BNT_t[m,n]\right)=(S_xS_y)\left(M\left(G;x,y\right)\right)|_{x=y=1}=\frac{m^2}{16}(9n^2-1),$
4. $R_a(G)=(D_x^{\alpha}D_y^{\alpha})(M(G;x,y))|_{(x=y=1)}=(m^2(729n^2-1620n+864))^{\alpha},$
5. $R_a(G(S_x^{\alpha}S_y^{\alpha})(M(G;x,y))|_{(x=y=1)}=(\frac{m^2}{16}(9n^2-1))^{\alpha},,$
6. $SDD(G)=(D_xS_y+S_xD_y)(M(G;x,y))|_{(x=y=1)}=\frac{m^2}{4}(162n^2-180n+12).$

Proposition 2. Let $BNT_t[m,n]$ is boron triangular nanotube, then

- $H\left(BNT_t[m\ n]?\right)=m/20\ 15n-1),$
- $I(BNT_t[m,n]=m/10\,(135n-156),$
- $A(BNT_t[m,n])=\frac{1}{125}m(26244n+176266)\,.$

Proof. Let $f\left(x,y\right)$ be M-polynomial of $BNT_t\left[m,n\right]$. Then

$$f\left(BNT_t[m,n]?\,x,y\right)=3mx^4y^4+6mx^4y^6+m/2\,(9n-24)x^6y^6,$$

$$J\left(f(BNT_t[m,n]?\,x,y)\right)=3mx^8+6mx^{10}+m/2\,(9n-24)x^{12},$$

$$S_xJ\left(f(BNT_t[m,n]?\,x,y)\right)=3/8\,mx^8+3/5\,mx^{10}+1/24\,m(9n-24)x^{12},$$

$$H\left(BNT_t[m,n]?\,x,y\right)=2S_xJ\left(BNT_t[m,n]?\,x,y\right)|_{x=1}=m/20\,(15n-1),$$

$$D_y\left(f(BNT_t[m,n]?\,x,y)\right)=12mx^4y^4+36mx^4y^6+3m(9n-24)x^6y^6,$$

$$D_xD_y\left(f\left(BNT_t[m,n]?\,x,y\right)\right)=48mx^4y^4+144mx^4y^6+18m(9n-24)x^6y^6,$$

$$JD_xD_y\left(f\left(BNT_t[m,n]?\,x,y\right)\right)|_{x=y=1}=48mx^8+144mx^{10}+18m(9n-24)x^{12},$$

$$I(BNT_t[m,n])=S_xJD_xD_y\left(BNT_t[m,n]?\,x,y\right)_{x=1}=m\!\!\diagup_{10}(135n-156),$$

$$D_y{}^3\left(f(BNT_t[m,n]?\,x,y)\right)=192mx^4y^4+1296mx^4y^6+108m(9n-24)x^6y^6,$$

$$D_x{}^3D_y{}^3\left(f(BNT_t[m,n]?\,x,y)\right)=12288mx^4y^4+82944mx^4y^6+23328m(9n-24)x^6y^6,$$

$$JD_x{}^3D_y{}^3\left(f(BNT_t[m,n]?,x\ \ y)\right)=12288mx^8+82944mx^{10}+23328m(9n-24)x^{12},$$

$$Q_{-2}JD_x{}^3D_y{}^3\left(f(BNT_t[m,n]?\,x,y)\right)=12288mx^6+82944mx^8+23328m(9n-24)x^{10},$$

$$A(BNT_t[m,n])=S_x{}^3Q_{-2}JD_x{}^3D_y{}^3\left(f(BNT_t[m,n]?\,x,y)\right)=\frac{1}{125}m(26244n+176266).$$

CONCLUSIONS AND DISCUSSION

In this article, we computed at first step, the closed form of M-polynomial for triangular boron nanotubes. Then we derive many degree-based topological indices for triangular Boron nanotubes. Topological indices thus calculated for these nanotubes can help us to understand the physical features, chemical reactivity, and biological activities. In this point of view, a topological index can be regarded as a score function which maps each molecular structure to a real number and is used as descriptors of the molecule under testing. These results can also play a vital part in the determination of the significance of triangular boron nanotubes in electronics and industry. We also want to remark that similar techniques can be used to determine M-polynomial and topological indices about α-boron nanotubes. A comparison of both types of boron Nanotubes can be given.

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