RESEARCH ARTICLE

Some topological indices of the family of nanostructures of polycyclic aromatic hydrocarbons (PAHs)

Najmeh Soleimani*, Esmaeel Mohseni1, Niloofar Maleki2 and Najmeh Imani2
1 Young Researchers and Elite Club, Karaj Branch, Islamic Azad University, Karaj, Iran.
2 Salehan Institute of Higher Education, Qumshahr, Iran.

Revised: 30 September 2017; Accepted: 19 October 2017

Abstract: Molecular descriptors play a significant role in many areas such as chemistry and pharmacology. Among these, topological indices have a prominent place. In this paper, we focus on the structure of polycyclic aromatic hydrocarbons and calculate theta, Pi and Sadhana indices of nanostructures. These indices on the ground of quasi-orthogonal cut ‘qoc’ edge strips in molecular graph. Also, the exact formulae for connectivity indices of nanotubes and nanotori are presented in this manuscript. These topological indices are useful for surveying structure of nanostructures, which have a relationship with degrees of their vertices.

Keywords: Connectivity indices, cut method, nanostructures, Pi index, Sadhana index, theta index.

INTRODUCTION

Graph theory models have extensively been used as predictors of properties of chemical compounds (Trinajstić, 1992; Todescini & Consonni, 2000 and references within). M.V. Diudea was the first scientist who considered graph theoretical problems of nanotechnology, and some works on computing topological indices of nanostructure, nanotubes and nanotori are presented in many papers (Diudea & John, 2001; Diudea & Kirby, 2001; Diudea, 2002; Diudea et al., 2003; 2004).

The present study is a continuation of our previous studies (Nikmehr et al., 2015; Soleimani et al., 2015; 2016) on computing some topological indices of nanostructures.

METHODOLOGY

From the point of graph theory, all organic molecular structures can be drawn as graphs in which atoms and bonds are represented by vertices and edges, respectively. Let G be a simple graph with vertex set V(G) and edge set E(G). The edge connecting the vertices u and v will be denoted by uv. The degree of the vertex u, denoted by du, is the number of first neighbours of u in the underlying graph. The distance between u and v in V(G), d(u, v), is the length of a shortest u-v path in G. Two edges e = uv and f = xy of G are called co-distant, ‘e co f’, if and only if they obey the following relation:

\[ d(u,v) + 1 = d(u,x) + 1 = d(u,y). \]

The above relation co is reflexive and symmetric for any edge e of G but in general is not transitive. A graph is called a co-graph if the relation co is also transitive and thus an equivalence relation.

Let \( C(e) = \{ f \in E(G) \mid f \text{ co } e \} \) be the set of edges in G that are co-distant to \( e \in E(G) \). The set \( C(e) \) can be obtained by an orthogonal edge cutting procedure: take a straight line segment, orthogonal to the edge e, and intersect it and all other edges (of a polygonal plane graph) parallel to e. The set of these intersections is called an orthogonal cut (oc for short) of G, with respect to e. If \( G \) is a co-graph then its orthogonal cuts \( C_1, C_2, ..., C_k \) form a partition of \( E(G) \):

* Corresponding author (soleimani.najme@gmail.com; https://orcid.org/0000-0002-2336-1066)

This article is published under the Creative Commons CC-BY-ND License (http://creativecommons.org/licenses/by-nd/4.0/). This license permits use, distribution and reproduction, commercial and non-commercial, provided that the original work is properly cited and is not changed anyway.
\[ E(G) = C_1 \cup C_2 \cup \ldots \cup C_k, C_i \cap C_j = \emptyset, \]
for \( i \neq j \) and \( i, j = 1, 2, \ldots, k \).

If any two consecutive edges \( e \) and \( f \) of a plane graph \( G \) of an edge-cut sequence are topologically parallel within the same face of the covering, such a sequence is called a quasi-orthogonal cut (qoc) strip. Obviously, any orthogonal cut strip is a qoc strip but the reverse is not always true. This means the transitivity relation of the co relation is not necessarily obeyed. Topological index is a real number that is derived from molecular graphs of chemical compounds. There are several topological indices already defined.

**Topological indices based on counting qoc strips**

Three topological indices have been defined on the ground of qoc strips:

**Theta index:**
\[ \theta(G) = \sum c m(G, c) \times c^2. \] ...

**Pi index:**
\[ \pi(G) = \sum c m(G, c) \times c \times (|E(G)| - c). \] ...

**Sadhana index:**
\[ Sd(G) = \sum c m(G, c) \times (|E(G)| - c). \] ...

with \( m(G, c) \) being the number of strips of length \( c \). In Khadikar et al. (2004a; 2004b; 2006) these topological indices and their polynomials of some graphs are computed.

**Connectivity indices**

Randić (1975) first addressed the problem of relating the physical properties of alkanes to the degree of branching across an isomeric series. The degree of branching of a molecule was quantified using a branching index, which subsequently became known as first-order molecular connectivity index \( \chi \). Kier and Hall (1986) extended this to higher orders and introduced modifications to account for heteroatoms.

Let \( G \) be a simple connected graph of order \( n \). For an integer \( m \geq 1 \), the m-order connectivity index of an organic molecule whose molecule graph \( G \) is defined as:

\[ m\chi(G) = \sum_{i_1, \ldots, i_{m+1}} \frac{1}{\sqrt{d_{i_1} \cdots d_{i_{m+1}}}}. \] ...

where \( i_1 \ldots i_{m+1} \) (for simplicity) runs over all paths of length \( m \) in \( G \), and \( d_v \) denote the degree of vertex \( v \).

Zhou and Trinajstić (2009) proposed another connectivity index, named the sum-connectivity index. It has been found that the sum-connectivity index correlates well with \( \pi \)-electronic energy of benzenoid hydrocarbons, and it is frequently applied in quantitative structure property and structure-activity studies. The m-order sum-connectivity index of \( G \) is defined as:

\[ m\chi(G) = \sum_{i_1, \ldots, i_{m+1}} \frac{1}{\sqrt{d_{i_1} + \cdots + d_{i_{m+1}}}}. \] ...

The second-order connectivity index is defined as follows:

\[ 2\chi(G) = \sum_{i_1, i_3} \frac{1}{\sqrt{d_{i_1}d_{i_3}d_{i_3}}} \] ...

The second-order sum-connectivity index is defined as follows:

\[ 2\chi(G) = \sum_{i_1, i_2, i_3} \frac{1}{\sqrt{d_{i_1}d_{i_2}d_{i_3}}} \] ...

**RESULTS AND DISCUSSION**

The explicit formulae for the theta, Pi, Sadhana, second-order connectivity and second-order sum-connectivity indices of vertical pentacenic nanotube, horizontal pentacenic nanotube and pentacenic nanotori are presented in this section.

Polycyclic aromatic hydrocarbons (PAHs) are organic compounds containing only carbon and hydrogen that are composed of multiple aromatic rings. Pentacenes are polycyclic aromatic hydrocarbons consisting of five linearly-fused benzene rings (Soleimani et al., 2014).

**Remark 1:** We denote a 2-dimensional lattice of vertical pentacenic nanotube by \( G = G[p, q] \) (Figure 1). Now we consider the molecular graph \( G \). It is easy to see that \(|V(G)| = 22pq \) and \(|E(G)| = 33pq - 5p \). Notice that the edges in the right side are affixed to the vertex in the left side of the figure to gain a tube in this way. First, we consider the following examples.

---

March 2018  
*Journal of the National Science Foundation of Sri Lanka* 46(1)
Example 1: Consider the graph of 2-dimensional lattice of $G[2,4]$ nanotube as depicted in Figure 1. One can see that, there are six distinct cases of qoc strips. We denote the corresponding edges by $e_1$, $e_2$, $e_3$, $c_1$, $c_2$, and $c_3$. By continuing method, it is easy to check that $|C(e_1)| = 12$, $|C(e_2)| = 10$, $|C(e_3)| = 8$, $|C(c_1)| = 2$, $|C(c_2)| = 4$, $|C(c_3)| = 6$ and $|C(c_4)| = 8$. On the other hand, there are 4, 3, 2, 4, 4, and 14 similar edges for each of the edges $e_1$, $e_2$, $e_3$, $c_1$, $c_2$, $c_3$, and $c_4$, respectively. So, the theta index of $V$-pentacenic nanotube $G = G[2,4]$ is

$$\theta(G) = \sum_c m(G, c) \times c^2$$

$$= (4 \times 12^2) + (3 \times 10^2) + (2 \times 8^2) + (4 \times 2^2) + (4 \times 4^2) + (4 \times 6^2)$$

$$= 2124.$$ 

Since the edge number of $G[2,4]$ is equal to 254, thus we obtain

$$II(G) = \sum_c m(G, c) \times c \times (|E(G)| - c)$$

$$= (4 \times 12 \times (254 - 12)) + (3 \times 10 \times (254 - 10)) + (2 \times 8 \times (254 - 8)) + (4 \times 2 \times (254 - 2)) + (4 \times 4 \times (254 - 4)) + (4 \times 6 \times (254 - 6)) + (14 \times 8 \times (254 - 8))$$

$$= 62392.$$ 

Also,

$$SD(G) = \sum_c m(G, c) \times (|E(G)| - c)$$

$$= (4 \times (254 - 12)) + (3 \times (254 - 10)) + (2 \times (254 - 8)) + (4 \times (254 - 2)) + (4 \times (254 - 4)) + (4 \times (254 - 6)) + (14 \times (254 - 8))$$

$$= 8636.$$ 

In general, for $G = G[p, q]$, we have the following theorems.

Theorem 1 Consider the graph of $G = G[p, q]$, $\forall p, q \in \mathbb{N} - \{1\}$. Then its theta index is as follows:

$$\theta(G) = \begin{cases} 
61p^2q^2 + 44pq^2 - 25p^2 - \frac{8}{3}p^3 + \frac{8}{3}q & \text{if } 5p \ge q - 1, \\
261p^2q + 4pq^2 - 25p^2 - \frac{1000}{3}p^3 + \frac{40}{3}p & \text{if } 5p < q - 1.
\end{cases}$$

Proof. Let $G = G[p, q]$ be the graph of $V$-pentacenic nanotube. To compute the theta index of $G$, it is enough to calculate $C(e)$ for every edge $e \in E(G)$. By using the cut method and Figure 1, one can see that there are some distinct cases of qoc strips. We denote the corresponding edges by $e_1, e_2, e_3, ..., e_q$. Regarding the different possible cases which $p$ and $q$ can be chosen, the following cases are considered.

Case 1. $5p \ge q - 1$:

![Figure 1: The 2-D graph lattice of $G = G[p, q]$ with $p = 2$ and $q = 4$.]

| Type of edges | Number of co-distinct edges | Number of qoc |
|---------------|----------------------------|---------------|
| $e_1$         | $6p$                       | $q$           |
| $e_2$         | $5p$                       | $q - 1$       |
| $e_3$         | $2q$                       | $p$           |
| $c_i$         | $2i$                       | $4$           |
| $\forall i = 1, 2, ..., q - 1$ | $2q$ | $10p - 2q + 2$ |
| $c_q$         | $2q$                       | $10p - 2q + 2$ |

If $5p \ge q - 1$ using the data in Table 1, the theta index of $G = G[p, q]$, for $p, q \in \mathbb{N} - \{1\}$, can be written as

$$\theta(G) = \sum_c m(G, c) \times c^2$$

$$= q \times (6p)^2 + (q - 1) \times (5p)^2 + p \times (2q)^2 + (2q - 10p + 2) \times (10p)^2 + 4 \sum_{i=1}^{q-1} (2i)^2.$$
This expression can be simplified to the following form:
\[
\Theta(G) = 61p^2q + 44pq^2 - 25p^2 - \frac{8}{3}q^3 + \frac{8}{3}q.
\]

**Case 2.** $5p < q - 1$:

| Type of edges | Number of co-distant edges | Number of qoc |
|---------------|----------------------------|---------------|
| $e_1$         | $6p$                       | $q$           |
| $e_2$         | $5p$                       | $q - 1$       |
| $e_3$         | $2q$                       | $p$           |
| $c_i$         | $2i$                       | $4$           |
| $\forall i = 1, 2, ..., 5p - 1$ |                       |               |
| $c_{5p}$      | $10p$                      | $2q - 10p + 2$|

If $5p < q - 1$ using the data in Table 2, similar to the previous case, we have
\[
\Theta(G) = \sum m(G, c) \times c^2
\]
\[
= q \times (6p)^2 + (q - 1) \times (5p)^2 + p \times (2q)^2 + (2q - 10p + 2) \times (10p)^2 + 4 \sum_{i=1}^{5p-1} (2i)^2.
\]
Therefore,
\[
\Theta(G) = 261p^2q + 4pq^2 - 25p^2 - \frac{1000}{3}p^3 + \frac{40}{3}q.
\]

Summing up contributions of the two parts completes the proof.

Similar to the proof of Theorem 1, we can prove the following theorems:

**Theorem 2** The Pi and Sadhana indices of $G = G[p, q]$, $\forall p, q \in \mathbb{N} - \{1\}$ are computed as:
\[
II(G) = \begin{cases}
1089p^2q^2 - 391p^2q - 44pq^2 + 50p^2 + \frac{8}{3}q^3 - \frac{8}{3}q & \text{if } 5p \geq q - 1, \\
1089p^2q^2 - 591p^2q - 4pq^2 + 50p^2 + \frac{1000}{3}p^3 - \frac{40}{3}q & \text{if } 5p < q - 1.
\end{cases}
\]
\[
Sd(G) = 363p^2q + 132pq^2 - 55p^2 - 152pq + 20p.
\]

**Proof.** By Table 1, Table 2 and the definition of Pi and Sadhana indices, the proof is straightforward.

**Theorem 3** The second order connectivity index of $G = G[p, q]$ is as follows:
\[
\chi^2(G) = \frac{22\sqrt{3}}{3}pq + \frac{51\sqrt{2} - 50\sqrt{3}}{9}p.
\]

**Proof.** Let us define $d_{ijk}$ as a number of 2-edges paths with vertices of degree $i, j$ and $k$, respectively. It is obvious, $d_{ijk} = d_{kij}$. First, we define $d_{232}$ to be the number of edges connecting the three vertices of degree 2, 3 and 2 (the red path in Figure 2), $d_{323}$ to be the number of edges connecting the three vertices of degree 3, 2 and 3 (the blue path in Figure 2), $d_{333}$ to be the number of edges connecting three vertices of degree 2, 3 and 3 (the green path in Figure 2), and $d_{333}$ to be the number of edges connecting the three vertices of degree 3 (the pink path in Figure 2).

---

**Figure 2:** Examples of 2-edges paths $d_{222}$, $d_{223}$, $d_{233}$ and $d_{333}$ of $G[2, 2]$.

**Table 3:** Categorisation of all 2-edges paths based on their first and end point

| 2-edges paths | Number of 2-edges paths |
|---------------|-------------------------|
| (2,3,2)       | 8p                      |
| (3,2,3)       | 10p                     |
| (2,3,3)       | 24p                     |
| (3,3,3)       | 66pq - 62p              |

By considering the general form of vertical pentacenic nanotube we can fill Table 3.

Now, by using the results in Table 3, we have the following computations:
\[
\chi^2(G) = \sum_{i,j,k} \frac{1}{\sqrt{a_1^2 + a_2^2 + a_3^2}}
\]
\[
= \left(8p \times \frac{1}{\sqrt{2 \times 3 \times 2}} \right) + \left(10p \times \frac{1}{\sqrt{3 \times 2 \times 3}} \right)
\]
\[
\left( 24p \times \frac{1}{\sqrt{2} \times 3 \times 3} \right) + \left( 66pq - 62p \times \frac{1}{\sqrt{3} \times 3 \times 3} \right)
\]
\[
= \frac{22\sqrt{3}}{3} pq + \frac{51\sqrt{3} - 50\sqrt{3}}{9} p.
\]

**Theorem 4** The 2-order sum-connectivity index of 
\( G = G[p,q] \) is as follows:
\[
2X(G) = 22pq + \left( \frac{8\sqrt{7}}{7} + \frac{17\sqrt{17}}{2} - \frac{62}{3} \right) p.
\]

**Proof.** By Table 3 and the definition of \( 2X(G) \).

**Remark 2:** We denote a 2-dimensional lattice of 
horizontal pentacene nanotube by \( H = H[p,q] \) 
(Figure 3). Now we consider the molecular graph 
\( H \). It is easy to see that \( |V(H)| = 22pq \) and 
\( |E(H)| = 33pq - 2q \). Notice that the edges in the top 
are affixed to the vertex in the bottom of the figure to 
gain a tube in this way.

**Example 2:** Consider the graph of 2-dimensional lattice 
of \( H[3,4] \) nanotube as depicted in Figure 3.

![Figure 3: The 2-D graph lattice of \( H = H[p,q] \) with \( p = 3 \) and 
\( q = 4 \)](image)

One can see that, there are eight distinct cases of \( qoc \) 
strips. We denote the corresponding edges by \( e_1, e_2, e_3, 
\ldots, e_p, c_1, c_2, c_3, c_4, c_5 \) and \( c_r \). By continuing 
method it is easy to check that \( |C(e_1)| = 18, |C(e_2)| = 15, 
|C(e_3)| = 8, |C(e_4)| = 8, |C(c_1)| = 1, |C(c_2)| = 3, |C(c_3)| = 5 
and \( |C(c_4)| = 7 \). On the other hand, there are \( 4, 4, 2, 22, 
4, 4, 4 \) and 4 similar edges for each of edges \( e_1, e_2, e_3, 
e_4, c_1, c_2, c_3, c_4, \) and \( c_r \), respectively. So, the theta index of 
\( H \)-pentacene nanotube \( H = H[3,4] \) is
\[
\theta(H) = \sum c m(H,c) \times c^2
\]
\[
= (4 \times 18^2) + (4 \times 15^2) + (2 \times 8^2) + (22 \times 8^2) + 
(4 \times 1^2) + (4 \times 3^2) + (4 \times 5^2) + (4 \times 7^2)
\]
\[
= 4068.
\]

Since the edge number of \( H[3,4] \) is equal to 388, thus we obtain
\[
\Pi(H) = \sum c m(H,c) \times c \times |E(H)| - c
\]
\[
= (4 \times 18 \times (388 - 18)) + (4 \times 15 \times (388 - 15)) + (2 \times 8 \times (388 - 8)) + 
(22 \times 8 \times (388 - 8)) + (4 \times 1 \times (388 - 1)) + (4 \times 3 \times (388 - 3)) + 
(4 \times 5 \times (388 - 5)) + (4 \times 7 \times (388 - 7))
\]
\[
= 146476.
\]

Also,
\[
\Phi(H) = \sum c m(H,c) \times |E(H)| - c
\]
\[
= (4 \times (388 - 18)) + (4 \times (388 - 15)) + (2 \times (388 - 8)) + 
(22 \times (388 - 8)) + (4 \times (388 - 1)) + (4 \times (388 - 3)) + 
(4 \times (388 - 5)) + (4 \times (388 - 7))
\]
\[
= 18236.
\]

In general, for \( H = H[p,q] \), we have the following 
thereoms.

**Theorem 5** The theta, Pi and Sadhana indices of 
\( H = H[p,q] \), \( \forall p, q \in \mathbb{N} - \{1\} \) are computed as:
\[
\theta(H) = \begin{cases} 
61p^2q + 44pq^2 - 4q^2 - \frac{8}{3}q^3 - \frac{4}{3}q & \text{if } 5p \geq q. \\
261p^2q + 4pq^2 - 4q^2 - \frac{1000}{3}p^3 - \frac{20}{3}p & \text{if } 5p < q.
\end{cases}
\]
\[
\Pi(H) = \begin{cases} 
1089pq^2 - 61pq^2 - 176pq^2 + \frac{8}{3}q^3 + 8q^2 + \frac{4}{3}q & \text{if } 5p \geq q. \\
1089pq^2 - 261pq^2 - 136pq^2 + 8q^2 + \frac{1000}{3}p^3 + \frac{20}{3}p & \text{if } 5p < q.
\end{cases}
\]
\[
Sd(H) = 363p^2q + 132pq^2 - 8q^2 - 88pq + 4q.
\]

**Proof.** Let \( H = H[p,q] \) be the graph of \( H \)-pentacene 
nanotube. Tables 4 and 5 show the number of co-
distant edges in \( H \). By using these tables the proof is 
straightforward.
Table 4: The number of co-distinct edges of \( H = H[p, q] \) for \( 5p \geq q \).

| Type of edges | Number of co-distinct edges | Number of qoc |
|---------------|----------------------------|---------------|
| \( e_1 \)     | \( 6p \)                   | \( q \)       |
| \( e_2 \)     | \( 5p \)                   | \( q \)       |
| \( e_3 \)     | \( 2q \)                   | \( p - 1 \)   |
| \( e_4 \)     | \( 2q \)                   | \( 10p - 2q \) |
| \( c_i \), \( i \) is odd. | \( i \)             | \( 4 \)       |

\( \forall i = 1, 3, ..., 2q - 1 \)

Table 5: The number of co-distinct edges of \( H = H[p, q] \) for \( 5p < q \).

| Type of edges | Number of co-distinct edges | Number of qoc |
|---------------|----------------------------|---------------|
| \( e_1 \)     | \( 6p \)                   | \( q \)       |
| \( e_2 \)     | \( 5p \)                   | \( q \)       |
| \( e_3 \)     | \( 2q \)                   | \( p - 1 \)   |
| \( e_4 \)     | \( 10p \)                  | \( 2q - 10p \) |
| \( c_i \), \( i \) is odd. | \( i \)             | \( 4 \)       |

\( \forall i = 1, 3, ..., 10p - 1 \)

**Theorem 6** The second-order connectivity index of \( H = H[p, q] \) is as follows:

\[
\begin{align*}
2\chi(H) &= \sum_{i,j,k} \frac{1}{\sqrt{d_{i}d_{j}d_{k}}} \\
&= \left(8q \times \frac{1}{\sqrt{2} \times 3 \times 3}\right) + \left(4q \times \frac{1}{\sqrt{3} \times 2 \times 2}\right) + \\
&\left((66pq - 20q) \times \frac{1}{\sqrt{3} \times 3 \times 3}\right) \\
&= \frac{22\sqrt{3}}{3}pq + \frac{12\sqrt{2} - 14\sqrt{3}}{9}q.
\end{align*}
\]

**Proof.** First, we define \( d_{233} \) to be the number of edges connecting three vertices of degree 2, 3 and 3 (the green path in Figure 4), \( d_{122} \) to be the number of edges connecting the three vertices of degree 3, 2 and 2 (the orange path in Figure 4), and \( d_{333} \) to be the number of edges connecting the three vertices of degree 3 (the pink path in Figure 4).

By considering the general form of horizontal pentacenic nanotube we can fill the Table 6.

Table 6: Categorisation of all 2-edges paths based on their first and end point

| 2-edges paths | Number of 2-edges paths |
|---------------|-------------------------|
| (2,3,3)       | 8q                      |
| (3,2,2)       | 4q                      |
| (3,3,3)       | 66pq - 20q              |

Now, by using the results in Table 6, we have the following computations:

\[
2\chi(H) = \frac{22\sqrt{3}}{3}pq + \frac{12\sqrt{2} - 14\sqrt{3}}{9}q.
\]

**Theorem 7** The second-order sum-connectivity index of \( H = H[p, q] \) is as follows:

\[
2\chi(H) = 22pq + \left(2\sqrt{2} + \frac{4\sqrt{7}}{7} - \frac{20}{3}\right)q.
\]

**Proof.** By Table 6 and the definition of \( 2\chi(G) \).

![Figure 4: Examples of 2-edges paths \( d_{233}, d_{122} \) and \( d_{333} \) of \( H[1,2] \)](image)

![Figure 5: The 2-D graph lattice of \( L = L[p, q] \) with \( p = 2 \) and \( q = 4 \)](image)
Remark 3: We denote a 2-dimensional lattice of pentacene nanotetra by $L = L[p,q]$ (Figure 5). Now we consider the molecular graph. It is easy to see that $|V(L)| = 22pq$ and $|E(L)| = 33pq$. Notice that the edges in the top are affixed to the vertex in the bottom of the figure and the edges in the right side are affixed to the vertex in the left side of the figure to gain a tori in this way.

Theorem 8 The theta, Pi and Sadhana indices of $L = L[p,q]$, $\forall p, q \in \mathbb{N} - \{1\}$ are computed as:

$$\begin{align*}
\theta(L) &= \begin{cases}\vspace{0.1cm}
61p^2q + 44pq^2 - \frac{8}{3}q^3 + \frac{8}{3}q & \text{if } 5p \geq q - 1, \\
261p^2q + 4pq^2 - \frac{1000}{3}p^3 + \frac{40}{3}p & \text{if } 5p < q - 1.
\end{cases}
\end{align*}$$

$$\begin{align*}
\pi(L) &= \begin{cases}\vspace{0.1cm}
1089p^2q^2 - 61p^2q - 44pq^2 + \frac{8}{3}q^3 - \frac{8}{3}q & \text{if } 5p \geq q - 1, \\
1089p^2q^2 - 261p^2q - 4pq^2 + \frac{1000}{3}p^3 - \frac{40}{3}p & \text{if } 5p < q - 1.
\end{cases}
\end{align*}$$

$Sd(L) = 363p^2q + 132pq^2 - 99pq$.

Table 7: The number of co-distant edges of $L = L[p,q]$ for $5p \geq q - 1$

| Type of edges | Number of co-distant edges | Number of qoc |
|---------------|-----------------------------|---------------|
| $e_1$         | $6p$                        | $q$           |
| $e_2$         | $5p$                        | $q$           |
| $e_3$         | $2q$                        | $p$           |
| $e_i$         | $2i$                        | $4$           |
| $\forall i = 1, 2, ..., q - 1$ |                     |               |
| $e_q$         | $2q$                        | $10p - 2q + 2$|

Table 8: The number of co-distant edges of $L = L[p,q]$ for $5p < q - 1$

| Type of edges | Number of co-distant edges | Number of qoc |
|---------------|-----------------------------|---------------|
| $e_1$         | $6p$                        | $q$           |
| $e_2$         | $5p$                        | $q$           |
| $e_3$         | $2q$                        | $p$           |
| $e_i$         | $2i$                        | $4$           |
| $\forall i = 1, 2, ..., 5p - 1$ |                     |               |
| $e_{5p}$      | $10p$                       | $2q - 10p + 2$|

Proof. By using Table 7 and Table 8, we give explicit computing formulae for topological indices of nanotetra, as shown in Figure 5.

Theorem 9 The second-order connectivity and second-order sum-connectivity indices of $L = L[p,q]$ are computed as follows:

$$\begin{align*}
\gamma^2x(L) &= \frac{22\sqrt{3}}{3}pq, \\
\gamma^2\chi(L) &= 22pq.
\end{align*}$$

Proof. We define $d_{33}$ to be the number of edges connecting three vertices of degree 3. It is easy to see that the number of 2-edges paths in $L = L[p,q]$ is equal to $66pq$. Therefore, the proof is clear.

CONCLUSION

In this paper, a simple method enabling to compute the number of co-distant edges and number of qoc of vertical and horizontal pentacene nanotube and nanotetra is presented. By our calculation it is possible to evaluate the omega and its related counting polynomials of these nanostructures for future works.

Acknowledgement

The authors would like to thank the anonymous referees for their helpful comments that have improved the presentation of results in this article.

REFERENCES

1. Diudea M.V. (2002). Toroidal graphenes from 4-valent torii. Bulletin of the Chemical Society of Japan 75: 487 – 492. DOI: https://doi.org/10.1246/bcsj.75.487
2. Diudea M.V. & John P.E. (2001). Covering polyhedral tori. MATCH Communications in Mathematical and in Computer Chemistry 44: 103 – 116.
3. Diudea M.V. & Kirby E.C. (2001). The energetic stability of tori and single-wall tubes. Fullerene Science and Technology 9: 445 – 465. DOI: https://doi.org/10.1081/FST-100107148
4. Diudea M.V., Parv B. & Kirby E.C. (2003). Azulenitic tori. MATCH Communications in Mathematical and in Computer Chemistry 47: 53 – 70.
5. Diudea M.V., Stefu M., Pârv B. & John P.E. (2004). Wiener index of armchair polyhex nanotubes. Croatica Chemica Acta 77: 111 – 115.
6. Khadikar P.V., Joshi S., Bajaj A.V. & Mandlei D. (2004a). Correlations between the benzene character of acenes or...
helicenes and simple molecular descriptors. *Bioorganic and Medicinal Chemistry Letters* **14**: 1187 – 1191.
DOI: https://doi.org/10.1016/j.bmcl.2003.12.062
7. Khadikar P.V., Mandoli D. & Karmakar S. (2006). Sadhana (Sd): a new cyclic index: QSPR/QSAR studies of linear polyacenes. *Bioinformatics Trends* **1**: 51 – 63.
8. Khadikar P.V., Singh S., Jaiswal M. & Mandoli D. (2004b). Topological estimation of electronic absorption bands: arene absorption spectra as a tool for modeling their toxicity environmental pollution. *Bioorganic and Medicinal Chemistry Letters* **14**: 4795 – 4801.
DOI: https://doi.org/10.1016/j.bmcl.2004.06.094
9. Kier L.B. & Hall L.H. (1986). *Molecular Connectivity in Structure Activity Analysis*. John Wiley and Sons, London, England.
10. Nikmehr M.J., Veylaki M. & Soleimani N. (2015). Some topological indices of V-Phenylenic nanotube and nanotori. *Optoelectronics and Advanced Materials-Rapid Communications* **9**(9): 1147 – 1149.
11. Randić M. (1975). On characterization of molecular branching. *Journal of the American Chemical Society* **97**: 6609 – 6615.

12. Soleimani N., Mohseni E. & Maleki N. (2016). Connectivity indices of some famous dendrimers. *Journal of Chemical and Pharmaceutical Research* **8**(8): 229 – 235.
13. Soleimani N., Nikmehr M.J. & Tavallaee H.A. (2014). Theoretical study of nanostructures using topological indices. *Studia Universitatis Babes-Bolyai, Chemia* **59**(4): 139 – 148.
14. Soleimani N., Nikmehr M.J. & Tavallaee H.A. (2015). Computation of the different topological indices of nanostructures. *Journal of the National Science Foundation of Sri Lanka* **43**(2): 127 – 133.
DOI: https://doi.org/10.4038/jnsfsr.v43i2.7940
15. Trinajstić N. (1992). *Chemical Graph Theory*. CRC Press, Boca Raton, Florida, USA.
16. Todescini R. & Consonni V. (2000). *Handbook of Molecular Descriptors*. Wiley-VCH, Weinheim, Germany.
DOI: https://doi.org/10.1002/9783527613106
17. Zhou B. & Trinajstić N. (2009). On a novel connectivity index. *Journal of Mathematical Chemistry* **46**: 1252 – 1270.
DOI: https://doi.org/10.1007/s10910-008-9515-z