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New degree-based topological descriptors *via* m-polynomial of boron α-nanotube

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The study of molecular structure having size less than 100 nm is called nanotechnology. Nano-materials have vast applications in different fields. Boron α-nanotube is very famous in Nano-science. In this article, we computed some important topological indices of this structure using their M-polynomial along with plotting the results.

KEYWORDS

M-polynomial; boron α-nanotube; topological indices.

Introduction

In the first half of 18th century, by solving the problem of Konigsberg Bridge, the L. Euler laied the foundation of important sub field of mathematical, known as graph theory. Graph theory has significant impact on various branches of science and technology and is flourishing rapidly now. Graph theoretical concepts are widely used to study and modeling the various applications, in different areas such as engineering, computer science, chemistry and biology [2,13,14-26].

A graph denoted by G, is a set of points, known as vertices or nodes. A node is the fundamental unit of a graph. An edge will be drawn between two vertices. In graph theory the number of lines meet at a vertex called the vertex degree. Here, we set V (G) as set of vertices, E(G) as the set of edges and d_v as the degree of vertex v and d_{uv} as a degree of the edge. Where $d_{uv}=d_u+d_v-2$.

In chemistry we study the structure of molecules and construction of bonds between the atoms. Chemical graph theory provides the different tools to analyze the molecular structure of the compounds. A basic concept of chemistry is that the properties of the chemical compound depend on the structure of the molecule. In chemical graph theory, molecule of the chemical compound is converted into molecular graph by representing atoms as vertices and chemical bonds as edges of the graphs.

In chemical graph theory, a graph is converted into some mathematical object such as matrix, polynomial, a numeric number or a sequence of numbers. These mathematical objects describe the different properties of the chemical graph. In this study, we computed topological descriptors via M-polynomial of Boron α-armchair nanotube $B_\alpha NT_{mn}$.

Boron α-nanotube

With the help of Nanoscience, scientists are expected to revolutionize the world. In nanotechnology, the use of carbon is very important but now boron is also used in nano-scale devices due to the fact that boron is lighter and more galvanically inert then carbon [3,11,12]. Boron α-nanotube is such a nonmaterial which has a bright future. The shape of Boron α-nanotube is formed with 2D boron-nanosheet consisting of m rows and n column. The first and the last column of 2D boron-nanosheet are connected to form a boron α-nanotube.

An important factor that controls the unique properties of the nano tubes structures is caused by the rolling up of the nano sheet into a nano tube. There are three ways for the nano sheet to do the rolling, depending upon its direction: Armchair, zigzag, and chiral [3]. Different properties of boron nano tubes are also discussed by J.B. Liu et al. [11]. We categorized the boron-armchair nanotubes into two classes with respect to number of rows m [11]. First class having m 0 (mod 3) is shown in Figure 1a, and the other class having m∈(mod 3) is shown in Figure 1b. In this article we investigated the boron-armchair nanotube for m 0 (mod 3) and represented as $B_\alpha NT_{mn}$.

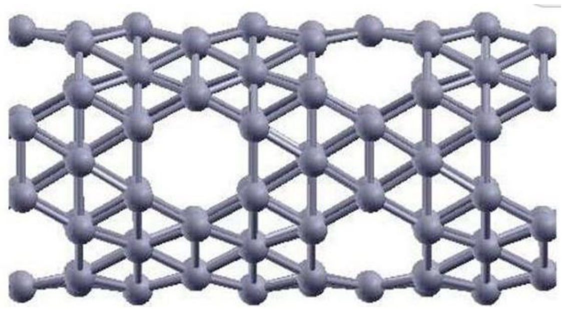


FIGURE 1 Boron α-armchair nanotube ($B_\alpha NT_{mn}$)

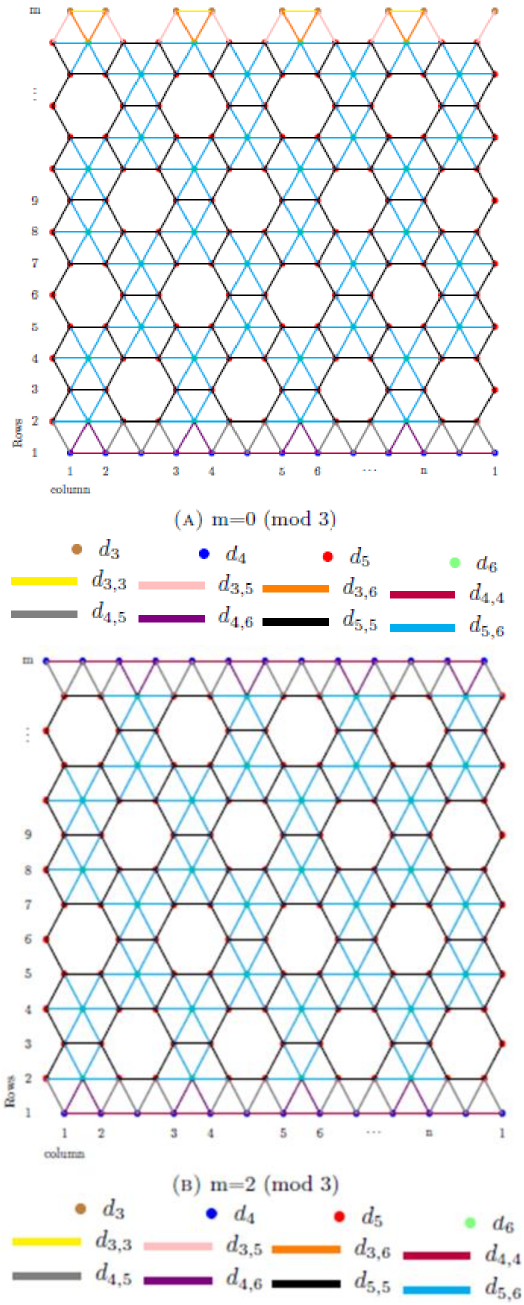


FIGURE 2 Boron $_\alpha$-nanosheet $B_\alpha NS_{mn}$

TABLE 1 Vertex Partition of boron α-nanotube ($B_\alpha NT_{mn}$)

d_u	3	4
Number of vertices	n	$\frac{3}{2}n$
5	6	Total vertices
n(m-2)	$\frac{1}{6}$n(2m-3)	$\frac{4}{3}$mn

Topological indices

A topological index is a numeric real number related to the topology of the molecular graph. There are many classes of molecular topological invariants but degree dependent topological indices have an important role in the field of chemical graph theory. These degree dependent indices are computed on the basis of degrees of vertices of molecular graph. Usually carbon-hydrogen bond is surpassed during the study of topological indices because this bond does not have any effect on the topological properties of the molecular compound. These topological indices have many application in QSAR and QSPR studies. Table 3 shows some important degree-based topological index.

TABLE 2 Edge Partition of boron α-nanotube ($B_\alpha NT_{mn}$)

$(d_u;d_v)$	Number of edges
(3,3)	$\frac{1}{2}n$
(3,5)	N
(3,6)	N
(4,4)	$\frac{3}{2}n$
(4,5)	2n
(4,6)	N
(5,5)	$\frac{1}{2}n(3m-8)$
(5,6)	$\frac{1}{2}n(2m-5)$
Total edges	$\frac{1}{2}n(7m-4)$

TABLE 3 Degree-based Topological indices

Atom-bond connectivity index[6]	$ABC[B_\alpha NT_{mn}]=\sum_{uv\in E(B_\alpha NT_{mn})}\sqrt{\frac{d_u+d_v-2}{d_u.d_v}}$
Geometric arithmetic index[15]	$GA[B_\alpha NT_{mn}]=\sum_{uv\in E(B_\alpha NT_{mn})}\frac{2\sqrt{d_u.d_v}}{d_u+d_v}$
First K Banhatti index[8]	$B_1[B_\alpha NT_{mn}]=\sum_{uv\in E(B_\alpha NT_{mn})}(d_u+d_{uv})$
Second K Banhatti index[8]	$B_2[B_\alpha NT_{mn}]=\sum_{uv\in E(B_\alpha NT_{mn})}(d_u.d_{uv})$
First K hyper Banhatti index[9]	$HB_1[B_\alpha NT_{mn}]=\sum_{uv\in E(B_\alpha NT_{mn})}(d_u+d_{uv})^2$
Second K hyper Banhatti index[9]	$HB_2[B_\alpha NT_{mn}]=\sum_{uv\in E(B_\alpha NT_{mn})}(d_u.d_{uv})^2$
Modified first K Banhatti index[10]	${}^mB_1[B_\alpha NT_{mn}]=\sum_{uv\in E(B_\alpha NT_{mn})}\frac{1}{d_u+d_{uv}}$
Modified second K Banhatti index[10]	${}^mB_2[B_\alpha NT_{mn}]=\sum_{uv\in E(B_\alpha NT_{mn})}\frac{1}{d_u.d_{uv}}$
Harmonic K Banhatti index[10]	$H_b[B_\alpha NT_{mn}]=\sum_{uv\in E(B_\alpha NT_{mn})}\frac{2}{d_u+d_{uv}}$

M-polynomial

An algebraic polynomial can also explain the behavior of the molecular structure. M-polynomial is also a graph representative mathematical object. With the help of M-polynomial, we computed many degree dependent topological invariants present in Table 4. For a graph G, the M-polynomial introduced in 2015 [5] is defined as:

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

Where $\delta = \min\{d_v \mid v \in V(G)\}$, $\Delta = \max\{d_v \mid v \in V(G)\}$ and $m_{ij}(G)$ is the number of edges uv∈E(G) such that $\{d_v;d_u\}=\{i;j\}$.

M-polynomial of many graphs were introduced in the past [4, 7]. In this work we computed M-polynomials and topological indices via M-polynomials given in [1] of $B_\alpha NT$. Table 4 gives formulas to compute some well-known degree based topological indices via M-Polynomial [1].

TABLE 4 M-Polynomial and Topological indices derived from boron α-nanotube *M(BαNTmn;x;y)=f(x;y).*

$ABC[B_\alpha NT_{mn}] = D_x^{\frac{1}{2}} Q_{-2} J S_x^{\frac{1}{2}} S_y^{\frac{1}{2}} [f(x,y)]_{x=1}$
$GA[B_\alpha NT_{mn}] = 2S_x J D_x^{\frac{1}{2}} D_y^{\frac{1}{2}} [f(x,y)]_{x=1}$
$B_1[B_\alpha NT_{mn}] = (D_x + D_y + 2D_x Q_{-2} J)[f(x,y)]_{x=y=1}$
$B_2[B_\alpha NT_{mn}] = D_x Q_{-2} J (D_x + D_y)[f(x,y)]_{x=1}$
$HB_1[B_\alpha NT_{mn}] = (D_x^2 + D_y^2 + 2D_x^2 Q_{-2} J + 2D_x Q_{-2} J (D_x + D_y))[f(x,y)]_{x=y=1}$
$HB_2[B_\alpha NT_{mn}] = D_x^2 Q_{-2} J (D_x^2 + D_y^2)[f(x,y)]_{x=1}^m$
$B_1[B_\alpha NT_{mn}] = S_x Q_{-2} J (L_x + L_y)[f(x,y)]_{x=1}^m$
$B_2[B_\alpha NT_{mn}] = S_x Q_{-2} J (S_x + S_y)[f(x,y)]_{x=1}$
$H_b[B_\alpha NT_{mn}] = 2S_x Q_{-2} J (L_x + L_y)[f(x,y)]_{x=1}$

Where the operator used is defined as

$D_x f(x,y) = x\frac{\partial(f(x,y))}{\partial x}$,

$D_y f(x,y) = y\frac{\partial(f(x,y))}{\partial y}$, $L_x f(x,y) = f(x^2, y)$,

$L_y f(x,y) = f(x, y^2)$,

$S_x f(x,y) = \int_0^x \frac{f(t,y)}{t} dt$, $S_y f(x,y) = \int_0^y \frac{f(x,t)}{t} dt$,

$Jf(x,y) = f(x,x)$, $Q_\alpha f(x,y) = x^\alpha f(x,y)$,

$D_x^{\frac{1}{2}} f(x,y) = \sqrt{x\frac{\partial(f(x,y))}{\partial x}} \cdot \sqrt{f(x,y)}$

$D_y^{\frac{1}{2}} f(x,y) = \sqrt{y\frac{\partial(f(x,y))}{\partial y}} \cdot \sqrt{f(x,y)}$,

$S_x^{\frac{1}{2}} f(x,y) = \sqrt{\int_0^x \frac{f(t,y)}{t} dt} \cdot \sqrt{f(x,y)}$,

$S_y^{\frac{1}{2}} f(x,y) = \sqrt{\int_0^y \frac{f(x,t)}{t} dt} \cdot \sqrt{f(x,y)}$.

Theorem 5.1. Let $B_\alpha NT_{mn}$ be a Boron α-nanotube where m is multiple of three then M-polynomial of $B_\alpha NT_{mn}$ is

$$M[B_\alpha NT_{mn}; x, y] = \frac{n}{2}x^3y^3 + nx^3y^5 + nx^3y^6 + \frac{3n}{2}x^4y^4$$
$$+2nx^4y^5 + nx^4y^6 + \frac{n}{2}(3m-8)x^5y^5 + n(2m-5)x^5y^6.$$

Proof. Let $B_\alpha NT_{mn}$ be a boron α-nanotube where m is multiple of 3 and represent the number of rows in a boron α-nanotube respectively then by using Figures 1a, 2 and Table 1, we have the following vertex partition [27-30].

$V_3 = \{u \in B_\alpha NT_{mn} : d_u = 3\} \Rightarrow |V_3| = n,$

$V_4 = \{u \in B_\alpha NT_{mn} : d_u = 4\} \Rightarrow |V_4| = \frac{3n}{2},$

$V_5 = \{u \in B_\alpha NT_{mn} : d_u = 5\} \Rightarrow |V_5| = mn - 2n,$

$V_6 = \{u \in B_\alpha NT_{mn} : d_u = 6\} \Rightarrow |V_6| = \frac{n}{6}(2m - 3n).$

Form Figures 1a, 2 and Table 2, the edge partition of boron α-nanotube is defined as:

$E_{3;3}(B_\alpha NT_{mn})=\{e=uv \in B_\alpha NT_{mn}: d_u=3; d_v=3\}$
$\rightarrow |E_{3;3}B_\alpha NT| = n/2,$

$E_{3;5}(B_\alpha NT_{mn})=\{e=uv \in B_\alpha NT_{mn}: d_u=3; d_v=5\}$
$\rightarrow |E_{3;5}B_\alpha NT| = n,$

$E_{3;6}(B_\alpha NT_{mn})=\{e=uv \in B_\alpha NT_{mn}: d_u=3; d_v=5\}$
$\rightarrow |E_{3;6}B_\alpha NT| = n,$

$E_{4;4}(B_\alpha NT_{mn})=\{e=uv \in B_\alpha NT_{mn}: d_u=4; d_v=5\}$
$\rightarrow |E_{4;4}B_\alpha NT| = 3n/2,$

$E_{4;5}(B_\alpha NT_{mn})=\{e=uv \in B_\alpha NT_{mn}: d_u=4; d_v=5\}$
$\rightarrow |E_{4;5}B_\alpha NT| = 2n,$

$E_{4;6}(B_\alpha NT_{mn})=\{e=uv \in B_\alpha NT_{mn}: d_u=4; d_v=6\}$
$\rightarrow |E_{4;6}B_\alpha NT| = n,$

$E_{5;5}(B_\alpha NT_{mn})=\{e=uv \in B_\alpha NT_{mn}: d_u=5; d_v=5\}$
$\rightarrow |E_{5;5}B_\alpha NT| = n/2\,(3m-8),$

$E_{5;6}(B_\alpha NT_{mn})=\{e=uv \in B_\alpha NT_{mn}: d_u=5; d_v=6\}$
$\rightarrow |E_{5;6}B_\alpha NT| = n(2m-5).$

Now, by using the definition of M-polynomial, we compute the M-polynomial of $B_\alpha NT_{mn}$

$$M(B_\alpha NT_{mn};x,y)=\sum_{\delta\le i\le j\le\Delta} m_{ij}(B_\alpha NT_{mn})x^i y^j$$
$$=\sum_{3\le i\le j\le 6} m_{ij}(B_\alpha NT_{mn})x^i y^j,$$
$$=\sum_{3\le 3} m_{33}(B_\alpha NT_{mn})x^3y^3+\sum_{3\le 5} m_{35}(B_\alpha NT_{mn})x^3y^5$$
$$+\sum_{3\le 6} m_{36}(B_\alpha NT_{mn})x^3y^6+\sum_{4\le 4} m_{44}(B_\alpha NT_{mn})x^4y^4$$
$$+\sum_{4\le 5} m_{45}(B_\alpha NT_{mn})x^4y^5+\sum_{4\le 6} m_{46}(B_\alpha NT_{mn})x^4y^6$$
$$+\sum_{5\le 5} m_{55}(B_\alpha NT_{mn})x^5y^5+\sum_{5\le 6} m_{56}(B_\alpha NT_{mn})x^5y^6,$$
$$=|E_{3,3}|x^3y^3+|E_{3,5}|x^3y^5+|E_{3,6}|x^3y^6$$
$$+|E_{4,4}|x^4y^4|E_{4,5}|x^4y^5+|E_{4,6}|x^4y^6$$
$$+|E_{5,5}|x^5y^5+|E_{5,6}|x^5y^6,$$
$$=\frac{n}{2}x^3y^3+nx^3y^5+nx^3y^6+\frac{3n}{2}x^4y^4+2nx^4y^5$$
$$+nx^4y^6+\frac{n}{2}(3m-8)x^5y^5+n(2m-5)x^5y^6.$$

Topological indices of boron $_\alpha$-nanotube

Theorem 6.1. Consider the $B_\alpha NT_{mn}$ be a boron $_\alpha$-nanotube and

$$M[B_\alpha NT_{mn};x,y]=\frac{n}{2}x^3y^3+nx^3y^5+nx^3y^6+\frac{3n}{2}x^4y^4$$
$$+2nx^4y^5+nx^4y^6+\frac{n}{2}(3m-8)x^5y^5+n(2m-5)x^5y^6,$$

Then,

$$[1.]ABC[B_\alpha NT_{mn}]=(\frac{3\sqrt{2}}{5}+\frac{\sqrt{30}}{5})mn+(\frac{1}{3}+\frac{\sqrt{10}}{5}$$
$$+\frac{\sqrt{14}}{6}+\frac{3\sqrt{6}}{8}+\frac{\sqrt{35}}{5}+\frac{\sqrt{3}}{3}-\frac{8\sqrt{2}}{5}+\frac{\sqrt{30}}{2})n,$$
$$[2.]GA[B_\alpha NT_{mn}]=(\frac{3}{2}+\frac{4\sqrt{30}}{11})mn+(\frac{\sqrt{15}}{4}$$
$$+\frac{2\sqrt{2}}{3}+\frac{8\sqrt{5}}{9}+\frac{2\sqrt{6}}{5}-\frac{10\sqrt{30}}{11}-2)n,$$
$$[3.]B_1[B_\alpha NT_{mn}]=97mn-97n,$$
$$[4.]B_2[B_\alpha NT_{mn}]=318mn-414n,$$
$$[5.]HB_1[B_\alpha NT_{mn}]=1349mn-1767n,$$
$$[6.]HB_2[B_\alpha NT_{mn}]=14682mn-24858n,$$
$$[7.]^m B_1[B_\alpha NT_{mn}]=\frac{692}{1365}mn-\frac{3457}{180180}n,$$
$$[8.]^m B_2[B_\alpha NT_{mn}]=\frac{169}{1080}mn-\frac{629}{4320}n,$$
$$[9.]H_b[B_\alpha NT_{mn}]=\frac{1384}{1365}mn-\frac{3457}{90090}n$$

Proof. Let $M[B_\alpha NT_{mn};x,y]=f(x,y)$

The atom-bond connectivity index

$$S_y^{\frac{1}{2}}f(x,y)=\frac{n}{2\sqrt{3}}x^3y^3+\frac{n}{\sqrt{5}}x^3y^5+\frac{n}{\sqrt{6}}x^3y^6+\frac{3n}{4}x^4y^4$$
$$+\frac{2n}{\sqrt{5}}x^4y^5+\frac{n}{\sqrt{6}}x^4y^6+\frac{n}{2\sqrt{5}}(3m-8)x^5y^5+\frac{n}{\sqrt{6}}(2m-5)x^5y^6,$$
$$S_x^{\frac{1}{2}}S_y^{\frac{1}{2}}f(x,y)=\frac{n}{6}x^3y^3+\frac{n}{\sqrt{15}}x^3y^5+\frac{n}{3\sqrt{2}}x^3y^6+\frac{3n}{8}x^4y^4$$
$$+\frac{n}{\sqrt{5}}x^4y^5+\frac{n}{2\sqrt{6}}x^4y^6+\frac{n}{10}(3m-8)x^5y^5+\frac{n}{\sqrt{30}}(2m-5)x^5y^6,$$
$$JS_x^{\frac{1}{2}}S_y^{\frac{1}{2}}f(x,y)=\frac{n}{6}x^6+\frac{n}{\sqrt{15}}x^8+\frac{n}{3\sqrt{2}}x^9+\frac{3n}{8}x^8+\frac{n}{\sqrt{5}}x^9$$
$$+\frac{n}{2\sqrt{6}}x^{10}+\frac{n}{10}(3m-8)x^{10}+\frac{n}{\sqrt{30}}(2m-5)x^{11},$$
$$Q_{-2}JS_x^{\frac{1}{2}}S_y^{\frac{1}{2}}f(x,y)=\frac{n}{6}x^4+\frac{n}{\sqrt{15}}x^6+\frac{n}{3\sqrt{2}}x^7+\frac{3n}{8}x^6+\frac{n}{\sqrt{5}}x^7$$
$$+\frac{n}{2\sqrt{6}}x^8+\frac{n}{10}(3m-8)x^8+\frac{n}{\sqrt{30}}(2m-5)x^9,$$
$$D_x^{\frac{1}{2}}Q_{-2}JS_x^{\frac{1}{2}}S_y^{\frac{1}{2}}f(x,y)=\frac{n}{3}x^4+\frac{\sqrt{6}n}{\sqrt{15}}x^6+\frac{\sqrt{7}n}{3\sqrt{2}}x^7+\frac{3\sqrt{6}n}{8}x^6$$
$$+\frac{\sqrt{7}n}{\sqrt{5}}x^7+\frac{\sqrt{8}n}{2\sqrt{6}}x^8+\frac{2\sqrt{2}n}{10}(3m-8)x^8+\frac{3n}{\sqrt{30}}(2m-5)x^9,$$
$$A[B_\alpha NT_{mn}]=D_x^{\frac{1}{2}}Q_{-2}JS_x^{\frac{1}{2}}S_y^{\frac{1}{2}}[f(x,y)]_{x=1},=(\frac{3\sqrt{2}}{5}+\frac{\sqrt{30}}{5})mn$$
$$+(\frac{1}{3}+\frac{\sqrt{10}}{5}+\frac{\sqrt{14}}{6}+\frac{3\sqrt{6}}{8}+\frac{\sqrt{35}}{5}+\frac{\sqrt{3}}{3}-\frac{8\sqrt{2}}{5}+\frac{\sqrt{30}}{2})n.$$

The geometric arithmetic index

$$D_y^{\frac{1}{2}}[f(x,y)]=\frac{\sqrt{3}n}{2}x^3y^3+\sqrt{5}nx^3y^5+\sqrt{6}nx^3y^6+3nx^4y^4$$
$$+2\sqrt{5}nx^4y^5+\sqrt{6}nx^4y^6+\frac{\sqrt{5}n}{2}(3m-8)x^5y^5+\sqrt{6}n(2m-5)x^5y^6,$$
$$D_x^{\frac{1}{2}}D_y^{\frac{1}{2}}[f(x,y)]=\frac{3n}{2}x^3y^3+\sqrt{15}nx^3y^5+3\sqrt{2}nx^3y^6+6nx^4y^4$$
$$+4\sqrt{5}nx^4y^5+2\sqrt{6}nx^4y^6+\frac{5n}{2}(3m-8)x^5y^5+\sqrt{30}n(2m-5)x^5y^6,$$
$$JD_x^{\frac{1}{2}}D_y^{\frac{1}{2}}[f(x,y)]=\frac{3n}{2}x^6+\sqrt{15}nx^8+3\sqrt{2}nx^9+6nx^8+4\sqrt{5}nx^9$$
$$+2\sqrt{6}nx^{10}+\frac{5n}{2}(3m-8)x^{10}+\sqrt{30}n(2m-5)x^{11},$$
$$S_xJD_x^{\frac{1}{2}}D_y^{\frac{1}{2}}[f(x,y)]=\frac{n}{4}x^6+\frac{\sqrt{15}n}{8}x^8+\frac{\sqrt{2}n}{3}x^9+\frac{3n}{4}x^8$$
$$+\frac{4\sqrt{5}n}{9}x^9+\frac{\sqrt{6}n}{5}x^{10}+\frac{n}{4}(3m-8)x^{10}+\frac{\sqrt{30}n}{11}(2m-5)x^{11},$$
$$2S_xJD_x^{\frac{1}{2}}D_y^{\frac{1}{2}}[f(x,y)]=\frac{n}{2}x^6+\frac{\sqrt{15}n}{4}x^8+\frac{2\sqrt{2}n}{3}x^9+\frac{3n}{2}x^8$$
$$+\frac{8\sqrt{5}n}{9}x^9+\frac{2\sqrt{6}n}{5}x^{10}+\frac{n}{2}(3m-8)x^{10}+\frac{2\sqrt{30}n}{11}(2m-5)x^{11},$$
$$GA[B_\alpha NT]=2S_xJD_x^{\frac{1}{2}}D_y^{\frac{1}{2}}[f(x,y)]_{x=1},=(\frac{3}{2}+\frac{4\sqrt{30}}{11})mn$$
$$+(\frac{\sqrt{15}}{4}+\frac{2\sqrt{2}}{3}+\frac{8\sqrt{5}}{9}+\frac{2\sqrt{6}}{5}-\frac{10\sqrt{30}}{11}-2)n.$$

The first K Banhatti index

$$D_x f(x,y)=\frac{3n}{2}x^3y^3+3nx^3y^5+3nx^3y^6+6nx^4y^4+8nx^4y^5$$
$$+4nx^4y^6+\frac{5n}{2}(3m-8)x^5y^5+5n(2m-5)x^5y^6,$$
$$D_y f(x,y)=\frac{3n}{2}x^3y^3+5nx^3y^5+6nx^3y^6+6nx^4y^4+10nx^4y^5$$
$$+6nx^4y^6+\frac{5n}{2}(3m-8)x^5y^5+6n(2m-5)x^5y^6,$$
$$(D_x+D_y)f(x,y)=3nx^3y^3+8nx^3y^5+9nx^3y^6+12nx^4y^4$$
$$+18nx^4y^5+10nx^4y^6+5n(3m-8)x^5y^5+11n(2m-5)x^5y^6,$$
$$(D_x+D_y)f(x,y)_{x=y=1}=37mn-35n,$$
$$Jf(x,y)=f(x,x)=\frac{n}{2}x^6+nx^8+nx^9+\frac{3n}{2}x^8+2nx^9$$
$$+nx^{10}+\frac{n}{2}(3m-8)x^{10}+n(2m-5)x^{11},$$
$$Q_{-2}Jf(x,y)=\frac{n}{2}x^4+nx^6+nx^7+\frac{3n}{2}x^6+2nx^7+nx^8$$
$$+\frac{n}{2}(3m-8)x^8+n(2m-5)x^9,$$
$$D_xQ_{-2}Jf(x,y)=2nx^4+6nx^6+7nx^7+9nx^6+14nx^7$$
$$+8nx^8+4n(3m-8)x^8+9n(2m-5)x^9,$$
$$2D_xQ_{-2}Jf(x,y)=4nx^4+12nx^6+14nx^7+18nx^6$$
$$+28nx^7+16nx^8+8n(3m-8)x^8+18n(2m-5)x^9,$$
$$2D_xQ_{-2}Jf(x,y)_{x=1}=60mn-62n,$$
$$B_1[B_\alpha NT_{mn}]=(D_x+D_y+2D_xQ_{-2}J)[f(x,y)]_{x=y=1},$$
$$B_1[B_\alpha NT_{mn}]=97mn-97n.$$

The second K Banhatti index

$$J(D_x+D_y)f(x,y)=3nx^6+8nx^8+9nx^9+12nx^8+18nx^9$$
$$+10nx^{10}+5n(3m-8)x^{10}+11n(2m-5)x^{11},$$
$$Q_{-2}J(D_x+D_y)f(x,y)=3nx^4+8nx^6+9nx^7+12nx^6$$
$$+18nx^7+10nx^8+5n(3m-8)x^8+11n(2m-5)x^9,$$
$$D_xQ_{-2}J(D_x+D_y)f(x,y)=12nx^4+48nx^6+63nx^7+72nx^6$$
$$+126nx^7+80nx^8+40n(3m-8)x^8+99n(2m-5)x^9,$$
$$B_2[B_\alpha NT_{mn}]=D_xQ_{-2}J(D_x+D_y)[f(x,y)]_{x=1},$$
$$B_1[B_\alpha NT_{mn}]=318mn-414n.$$

The first K hyper Banhatti index

$$D_x^2 f(x,y)=\frac{9n}{2}x^3y^3+9nx^3y^5+9nx^3y^6+24nx^4y^4+32nx^4y^5$$
$$+16nx^4y^6+\frac{25n}{2}(3m-8)x^5y^5+25n(2m-5)x^5y^6,$$
$$D_x^2 f(x,y)_{x=y=1}=\frac{175}{2}mn-\frac{261}{2}n,$$
$$D_y^2 f(x,y)=\frac{9n}{2}x^3y^3+25nx^3y^5+36nx^3y^6+24nx^4y^4$$
$$+50nx^4y^5+36nx^4y^6+\frac{25n}{2}(3m-8)x^5y^5+36n(2m-5)x^5y^6,$$
$$D_y^2 f(x,y)_{x=y=1}=\frac{219}{2}mn-\frac{209}{2}n,$$
$$D_x^2Q_{-2}Jf(x,y)=8nx^4+36nx^6+49nx^7+54nx^6+98nx^7$$
$$+64nx^8+32n(3m-8)x^8+81n(2m-5)x^9,$$
$$2D_x^2Q_{-2}Jf(x,y)=16nx^4+72nx^6+98nx^7+108nx^6+196nx^7$$
$$+128nx^8+64n(3m-8)x^8+162n(2m-5)x^9,$$
$$2D_x^2Q_{-2}Jf(x,y)_{x=1}=516mn-704n,$$
$$2D_xQ_{-2}J(D_x+D_y)f(x,y)=24nx^4+96nx^6+126nx^7+144nx^6$$
$$+252nx^7+160nx^8+80n(3m-8)x^8+198n(2m-5)x^9,$$
$$2D_xQ_{-2}J(D_x+D_y)[f(x,y)]_{x=1}=636mn-828n,$$
$$HB_1[B_\alpha NT_{mn}]=(D_x^2+D_y^2+2D_x^2Q_{-2}J+2D_xQ_{-2}J(D_x+D_y))[f(x,y)]_{x=y=1},$$
$$HB_1[B_\alpha NT_{mn}]=1349mn-1767n.$$

The second K hyper Banhatti index

$$(D_x^2+D_y^2)f(x,y)=9nx^3y^3+34nx^3y^5+45nx^3y^6+48nx^4y^4$$
$$+82nx^4y^5+52nx^4y^6+25n(3m-8)x^5y^5+61n(2m-5)x^5y^6,$$
$$J(D_x^2+D_y^2)f(x,y)=9nx^6+34nx^8+45nx^9+48nx^8$$
$$+82nx^9+52nx^{10}+25n(3m-8)x^{10}+61n(2m-5)x^{11},$$
$$Q_{-2}J(D_x^2+D_y^2)f(x,y)=9nx^4+34nx^6+45nx^7+48nx^6$$
$$+82nx^7+52nx^8+25n(3m-8)x^8+61n(2m-5)x^9,$$
$$D_x^2Q_{-2}J(D_x^2+D_y^2)f(x,y)=144nx^4+1224nx^6+2205nx^7+1728nx^6$$
$$+4018nx^7+3328nx^8+1600n(3m-8)x^8+4941n(2m-5)x^9,$$
$$HB_2[B_\alpha NT_{mn}]=D_x^2Q_{-2}J(D_x^2+D_y^2)[f(x,y)]_{x=1},=14682mn-24858n.$$

Modified first K Banhatti index

$$L_x f(x,y)=\frac{n}{2}x^6y^3+nx^6y^5+nx^6y^6+\frac{3n}{2}x^8y^4+2nx^8y^5$$
$$+nx^8y^6+\frac{n}{2}(3m-8)x^{10}y^5+n(2m-5)x^{10}y^6,$$
$$L_y f(x,y)=\frac{n}{2}x^3y^6+nx^3y^{10}+nx^3y^{12}+\frac{3n}{2}x^4y^8+2nx^4y^{10}$$
$$+nx^4y^{12}+\frac{n}{2}(3m-8)x^5y^{10}+n(2m-5)x^5y^{12},$$
$$J(L_x+L_y)f(x,y)=\frac{n}{2}x^9+nx^{11}+nx^{12}+\frac{3n}{2}x^{12}+2nx^{13}$$
$$+nx^{14}+\frac{n}{2}(3m-8)x^{15}+n(2m-5)x^{16}+\frac{n}{2}x^9+nx^{13}$$
$$+nx^{15}+\frac{3n}{2}x^{12}+2nx^{14}+nx^{16}+\frac{n}{2}(3m-8)x^{15}+n(2m-5)x^{17},$$
$$Q_{-2}J(L_x+L_y)f(x,y)=\frac{n}{2}x^7+nx^9+nx^{10}+\frac{3n}{2}x^{10}$$
$$+2nx^{11}+nx^{12}+\frac{n}{2}(3m-8)x^{13}+n(2m-5)x^{14}$$
$$+\frac{n}{2}x^7+nx^{11}+nx^{13}+\frac{3n}{2}x^{10}+2nx^{12}+nx^{14}$$
$$+\frac{n}{2}(3m-8)x^{13}+n(2m-5)x^{15},$$

$$S_xQ_{-2}J(L_x+L_y)f(x,y)=\frac{n}{14}x^7+\frac{n}{9}x^9+\frac{n}{10}x^{10}$$
$$+\frac{3n}{20}x^{10}+\frac{2n}{11}x^{11}+\frac{n}{12}x^{12}+\frac{n}{26}(3m-8)x^{13}$$
$$+\frac{n}{14}(2m-5)x^{14}+\frac{n}{14}x^7+\frac{n}{11}x^{11}+\frac{n}{13}x^{13}+\frac{3n}{20}x^{10}$$
$$+\frac{n}{6}x^{12}+\frac{n}{14}x^{14}+\frac{n}{26}(3m-8)x^{13}+\frac{n}{15}(2m-5)x^{15},$$
$${}^{m}B_1[B_\alpha NT_{mn}]=S_xQ_{-2}J(L_x+L_y)[f(x,y)]_{x=1},$$
$${}^{m}B_1[B_\alpha NT_{mn}]=\frac{692}{1365}mn+\frac{3457}{180180}n.$$

Modified second K Banhatti index

$$S_xf(x,y)=\frac{n}{6}x^3y^3+\frac{n}{3}x^3y^5+\frac{n}{3}x^3y^6+\frac{3n}{8}x^4y^4+\frac{n}{2}x^4y^5$$
$$+\frac{n}{4}x^4y^6+\frac{n}{10}(3m-8)x^5y^5+\frac{n}{5}(2m-5)x^5y^6,$$
$$S_yf(x,y)=\frac{n}{6}x^3y^3+\frac{n}{5}x^3y^5+\frac{n}{6}x^3y^6+\frac{3n}{8}x^4y^4+\frac{2n}{5}x^4y^5$$
$$+\frac{n}{6}x^4y^6+\frac{n}{10}(3m-8)x^5y^5+\frac{n}{6}(2m-5)x^5y^6,$$
$$(S_x+S_y)f(x,y)=\frac{n}{3}x^3y^3+\frac{8n}{15}x^3y^5+\frac{n}{2}x^3y^6+\frac{3n}{4}x^4y^4$$
$$+\frac{9n}{10}x^4y^5+\frac{5n}{12}x^4y^6+\frac{n}{5}(3m-8)x^5y^5+\frac{11n}{30}(2m-5)x^5y^6,$$
$$J(S_x+S_y)f(x,y)=\frac{n}{3}x^6+\frac{8n}{15}x^8+\frac{n}{2}x^9+\frac{3n}{4}x^8+\frac{9n}{10}x^9$$
$$+\frac{5n}{12}x^{10}+\frac{n}{5}(3m-8)x^{10}+\frac{11n}{30}(2m-5)x^{11},$$
$$Q_{-2}J(S_x+S_y)f(x,y)=\frac{n}{3}x^4+\frac{8n}{15}x^6+\frac{n}{2}x^7+\frac{3n}{4}x^6$$
$$+\frac{9n}{10}x^7+\frac{5n}{12}x^8+\frac{n}{5}(3m-8)x^8+\frac{11n}{30}(2m-5)x^9,$$
$$S_xQ_{-2}J(S_x+S_y)f(x,y)=\frac{n}{12}x^4+\frac{4n}{45}x^6+\frac{n}{14}x^7+\frac{n}{8}x^6$$
$$+\frac{9n}{70}x^7+\frac{5n}{96}x^8+\frac{n}{40}(3m-8)x^8+\frac{11n}{270}(2m-5)x^9,$$
$${}^{m}B_2[B_\alpha NT_{mn}]=S_xQ_{-2}J(S_x+S_y)[f(x,y)]_{x=1},$$
$${}^{m}B_2[B_\alpha NT_{mn}]=\frac{169}{1080}mn+\frac{629}{4320}n.$$

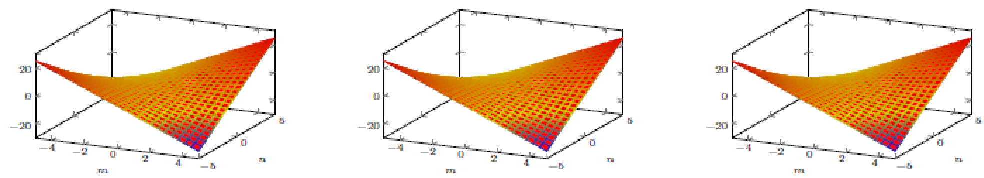
Harmonic K Banhatti index

$$2S_xQ_{-2}J(L_x+L_y)f(x,y)=\frac{n}{7}x^7+\frac{2n}{9}x^9+\frac{n}{5}x^{10}+\frac{3n}{10}x^{10}$$
$$+\frac{4n}{11}x^{11}+\frac{n}{6}x^{12}+\frac{n}{13}(3m-8)x^{13}+\frac{n}{7}(2m-5)x^{14}$$
$$+\frac{n}{7}x^7+\frac{2n}{11}x^{11}+\frac{2n}{13}x^{13}+\frac{3n}{10}x^{10}+\frac{n}{3}x^{12}+\frac{n}{7}x^{14}$$
$$+\frac{n}{13}(3m-8)x^{13}+\frac{2n}{15}(2m-5)x^{15},$$
$$H_b[B_\alpha NT_{mn}]=2S_xQ_{-2}J(L_x+L_y)[f(x,y)]_{x=1},$$
$$H_b[B_\alpha NT_{mn}]=\frac{1384}{1365}mn+\frac{3457}{90090}n.$$

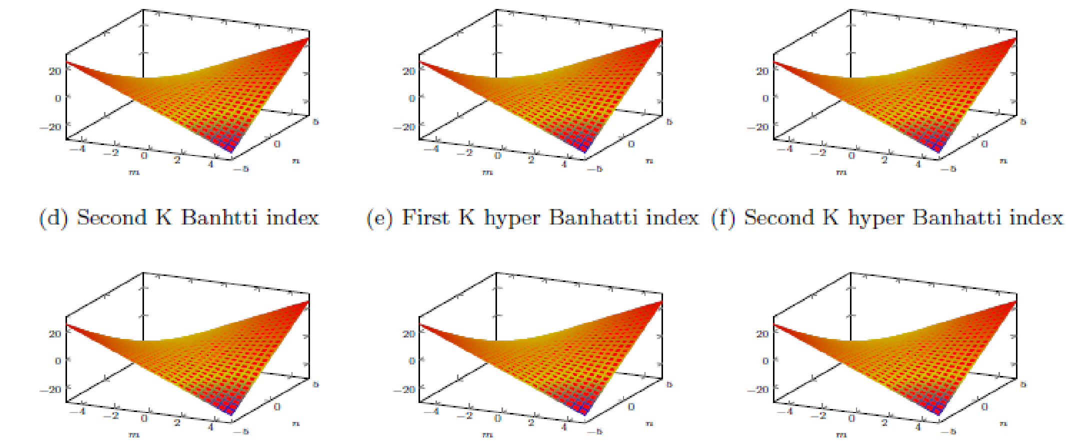
Figure 3 represents the graphically view of degree dependent topological indices of $B_\alpha NT$. These graphs show the connection between topological indices and parameters involved. Although this representations seem to be very much alike, all have different gradients.

Conclusion

In the present work, we computed *$M(B_\alpha NT_{mn};x;y)$* and with the help of this polynomial and found the various degree based topological invariants given in Table 4. Topological indices that were decoded the information were stored in the molecular structure. We also showed the behavior of M-Polynomial and topological invariants by drawing graphics. This graphical description enabled us to understand the results against the parameters.



(a) Atom-bond connectivity index (b) Geometric arithmetic index (c) First K Banhtti index



(d) Second K Banhtti index (e) First K hyper Banhatti index (f) Second K hyper Banhatti index

(g) Modified first K Banhatti index (h) Modified second K Banhatti index (i) Harmonic K Banhatti index

FIGURE 3 3D plots of topological indices of $B_{\alpha}NT_{mn}$.

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