

Research Article

On Computation of Face Index of Certain Nanotubes

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Topological index is a number that can be used to characterize the graph of a molecule. Topological indices describe the physical, chemical, and biological properties of a chemical structure. In this paper, we derive the analytical closed formulas of face index of some planar molecular structures such as TUC_4 , $TUC_4C_8(S)$, $TUHC_6$, $TUC_4C_8(R)$, and armchair $TUVC_6$.

1. Introduction

In this time of rapid technological development, the pharmacological techniques have evolved rapidly during the recent years. Consequently, a large number of new drugs and chemical compounds have been obtained. A huge amount of work is required to study the biological, chemical, and pharmacological aspects of these new drugs and chemical compounds. This workload is becoming more and more cumbersome as it requires sufficient tools, reagents, human resources, and a lot of time to check the performance of these new chemical compounds. However, the developing countries cannot afford these equipment and reagents to check up these biochemical properties and are resultantly unable to compete with the developed world in the areas of medical science and industry. To some extent, the chemical graph theory solved this problem as it assists to measure the pharmaceutical, chemical, and physical properties of the chemical compounds. Fortunately, previous research has revealed that chemical properties of a molecule such as boiling point, melting point, and toxicity are closely related to their molecular structures (see [1, 2]). This relationship is

one of the key reasons for the development of the mathematical chemistry. In the chemical graph theory, a molecular structure can be represented in the form of a graph $G = (V(G), E(G))$, where vertices $V = V(G)$ and edges $E = E(G)$ of a graph G show the atoms and the bonds of a molecular structure, respectively.

A topological index (TI) is an invariant that is assigned to a molecular structure (graph) and is used to characterize the molecule. It may be thought as a convenient device which converts a chemical constitution into a unique number, which is independent of the way in which the corresponding graph has been drawn or labeled. TIs were employed in developing a suitable correlation between the chemical structure and chemical or biological activities and physical properties. Several researchers working in the area of chemical and mathematical sciences have introduced TIs, such as the Wiener index, Randić indices, Zagreb indices, PI index, eccentric index, atom-bond connectivity index, and forgotten index, which have been used to predict the characteristics of the nanomaterials, drugs, and other chemical compounds. There are several papers to calculate the topological indices of some special molecular graphs [3–12].

The notions of a planar graph, its faces, and an infinite face are well known in the literature. Let $G = (V(G), E(G), F(G))$ be a finite simple connected planar graph, where $V(G)$, $E(G)$, and $F(G)$ represent the vertex, edge, and face sets, respectively. A face $f \in F(G)$ is incident to an edge $e \in E(G)$ if e is one of those which surrounds the face. Similarly, a face $f \in F(G)$ is incident to a vertex v in G if v is at the end of one of those incident edges; the incidence of v to the face f is represented by $v \sim f$. The face degree f in G is given as $d(f) = \sum_{v \sim f} d(v)$. For the notions and notations not given here, we refer [13] to the readers.

Recently, Jamil et al. [14] introduced a novel topological index named as the face index. The face index helped to predict the energy and the boiling points of selected benzenoid hydrocarbons with the correlation coefficient $r > 0.99$. For a graph G , the face index (FI) can be defined as

$$FI(G) = \sum_{f \in F(G)} d(f) = \sum_{v \sim f \in F(G)} d(v). \quad (1)$$

In this paper, we calculate the face index of some special molecular graphs which have been widely used in drugs.

2. Main Results

In this section, we investigate the exact formulas of the face index for the molecular structures of vastly studied nanotubes with wide range of applications: $TUC_4C_8(S)$, $TUC_4C_8(R)$, $TUHC_6$, TUC_4 , and $TUVC_6$. To find the face indices of the molecular graphs of these nanotubes, we partitioned the face set depending on the degrees of each face.

2.1. Face Index of $TUC_4C_8(S)[n, q, r]$ and $TUC_4C_8(R)[n, q, r]$ Nanotubes. The 2-dimensional lattice of $TUC_4C_8(S)$ is constructed by the alternately positioned squares C_4 and octagons C_8 (see Figure 1(a)), where n, q , and r represent the number of rows, octagons in each row, and squares in each row. A $TUC_4C_8(S)[n, q, r]$ nanotube can be constructed by rolling the 2D lattice of carbon atoms and can be seen in Figure 1(b).

Firstly, we prove the following formula which provides the exact values of the face index for $TUC_4C_8(S)[n, q, r]$.

Theorem 1. *Let $G = TUC_4C_8(S)[n, q, r]$, where $n, q, r \geq 1$, be the 2-dimensional lattice of $TUC_4C_8(S)$ nanotube; then, the face index of G is given as*

$$FI(G) = 24nq + 12nr + 4q + 12r. \quad (2)$$

Proof. Let G be the 2-dimensional lattice of $TUC_4C_8(S)[n, q, r]$ nanotube with n number of rows and let q and r be the number of octagons and number of squares in each row, respectively. In $TUC_4C_8(S)[n, q, r]$, the total number of faces in one row is $q + r$. Let f_j denote the faces having $\sum_{w \sim f_j} d_w = j$ and $|f_j|$ denote the number of faces with degree j . From Figure 1(a), it can be noticed that 2D lattice of $TUC_4C_8(S)[7, 4, 4]$ contains four types of internal faces f_{12} , f_{20} , f_{22} , and f_{24} and an external face, f_∞ . When

$TUC_4C_8(S)[n, q, r]$ has n rows, then sum of vertex degrees of external face is $8q + 12r$. The number of internal faces in each row is given in Table 1.

The face index of $TUC_4C_8(S)[n, q, r]$ is

$$\begin{aligned} FI(G) &= \sum_{w \sim f \in F(G)} d_w \\ &= \sum_{w \sim f_{12}} d_w + \sum_{w \sim f_{22}} d_w + \sum_{w \sim f_{24}} d_w + \sum_{w \sim f_\infty} d_w \\ &= |f_{12}|(12) + |f_{22}|(22) + |f_{24}|(24) + 8q + 12r \quad (3) \\ &= nr(12) + 2q(22) + q(n-2)(24) + 8q + 12r \\ &= 12nr + 44q + 24nq - 48q + 8q + 12r \\ &= 24nq + 12nr + 4q + 12r. \end{aligned}$$

This completes the proof. \square

Theorem 2. *Let $n, q, r \geq 1$ and $H = TUC_4C_8(R)[n, q, r]$ be the graph of 2-dimensional lattice of $TUC_4C_8(R)$ nanotube. Then, the face index of the graph H is given as*

$$FI(H) = 24nq + 6nr + 12q + 18r. \quad (4)$$

Proof. Consider a $TUC_4C_8(R)[n, q, r]$ nanotube with n number of rows, q number of octagons, and r number of squares in each row as shown in Figure 2(a). The 2-dimensional lattice (H) of $TUC_4C_8(R)[n, q, r]$ is shown in Figure 2(b). In H , the total number of faces in one row is $q + r$. Let f_j and $|f_j|$ denote the face with degree j and the number of faces with degree j , respectively. From the structure of H , one can notice that there are three types of internal faces f_{11} , f_{12} , and f_{24} and an external face f_∞ . The external face has degree $12q + 2r$. Table 2 illustrates the number of internal faces in $TUC_4C_8(R)[n, q, r]$ based on the degree of each face.

The face index of the graph $H = TUC_4C_8(R)[n, q, r]$ is

$$\begin{aligned} FI(H) &= \sum_{w \sim f \in F(H)} d_w \\ &= \sum_{w \sim f_{11}} d_w + \sum_{w \sim f_{12}} d_w + \sum_{w \sim f_{24}} d_w + \sum_{w \sim f_\infty} d_w \\ &= |f_{11}|(11) + |f_{12}|(12) + |f_{24}|(24) + 12q + 2r \\ &= r(11) + \frac{(n-1)r}{2}(12) + nq(24) + 12q + 2r \\ &= 11r + 6nr - 6r + 24nq + 12q + 2r \\ &= 24nq + 6nr + 12q + 7r. \end{aligned} \quad (5)$$

This completes the proof. \square

2.2. Face Index of $TUC_4[p, q]$ Nanotube. For $p \geq 2$ and $q \geq 3$, the 2-dimensional lattice of $TUC_4[p, q]$ nanotube is obtained by the Cartesian product of the path P_p and the cycle C_q . For $p = 8$ and $q = 4$, the example of $TUC_4[p, q]$ is shown in Figure 3(b).

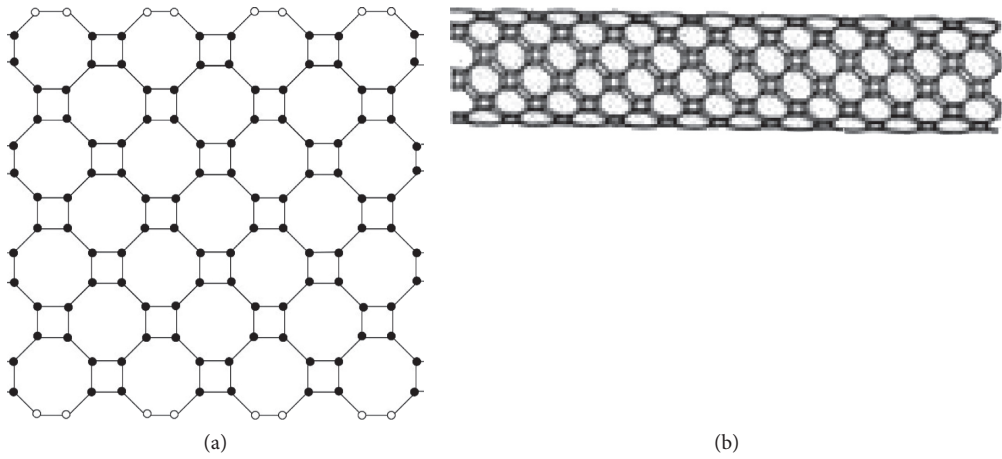


FIGURE 1: (a) 2D lattice of $TUC_4C_8(S)[7,4,4]$. (b) 3D nanotube $TUC_4C_8(S)$.

TABLE 1: Numbers of f_{12} , f_{20} , f_{22} , and f_{24} with given number of rows.

n	$ f_{12} $	$ f_{20} $	$ f_{22} $	$ f_{24} $
1	R	q	—	—
2	$2r$	—	$2q$	—
3	$3r$	—	$2q$	Q
4	$4r$	—	$2q$	$2q$
⋮	⋮	⋮	⋮	⋮
⋮	⋮	⋮	⋮	⋮
N	Nr	—	$2q$	$(n-2)q$

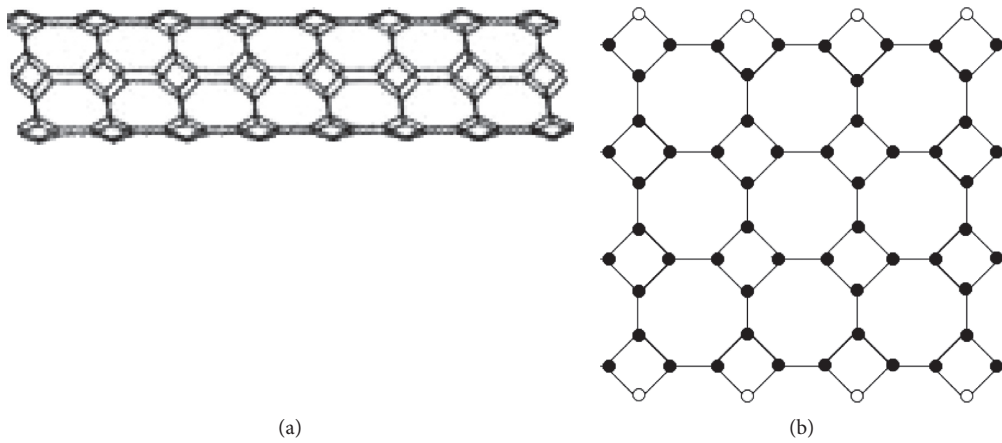


FIGURE 2: (a) 3D nanotube $TUC_4C_8(R)$. (b) 2D lattice of $TUC_4C_8(R)$.

TABLE 2: Numbers of f_{11} , f_{12} , and f_{24} with given number of rows.

n	$ f_{11} $	$ f_{12} $	$ f_{24} $
1	R	—	Q
2	R	$r/2$	$2q$
3	R	R	$3q$
4	R	$3r/2$	$4q$
5	5	$2r$	$5q$
⋮	⋮	⋮	⋮
⋮	⋮	⋮	⋮
N	R	$(n-1)r/2$	Nq

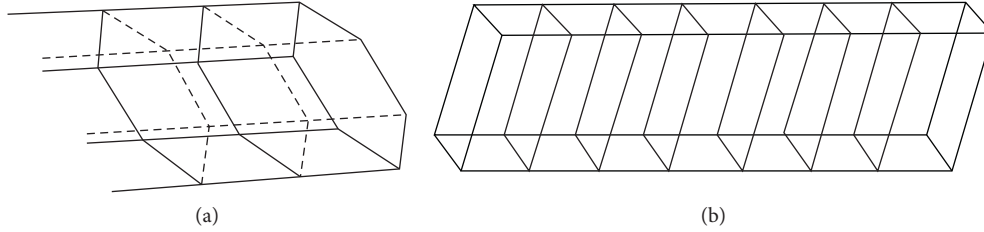


FIGURE 3: (a) Nanotube $TUC_4[p, 6]$. (b) Nanotube $TUC_4[8, 4]$.

Theorem 3. Let K be the graph of $TUC_4[p, q]$ nanotube structure, where $p \geq 2$ and $q \geq 3$. Then, the face index of K is equal to

$$FI(K) = \begin{cases} 18q; & \text{if } p = 2, \\ 34q; & \text{if } p = 3, \\ 2q(8p - 7); & \text{if } p > 3. \end{cases} \quad (6)$$

Proof. We will prove the result for $p > 3$. Let K denote the graph of $TUC_4C[p, q]$ nanotube structure. From Figure 3, we can notice that the graph K contains three types of internal faces, namely, f_{3q} , f_{14} , and f_{16} , and an external face of degree $3q$. By applying the definition and using the values from Table 3, the face index of K can be computed as

$$\begin{aligned} FI(K) &= \sum_{w \sim f \in F(K)} d_w \\ &= \sum_{w \sim f_{3q}} d_w + \sum_{w \sim f_{14}} d_w + \sum_{w \sim f_{16}} d_w \\ &= |f_{3q}|(3q) + |f_{14}|(14) + |f_{16}|(16) \\ &= 2(3q) + 14(2q) + 16(p - 3)q \\ &= 2q(8p - 7). \end{aligned} \quad (7)$$

This completes the proof.

2.3. Zig-Zag $TUHC_6[n, q]$ Nanotube. Consider the graph K of $TUHC_6[n, q]$ zig-zag polyhex nanotube structure, where n denotes the number of rows and the number of hexagons in each row is represented by q . Figure 4 illustrates the nanotube $TUHC_6[n, q]$ and its 2-dimensional structure.

Theorem 4. For $n, q \geq 1$, let K represent the 2-dimensional graph of $TUHC_4[n, q]$ structure. The face index of K is

$$FI(K) = 18nq + 8q. \quad (8)$$

Proof. Let $TUHC_6[n, q]$ be a polyhex nanotube with n number of rows and q number of hexagons in each row and K be the 2-dimensional graph of $TUHC_6[n, q]$ structure. The molecular graph of $TUHC_6[n, q]$ is shown in Figure 4. Let f_j denote the face having degree j , i.e., $\sum_{w \sim f_j} d_w = j$, and let $|f_j|$ denote the number of f_j . The molecular graph of $TUHC_6[n, q]$ contains two types of internal faces f_{17} and f_{18} and an external face f_{∞} . When $TUHC_6[n, q]$ has n rows, then the face degree of f_{∞} is $10q$. The number of internal faces with the given number of rows is listed in Table 4.

TABLE 3: Numbers of f_{11} , f_{12} , and f_{24} with given number of rows.

$TUC_4[k, q]$	$ f_{3q} $	$ f_{12} $	$ f_{14} $	f_{16}
$k=2$	2	Q	—	—
$k=3$	2	—	$2q$	—
$k=4$	2	—	$2q$	Q
$k=5$		—	$2q$	$2q$
\vdots	\vdots	\vdots	\vdots	\vdots
\vdots	\vdots	\vdots	\vdots	\vdots
\vdots	\vdots	\vdots	\vdots	\vdots
$k=p$	2	—	$2q$	$(p-3)q$

The face index of the graph $K = TUHC_6[n, q]$ is

$$\begin{aligned} FI(K) &= \sum_{w \sim f \in F(K)} d_w \\ &= \sum_{w \sim f_{17}} d_w + \sum_{w \sim f_{18}} d_w + \sum_{w \sim f_{\infty}} d_w \\ &= |f_{17}|(17) + |f_{18}|(18) + 10q \\ &= 2q(17) + (n - 2)q(18) + 10q \\ &= 34q + 18nq - 36q + 10q \\ &= 18nq + 8q, \end{aligned} \quad (9)$$

which is the required result. \square

2.4. $TUVC_6[n, q]$ Nanotube. The 2-dimensional graph of $TUVC_6[n, q]$ is shown in Figure 5(b), and the $TUVC_6[n, q]$ nanotube can be constructed by rolling this lattice of carbon atoms (Figure 5(a)), where n represents the number of rows and q is the hexagons in each row.

Theorem 5. Let $L = TUVC_4[n, q]$, where $n, q \geq 1$, be the graph of 2-dimensional lattice of $TUVC_6[n, q]$ armchair polyhex nanotube. The face index of L is

$$FI(L) = 36nq - 8q. \quad (10)$$

Proof. Let L represent the 2-dimensional molecular graph of $TUVC_6[n, q]$ with n number of rows and q number of hexagons in each row. From Figure 5(b), we can easily notice that L contains 2 types of internal faces f_{16} and f_{18} and an external face, and the degree of external face is $14q$. The cardinalities of internal faces with given degree and given number of rows are explained in Table 5.

The face index of $L = TUVC_6[n, q]$ is

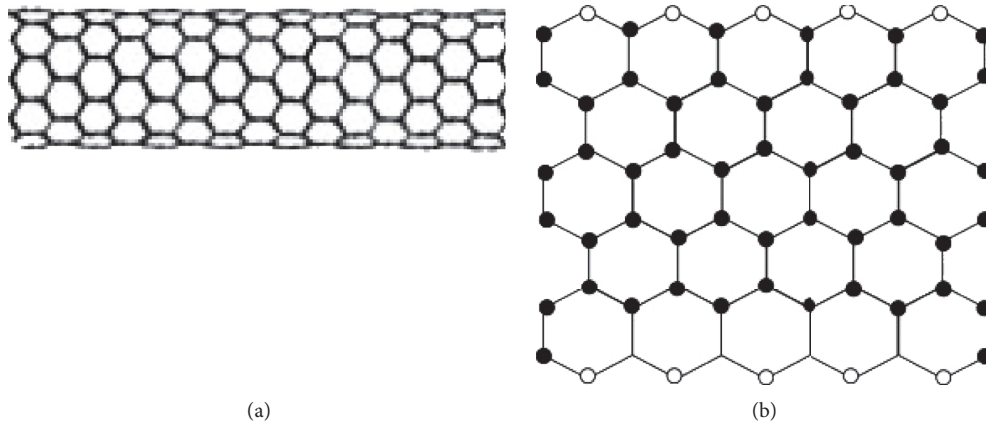


FIGURE 4: (a) 3D nanotube TUHC₆[n, q]. (b) 2D lattice of TUHC₆[5, 5].

TABLE 4: The cardinalities of the faces with given degree for given number of rows.

n	$ f_{16} $	$ f_{17} $	$ f_{18} $
1	q	—	—
2	—	$2q$	—
3	—	$2q$	Q
4	—	$2q$	$2q$
⋮	⋮	⋮	⋮
⋮	⋮	⋮	⋮
N	—	$2q$	$(n-2)q$

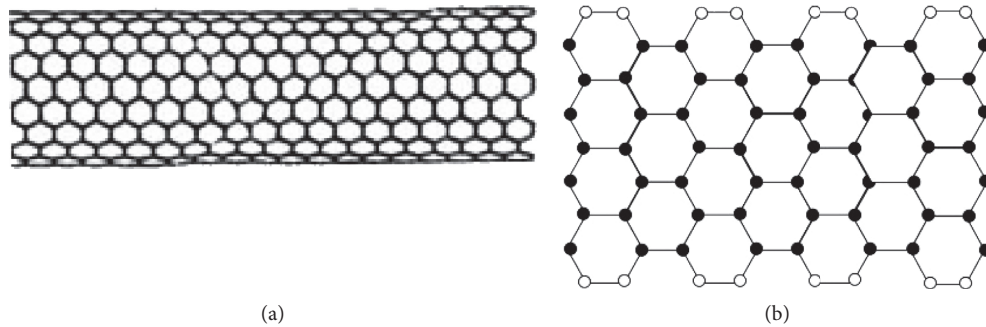


FIGURE 5: (a) Armchair 3D nanotube TUV C₆[n, q]. (b) 2D lattice of TUV C₆[4, 4].

TABLE 5: The cardinalities of f_{14} , f_{16} , and f_{18} with given number of rows.

n	$ f_{14} $	$ f_{16} $	$ f_{18} $
1	q	—	—
2	—	$2q$	Q
3	—	$2q$	$3q$
4	—	$2q$	$5q$
⋮	⋮	⋮	⋮
⋮	⋮	⋮	⋮
N	—	$2q$	$(2n-3)q$

$$\begin{aligned}
 FI(L) &= \sum_{w \sim f \in F(L)} d_w \\
 &= \sum_{w \sim f_{16}} d_w + \sum_{w \sim f_{18}} d_w + \sum_{w \sim f_{\infty}} d_w \\
 &= |f_{16}|(16) + |f_{18}|(18) + 14q \\
 &= 2q(16) + (2n-3)q(18) + 14q \\
 &= 32q + 36nq - 54q + 14q \\
 &= 36nq - 8q,
 \end{aligned}
 \tag{11}$$

and the proof is complete. \square

3. Conclusion

In [14], using multiple linear regression, it has been shown that the novel face index can predict the π electron energy and boiling point of benzenoid hydrocarbon with a correlation coefficient greater than 0.99. Therefore, this index can be useful in QSPR/QSAR studies. In this paper, we have computed the novel face index of some nanotubes.

Data Availability

No data were used to support the study.

Disclosure

This research was carried out as a part of the employment of the authors.

Conflicts of Interest

The authors declare that they have no conflicts of interest.

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