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Analysis of K-Banhatti Polynomials and Calculation of Some Degree Based Indices Using (a, b)-Nirmala Index in Molecular Graph and Line Graph of $TUC_4C_8(S)$ Nanotube

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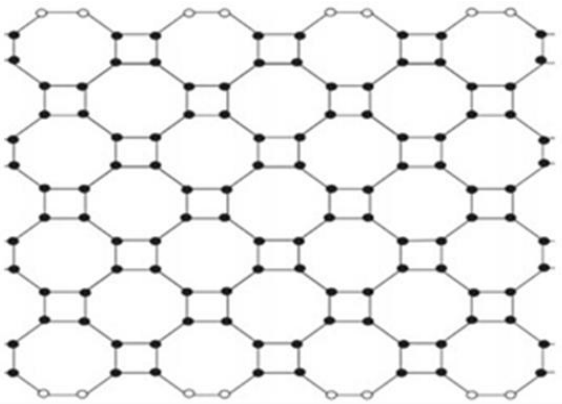
ABSTRACT

Mathematical chemistry is a branch of theoretical chemistry that studies molecular structure without considering their quantum mechanics using mathematical methods. Carbon nanotubes are a particular type of fullerenes. In this article, K-Banhatti indices are obtained with the help of K-Banhatti polynomials for the molecular graph and the line graph of the $TUC_4C_8(S)$ nanotube. Next, first, the (a, b)- Nirmala index is calculated for the molecular graph and line graph of $TUC_4C_8(S)$ nanotube, and then using them, Y-index and some topological indices are computed.

GRAPHICALABSTRACT



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Introduction

The analysis of a chemical molecular structure smaller than 100 nm is known as nanotechnology. Nanomaterials have many applications in different fields of nanoscience [1].

Carbon nanotubes (CNTs) were initially discovered in 1991 [2]. So far, much research has been done on their structure and determination of their physical and chemical properties by direct measurement and prediction methods using modelling techniques.

The production capacity of carbon nanotubes is increasing exponentially every year, and as a result, their prices are decreasing. Carbon nanotubes are structures of nanometre diameter, and their length/diameter ratio is a large number. Important features of carbon nanotubes include high young modulus, high tensile strength, high electronic current, and superconductivity (at low temperatures). Likewise, at room temperature, the thermal conductivity of nanotubes is higher than natural diamond. These properties of carbon nanotubes have led to their many applications in nanotechnology, electronics, materials science, and architecture [3].

Despite all efforts, the lack of reliable production capacity in a high volume and the high price of nanotubes have prevented the commercialization of carbon nanotube technologies.

One of the most widely used nanotubes is the $TUC_4C_8(S)$. It is a trivalent decoration made by alternating the squares C_4 and octagons C_8. Such a covering can be derived from square net by the leapfrog operation, which has attracted the attention of many scientists in the recent years due to its wide applications [3].

Ashrafi and Yousefi computed Wiener index of the $TUC_4C_8(S)$ nanotorus [4]. Loghman and Badakhshian calculated the PI polynomial of the $TUC_4C_8(S)$ nanotube and nanotorus [5].

The essential role of molecular descriptors is in mathematical chemistry. Chemical graph theory is a branch of mathematical chemistry that deals with the relationship between mathematics, chemistry, and graph theory.

By obtaining a real number called a topological index for a chemical molecule using chemical graph theory techniques, its molecular structure can be analysed through topological indices.

Figure 1 displays the molecular graph structure of the $TUC_4C_8(S)$ nanotube.

In the molecular graph, its vertices correspond to atoms, and its edges correspond to bonds. Topological indices are numerical values related to a chemical structure that describe the correlation of chemical structure with different physical properties and chemical reactions.

We represent the set of edges with E and denote the degree of vertex v by d_v. Let $d_G(e)$ denote the degree of an edge e=uv in G and $d_G(e)$ is defined by $d_G(e) = d_u + d_v - 2$.

Definition 1.1. In graph G= (V, E), the first Zagreb index is defined as follows [6]:

$$M_1(G) = \sum_{uv \in E(G)} [d_u + d_v].$$

Definition 1.2. The Y-index of a graph G defines as [7]:

$$Y(G) = \sum_{uv \in E(G)} [d_u^3 + d_v^3].$$

Definition 1.3. The Nirmala index and the $(a,b)-$ Nirmala index for graph G are defined as [1, 2]:

$$N(G) = \sum_{uv \in E(G)} \sqrt{d_u + d_v},$$

$$N_{(a,b)}(G) = \sum_{uv \in E(G)} \left(\frac{d_u^{\,a} + d_v^{\,a}}{2}\right)^b.$$

Definition 1.4. The first and the second K-Banhatti indices for graph G are defined as [8]:

$$B_1(G) = \sum_{ue} [d_u + d_G(e)], \quad B_2(G) = \sum_{ue} d_u d_G(e),$$

Where, ue means that the vertex u and edge e are incident in G.

Definition 1.5. The first and the second K-Banhatti polynomials for graph G are defined as [8]:

$$KB_1(G, x) = \sum_{ue} x^{d_u + d_G(e)}, \quad KB_2(G, x) = \sum_{ue} x^{d_u \cdot d_G(e)}.$$

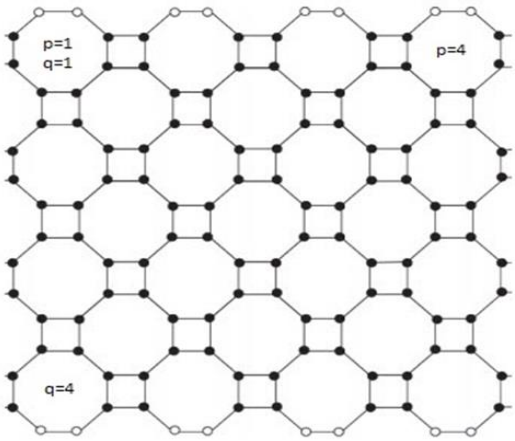

Figure 1: The graph structure of the $TUC_4C_8(S)$ nanotube

Table 1: Topological indices definitions and relationships between them and (a, b)-Nirmala index.

Topological index	Topological index definition	Relationship between topological index and (a, b)-Nirmala
First Zagreb index	$M_1(G)=\sum_{uv\in E(G)}(d_u+d_v)$	$N_{1,1}(G)=\frac{1}{2}M_1(G)$
Sombor index [10]	$SO(G)=\sum_{uv\in E(G)}\sqrt{d_u^2+d_v^2}$	$N_{2,\frac{1}{2}}(G)=\frac{1}{\sqrt{2}}SO(G)$
Harmonic index [11]	$H(G)=\sum_{uv\in E(G)}\frac{2}{d_u+d_v}$	$N_{1,-1}(G)=H(G)$
Sum connectivity index [12]	$SCI(G)=\sum_{uv\in E(G)}\frac{1}{\sqrt{d_u+d_v}}$	$N_{1,-\frac{1}{2}}(G)=\sqrt{2}SCI(G)$
Inverse sum indeg index [13]	$ISI(G)=\sum_{uv\in E(G)}\frac{d_ud_v}{d_u+d_v}$	$N_{-1,-1}(G)=2ISI(G)$
Nirmala index [14]	$N(G)=\sum_{uv\in E(G)}\sqrt{d_u+d_v}$	$N_{1,\frac{1}{2}}(G)=\frac{1}{\sqrt{2}}N(G)$

Table 2: Number of edges in the molecular graph of the $TUC_4C_8(S)$ nanotube

Edge type	Number of edges	$d_G(e)$
E_1'	2p	2
E_2'	4p	3
E_3'	2p(6q-4)	4

Some topological indices of graph G can be obtained from the (a, b)$^{-}$ Nirmala index (Table 1) by assigning specific values to the parameters a and b [9].

Definition 1.6. In a non-empty graph G, if each edge is considered as a vertex and the two vertices are connected, if the corresponding edges of the two vertices are adjacent to G, the resulting graph

is denoted by L(G) and is called the line graph of G [15].

In this article, we compute K-Banhatti polynomials and (a, b)¯ Nirmala index for the $TUC_4C_8(S)$ and its line graph. In the next section, we compute K-Banhatti indices and find some new relationship between (a, b)¯ Nirmala index and Y-index.

Main results

The molecular graph of the $TUC_4C_8(S)$ nanotube is denoted by G, its line graph by L(G). There are three types of edges in $TUC_4C_8(S)$ nanotube as follows:

$$E_1^{'} = \{(d_u, d_v) | uv \in E(\mathrm{G}), \mathrm{d}_u = 2, d_v = 2\},$$

$$E_2^{'} = \{(d_u, d_v) | uv \in E(\mathrm{G}), \mathrm{d}_u = 2, d_v = 3\},$$

$$E_3^{'} = \{(d_u, d_v) | uv \in E(\mathrm{G}), \mathrm{d}_u = 3, d_v = 3\}.$$

$$|E| = |E_1^{'}| + |E_2^{'}| + |E_3^{'}| = 2p + 4p + 2p(6q-4) = 12pq - 2p.$$

The status of the rows and columns in the line graph of the $TUC_4C_8(S)$ nanotube is depicted in Figure 2. p and q represent the number of octagons in each row and column of the line graph, respectively.

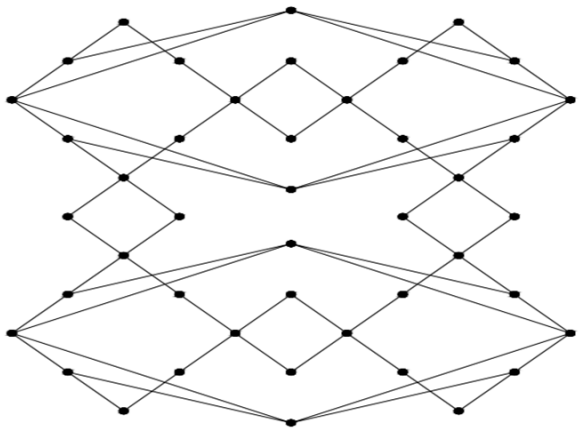

Figure 2: The line graph of $TUC_4C_8(S)$ nanotube for p=q=2

There are five types of edges in the line graph of the TUC_4C_8 (S) nanotube as follows:

$$E_1 = \{(d_u, d_v) | uv \in E(\mathrm{L(G)}), \mathrm{d}_u = 2, d_v = 2\},$$

$$E_2 = \{(d_u, d_v) | uv \in E(\mathrm{L(G)}), \mathrm{d}_u = 2, d_v = 3\},$$

$$E_3 = \{(d_u, d_v) | uv \in E(\mathrm{L(G)}), \mathrm{d}_u = 2, d_v = 4\},$$

$$E_4 = \{(d_u, d_v) | uv \in E(\mathrm{L(G)}), \mathrm{d}_u = 3, d_v = 4\},$$

$$E_5 = \{(d_u, d_v) | uv \in E(\mathrm{L(G)}), \mathrm{d}_u = 4, d_v = 4\}.$$

Table 3: Number of edges in the line graph of TUC_4C_8 (S) nanotube

Edge type	Number of edges	$d_G(e)$
E_1	4(p-1)	2
E_2	4	3
E_3	4[4pq-3q-2p+1]	4
E_4	12q-4	5
E_5	4q	6

As a result, the number of edges and vertices in the line graph of the TUC_4C_8 (S) nanotube is equal to:

$$|E(L(G))| = 4(p-1)+4+4(4pq-3q-2p+1)+12q-4+4q$$
$$=16pq-4p+4q.$$

Theorem 2.1. Let G be the graph of the TUC_4C_8 (S) nanotube. Then, the first and the second K-Banhatti polynomials of G are as follows:

$$KB_1(G,\mathrm{x}) = 2p\,x^8 + 4px^{11} + 2p\left(6q-4\right)x^{14},$$
$$KB_2(G,\mathrm{x}) = 2p\,x^8 + 4px^{15} + 2p\left(6q-4\right)x^{24}.$$

Proof

$$KB_1(G,\mathrm{x}) = \sum_{ue} x^{d_u+d_G(e)} = \sum_{uv\in E(G)} x^{(d_u+d_G(e))+(d_v+d_G(e))}$$
$$= (2p)x^{[(2+2)+(2+2)]} + (4p)x^{[(2+3)+(3+3)]} + (2p\left(6q-4\right))x^{[(3+4)+(3+4)]}$$
$$= 2p\,x^8 + 4px^{11} + 2p\left(6q-4\right)x^{14},$$
$$KB_2(G,\mathrm{x}) = \sum_{ue} x^{d_u.d_G(e)} = \sum_{uv\in E(G)} x^{(d_u.d_G(e))+(d_v.d_G(e))}$$
$$= (2p)x^{[(2\times2)+(2\times2)]} + (4p)x^{[(2\times3)+(3\times3)]} + (2p\left(6q-4\right))x^{[(3\times4)+(3\times4)]}$$
$$= 2p\,x^8 + 4px^{15} + 2p\left(6q-4\right)x^{24}.$$

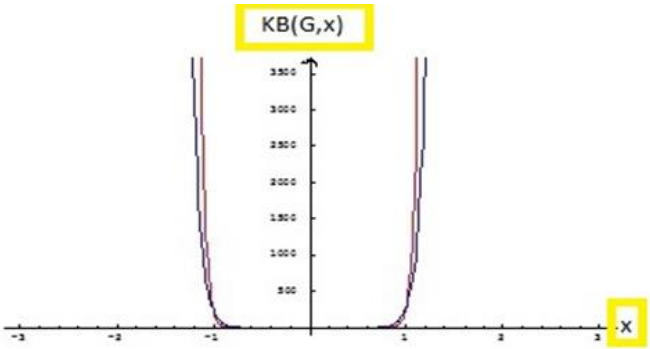

Figure 3: The behavior of the first and the second K-Banhatti polynomials, with Blue and Red, respectively, in the molecular graph of the TUC_4C_8 (S) nanotube for p=q=10

Theorem 2.2. Consider G be the graph of the TUC_4C_8 (S) nanotube. Then, we have

$$KB_1(G) = 168pq - 52p,$$
$$KB_2(G) = 288pq - 116p.$$

Proof

$$KB_1(G) = \left.\frac{\partial KB_1(G,x)}{\partial x}\right|_{x=1} = 8(2p)+11(4p)+14(2p\left(6q-4\right))$$
$$=16p+44p+168pq-112p = 168pq-52p,$$
$$KB_2(G) = \left.\frac{\partial KB_2(G,x)}{\partial x}\right|_{x=1} = 8(2p)+15(4p)+24(2p\left(6q-4\right))$$
$$=16p+60p+288pq-192p = 288pq-116p.$$

Theorem 2.3. Suppose L(G) be the line graph of the TUC_4C_8 (S) nanotube. Then, we have

$$KB_1(\mathrm{L}(G),\mathrm{x}) = 4(p-1)x^8 + 4x^{11} + 4[4pq-3q-2p+1]x^{14} + (12q-4)x^{17} + 4qx^{20},$$
$$KB_2(\mathrm{L}(G),\mathrm{x}) = 4(p-1)x^8 + 4x^{15} + 4[4pq-3q-2p+1]x^{24} + (12q-4)x^{35} + 4qx^{48}.$$

Proof

$$\begin{aligned}
KB_1(G,\mathrm{x}) &= \sum_{ue} x^{d_u+d_G(e)} = \sum_{uv\in E(G)} x^{(d_u+d_G(e))+(d_v+d_G(e))} \\
&= (4(p-1))x^{[(2+2)+(2+2)]} + (4)x^{[(2+3)+(3+3)]} + (4[4pq-3q-2p+1])x^{[(2+4)+(4+4)]} \\
&+ (12q-4)x^{[(3+5)+(4+5)]} + (4q)x^{[(4+6)+(4+6)]} \\
&= 4(p-1)x^8 + 4x^{11} + 4[4pq-3q-2p+1]x^{14} + (12q-4)x^{17} + 4qx^{20}, \\
KB_2(G,\mathrm{x}) &= \sum_{ue} x^{d_u.d_G(e)} = \sum_{uv\in E(G)} x^{(d_u.d_G(e))+(d_v.d_G(e))} \\
&= (4(p-1))x^{[(2\times2)+(2\times2)]} + (4)x^{[(2\times3)+(3\times3)]} + (4[4pq-3q-2p+1])x^{[(2\times4)+(4\times4)]} \\
&+ (12q-4)x^{[(3\times5)+(4\times5)]} + (4q)x^{[(4\times6)+(4\times6)]} \\
&= 4(p-1)x^8 + 4x^{15} + 4[4pq-3q-2p+1]x^{24} + (12q-4)x^{35} + 4qx^{48}.
\end{aligned}$$

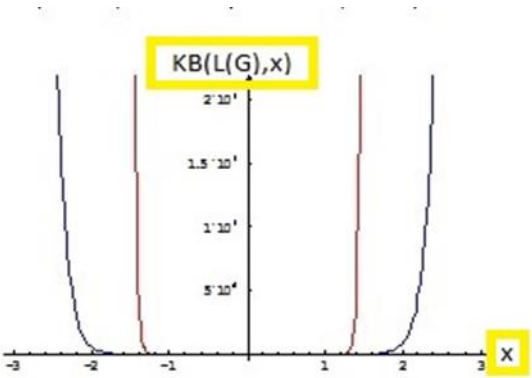

Figure 4: The behaviour of the first and second K-Banhatti polynomials, with Blue and Red, respectively, in the line graph of the TUC_4C_8 (S) nanotube for p=q=10

Theorem 2.4: Let L(G) be the line graph of the TUC_4C_8 (S) nanotube. Then the K-Banhatti indices of L(G) are as follows,

$$KB_1(\mathrm{L}(G)) = 224pq + 80p + 116q,$$
$$KB_2(\mathrm{L}(G)) = 384pq - 160p + 324q - 16.$$

Proof

$$\begin{aligned}
KB_1(\mathrm{L}(G)) &= \left.\frac{\partial KB_1(\mathrm{L}(G),x)}{\partial x}\right|_{x=1} \\
&= 8(4(p-1)) + 44 + 14(4[4pq-3q-2p+1]) + 17(12q-4) + 20(4q) \\
&= 32p - 32 + 44 + 224pq - 168q - 112p + 56 + 204q - 68 + 80q \\
&= 224pq - 80p + 116q,
\end{aligned}$$

$$KB_2(\mathrm{L}(G)) = \left.\frac{\partial KB_2(\mathrm{L}(G),x)}{\partial x}\right|_{x=1}$$
$$= 8(4(p-1)) + 60 + 24(4[4pq-3q-2p+1]) + 35(12q-4) + 48(4q)$$
$$= 32p - 32 + 60 + 384pq - 288q - 192p + 96 + 420q - 140 + 192q$$
$$= 384pq - 160p + 324q - 16.$$

Remark 2.5. Let $N_{a,b}(G)$ be the (a, b)$^-$ Nirmala index for the graph G. Then, Y-index of G is computed as follow:
$Y(G) = 2N_{3,1}$.

Proof.
According to definition 1.2, it is clear.

Theorem 2.6. Let (G) be the molecular graph of the TUC_4C_8 (S) nanotube. Then, (a, b)$^-$ Nirmala index of G is computed as follow:

$$N_{a,b}(G) = 2^{ab+1}p + (4p)(\frac{2^a+3^a}{2})^b + (2p(6q-4))3^{ab}.$$

Proof.

$$N_{(a,b)}(G) = \sum_{uv\in E(G)}(\frac{d_u{}^a + d_v{}^a}{2})^b = (2p)(\frac{2^a+2^a}{2})^b + (4p)(\frac{2^a+3^a}{2})^b + (2p(6q-4))(\frac{3^a+3^a}{2})^b$$
$$= 2^{ab+1}p + (4p)(\frac{2^a+3^a}{2})^b + (2p(6q-4))3^{ab}.$$

Corollary 2.7. Let $N_{a,b}$ be the (a, b)$^-$ Nirmala index of the TUC_4C_8 (S) nanotube. Then,

1. $\mathrm{M_1(G)} = 72pq - 20p$,
2. $\mathrm{SO(G)} = (4\sqrt{13} - 20\sqrt{2})p + 36\sqrt{2}pq$,
3. $\mathrm{H(G)} = -\frac{16}{15}p + 4pq$,
4. $\mathrm{SCI(G)} = (\frac{15+12\sqrt{5}-40\sqrt{3}}{15})p + 4\sqrt{3}pq$
5. $\mathrm{ISI(G)} = -\frac{62}{5}p + 36pq$,
6. $\mathrm{N(G)} = (4+4\sqrt{5}-8\sqrt{6})p + 12\sqrt{6}pq$,
7. $Y(\mathrm{G}) = -114p + 324pq$.

Proof

1. $\mathrm{M_1(G)} = 2N_{1,1}(G) = 2[2^{1+1}p + (4p)(\frac{2^1+3^1}{2})^1 + (2p(6q-4))3^1] = 72pq - 20p$,

2. $\mathrm{SO(G)} = \sqrt{2}N_{2,\frac{1}{2}}(G) = \sqrt{2}[2^{1+1}p + (4p)(\frac{2^2+3^2}{2})^{\frac{1}{2}} + (2p(6q-4))3^1]$
$$= \sqrt{2}[4\mathrm{p} + (4\mathrm{p})\sqrt{\frac{13}{2}} + 6p(6q-4)] = 4\sqrt{2}p + 4\sqrt{13}p + 36\sqrt{2}pq - 24\sqrt{2}p$$
$$= (4\sqrt{13} - 20\sqrt{2})p + 36\sqrt{2}pq,$$

3. $\mathrm{H(G)} = N_{1,-1}(G) = (4p)(\frac{2+3}{2})^{-1} + (2p(6q-4))3^{-1} = \frac{8}{5}p + 4pq - \frac{8}{3}p = -\frac{16}{15}p + 4pq$,

4. $\mathrm{SCI(G)} = \frac{\sqrt{2}}{2}N_{1,-\frac{1}{2}}(G) = \frac{\sqrt{2}}{2}[\sqrt{2}p + (4p)(\sqrt{\frac{2}{5}}) + (2p(6q-4))\frac{1}{\sqrt{3}}]$
$$= \mathrm{p} + \frac{4\sqrt{5}}{5}p + 4\sqrt{3}pq - \frac{8\sqrt{3}}{3}p = (1 + \frac{4\sqrt{5}}{5} - \frac{8\sqrt{3}}{3})p + 4\sqrt{3}pq$$
$$= (\frac{15+12\sqrt{5}-40\sqrt{3}}{15})p + 4\sqrt{3}pq,$$

$$5.\mathrm{ISI(G)} = \frac{1}{2}N_{-1,-1}(G) = \frac{1}{2}[2^2 p + (4p)(\frac{2^{-1}+3^{-1}}{2})^{-1} + (2p(6q-4))3]$$
$$= 2\mathrm{p} + \frac{48}{5}p + 36pq - 24p = -\frac{62}{5}p + 36pq,$$

$$6.\mathrm{N(G)} = \sqrt{2}N_{1,\frac{1}{2}}(G) = \sqrt{2}[2\sqrt{2}p + (4p)(\sqrt{\frac{5}{2}}) + (2p(6q-4))\sqrt{3}]$$
$$= 4\mathrm{p} + 4\sqrt{5}p + 12\sqrt{6}pq - 8\sqrt{6}p = (4+4\sqrt{5}-8\sqrt{6})p + 12\sqrt{6}pq,$$

$$7.Y(\mathrm{G}) = 2N_{3,1} = 2[2^4 p + (4p)(\frac{2^3+3^3}{2}) + (2p(6q-4))3^3]$$
$$= 32\mathrm{p} + 70\mathrm{p} + 324pq - 216p = -114p + 324pq.$$

Theorem 2.8. Let L(G) be the line graph of the TUC_4C_8 (S) nanotube. Then, (a, b)$^-$ Nirmala index of L(G) is as follows:

$$N_{a,b}(\mathrm{L}(G)) = 2^{ab+2}(p-1) + 4(\frac{2^a+3^a}{2})^b + (4[4pq-3q-2p+1])(\frac{2^a+4^a}{2})^b$$
$$+ (12q-4)((\frac{3^a+4^a}{2})^b) + (4q)4^{ab}.$$

Proof

$$N_{(a,b)}(L(G)) = \sum_{uv \in E(L(G))} (\frac{d_u{}^a + d_v{}^a}{2})^b$$
$$= (4(p-1))((\frac{2^a+2^a}{2})^b) + 4((\frac{2^a+3^a}{2})^b) + (4[4pq-3q-2p+1])((\frac{2^a+4^a}{2})^b)$$
$$+ (12q-4)((\frac{3^a+4^a}{2})^b) + (4q)((\frac{4^a+4^a}{2})^b)$$
$$= 2^{ab+2}(p-1) + 4(\frac{2^a+3^a}{2})^b + (4[4pq-3q-2p+1])(\frac{2^a+4^a}{2})^b$$
$$+ (12q-4)((\frac{3^a+4^a}{2})^b) + (4q)4^{ab}.$$

Corollary 2.9. Let L(G) be the line graph of the TUC_4C_8 (S) nanotube and $N_{a,b}$ be the (a, b)$^-$ Nirmala index of L(G). Then,

$$1.\mathrm{M_1(L(G))} = 96pq - 32p + 44q,$$
$$2.\mathrm{SO(L(G))} = 32\sqrt{5}pq + (8\sqrt{2}-16\sqrt{5})p + (-24\sqrt{5}+60+16\sqrt{2})q - 8\sqrt{2} + 4\sqrt{13} + 8\sqrt{5} - 20,$$
$$3.\mathrm{H(L(G))} = \frac{16}{3}pq - \frac{2}{3}p + \frac{3}{7}q - \frac{8}{120},$$
$$4.\mathrm{SCI(L(G))} = \frac{16\sqrt{6}}{6}pq + \frac{-8\sqrt{6}+12}{6}p + (\frac{-84\sqrt{6}+72+42\sqrt{2}}{42})\mathrm{q} + \frac{140\sqrt{6}+168\sqrt{5}+300}{210},$$
$$5.\mathrm{ISI(L(G))} = \frac{64}{3}\mathrm{pq} - \frac{20}{3}\mathrm{p} + \frac{88}{7}\mathrm{q} - \frac{76}{105},$$

$6.\mathrm{N(L(G))} = 16\sqrt{6}\,\mathrm{pq} + (4-8\sqrt{6})p + (-12\sqrt{6}+12\sqrt{7}+8\sqrt{2})q + 4\sqrt{5}+4\sqrt{6}-4\sqrt{7}-4,$

$7.Y(\mathrm{L(G)}) = 1152pq - 521p + 740q.$

Proof.

$$1.\mathrm{M_1(L(G))} = 2N_{1,1}(\mathrm{L}(G)) = 2[2^{1+2}(p-1) + 4(\frac{2+3}{2}) + (4[4pq-3q-2p+1])(\frac{2+4}{2})$$

$$+(12q-4)((\frac{3+4}{2}))+(4q)4\ ]$$

$$= 2[8(\mathrm{p}-1)+10+12[4pq-3q-2p+1]+\frac{7}{2}(12q-4)+16\mathrm{q}]$$

$$= 16\mathrm{p}-16+20+96pq-72q-48p+24+84q-28+32q$$

$$= 96pq-32p+44q,$$

$$2.\mathrm{SO(L(G))} = \sqrt{2}N_{2,\frac{1}{2}}(\mathrm{L}(G)) = \sqrt{2}[2^{1+2}(p-1)+4(\frac{2^2+3^2}{2})^{\frac{1}{2}} + (4[4pq-3q-2p+1])(\frac{2^2+4^2}{2})^{\frac{1}{2}}$$

$$+(12q-4)((\frac{3^2+4^2}{2})^{\frac{1}{2}})+(4q)4^1]$$

$$= 8\sqrt{2}(p-1)+4\sqrt{13}+\sqrt{20}(4[4pq-3q-2p+1])+5(12q-4)+16\sqrt{2}q$$

$$= 8\sqrt{2}p-8\sqrt{2}+4\sqrt{13}+16\sqrt{20}pq-12\sqrt{20}q-8\sqrt{20}p+4\sqrt{20}+60q-20+16\sqrt{2}q$$

$$= 32\sqrt{5}pq+(8\sqrt{2}-16\sqrt{5})p+(-24\sqrt{5}+60+16\sqrt{2})q-8\sqrt{2}+4\sqrt{13}+8\sqrt{5}-20,$$

$$3.\mathrm{H(L(G))} = N_{1,-1}(\mathrm{L}(G)) = [2^{-1+2}(p-1)+4(\frac{2+3}{2})^{-1} + (4[4pq-3q-2p+1])(\frac{2+4}{2})^{-1}$$

$$+(12q-4)((\frac{3+4}{2})^{-1})+(4q)4^{-1}]$$

$$= 2\mathrm{p}-2+\frac{8}{5}+\frac{4}{3}[4pq-3q-2p+1]+\frac{2}{7}(12q-4)+q = \frac{16}{3}pq-\frac{2}{3}p+\frac{3}{7}q-\frac{8}{120},$$

$$4.\mathrm{SCI(L(G))} = \frac{\sqrt{2}}{2}N_{1,-\frac{1}{2}}(\mathrm{L}(G)) = \frac{\sqrt{2}}{2}[2^{-\frac{1}{2}+2}(p-1)+4(\frac{2+3}{2})^{-\frac{1}{2}}$$

$$+(4[4pq-3q-2p+1])(\frac{2+4}{2})^{-\frac{1}{2}}+(12q-4)((\frac{3+4}{2})^{-\frac{1}{2}})+(4q)4^{-\frac{1}{2}}]$$

$$= \frac{\sqrt{2}}{2}[2\sqrt{2}(p-1)+4\sqrt{\frac{2}{5}}+\frac{4\sqrt{3}}{3}(4pq-3q-2p+1)+\sqrt{\frac{2}{7}}(12q-4)+2q]$$

$$= 2p-2+\frac{4\sqrt{5}}{5}+\frac{4\sqrt{6}}{6}(4pq-3q-2p+1)+\frac{12q-4}{7}+\sqrt{2}q$$

$$= \frac{16\sqrt{6}}{6}pq+\frac{-8\sqrt{6}+12}{6}p+(\frac{-84\sqrt{6}+72+42\sqrt{2}}{42})\mathrm{q}+\frac{140\sqrt{6}+168\sqrt{5}+300}{210},$$

$$5.\mathrm{ISI(L(G))}=\frac{1}{2}N_{-1,-1}(\mathrm{L}(G))=\frac{1}{2}[2^{1+2}(p-1)+4(\frac{2^{-1}+3^{-1}}{2})^{-1}+(4[4pq-3q-2p+1])(\frac{2^{-1}+4^{-1}}{2})^{-1}$$
$$+(12q-4)((\frac{3^{-1}+4^{-1}}{2})^{-1})+(4q)4^{1}]$$
$$=4(\mathrm{p}-1)+\frac{24}{5}+\frac{16}{3}(4pq-3q-2p+1)+\frac{12}{7}(12q-4)+8q=+\frac{64}{3}\mathrm{pq}-\frac{20}{3}\mathrm{p}+\frac{88}{7}\mathrm{q}-\frac{76}{105},$$

$$6.\mathrm{N(L(G))}=\sqrt{2}N_{1,\frac{1}{2}}(\mathrm{L}(G))=\sqrt{2}[2^{\frac{1}{2}+2}(p-1)+4(\frac{2\ +3}{2})^{\frac{1}{2}}+(4[4pq-3q-2p+1])(\frac{2\ +4}{2})^{\frac{1}{2}}$$
$$+(12q-4)((\frac{3\ +4}{2})^{\frac{1}{2}})+(4q)4^{\frac{1}{2}}]$$
$$=\sqrt{2}[2\sqrt{2}(p-1)+4\sqrt{\frac{5}{2}}+4\sqrt{3}(4pq-3q-2p+1)+\sqrt{\frac{7}{2}}(12q-4)+8q]$$
$$=4p-4+4\sqrt{5}+16\sqrt{6}\,\mathrm{pq}-12\sqrt{6}q-8\sqrt{6}p+4\sqrt{6}+12\sqrt{7}\,\mathrm{q}-4\sqrt{7}+8\sqrt{2}\,\mathrm{q}$$
$$=16\sqrt{6}\,\mathrm{pq}+(4-8\sqrt{6})p+(-12\sqrt{6}+12\sqrt{7}+8\sqrt{2})q+4\sqrt{5}+4\sqrt{6}-4\sqrt{7}-4,$$

$$7.Y(\mathrm{L(G)})=2N_{3,1}(L(G))=2[2^{3+2}(p-1)+4(\frac{2^3+3^3}{2})\ +(4[4pq-3q-2p+1])(\frac{2^3+4^3}{2})$$
$$+(12q-4)((\frac{3^3+4^3}{2})\ )+(4q)4^{ab3}]$$
$$=64p-64+140+1152pq-864q-576p+288+1092q-364+512q$$
$$=+1152pq-521p+740q.$$

Conclusion

In this article, Banhatti polynomials for the TUC_4C_8 (S) nanotube are investigated and the corresponding diagram is drawn. Then, the relationship between Y-index and (a, b)-Nirmala index was proved and with the help of (a, b)-Nirmala index, some topological indices were calculated for the molecular graph and line graph of the TUC_4C_8 (S) nanotube. According to the diagrams drown in Figures 3 and 4, the K-Banhatti polynomials of the line graph and the molecular graph intersect at the points x=1, x=-1, but since the degree of the second K-Banhatti polynomial is more, the second K-Banhatti for the molecular graph and the line graph are greater than the first K-Banhatti index. This method can also be used to calculate the topological indices of the other nanotubes.

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Authors' contributions

All authors contributed to data analysis, drafting, and revising of the paper and agreed to be responsible for all the aspects of this work.

Conflict of Interest

We have no conflicts of interest to disclose.

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