ACTA CHEMICA IASI, **24_2**, 122-138 (2016)
DOI: 10.1515/achi-2016-0011

SOME FORMULAS FOR THE POLYNOMIALS AND TOPOLOGICAL INDICES OF NANOSTRUCTURES

Najmeh Soleimani[a*], Esmaeel Mohseni[b], Fahimeh Rezaei[b], Fatemeh Khati[b]

[a]*Young Researchers and Elite Club, Karaj Branch, Islamic Azad University, Karaj, Iran*

[b]*Salehan Institute of Higher Education, Qaemshahr, Iran*

Abstract: In this paper, we focus on the structure of Polycyclic Aromatic Hydrocarbons (PAHs) and calculate the Omega and its related counting polynomials of nanostructures. Also, the exact expressions for the Theta, Sadhana, Pi, Hyper Zagreb and Forgotten Zagreb indices of linear [n]-Tetracene, V-Tetracenic nanotube, H-Tetracenic nanotube and Tetracenic nanotori were computed for the first time. These indices can be used in QSAR/QSPR studies.

***Keywords*:** Polycyclic Aromatic Hydrocarbons (PAHs); Nanostructures; Polynomials; Topological indices.

Introduction

Graph theory has found considerable use in Chemistry, notably in modelling chemical structures. In chemical graph theory, the vertices correspond to the atoms and also the edges correspond to the bonds. Topological indices have some applications in theoretical chemistry, particularly in QSPR/QSAR research.[1] There is a lot of research which has been done on topological indices of various graph families so far, and is of

* Najmeh Soleimani, *email*: soleimani.najmeh@gmail.com

much importance due to their chemical significance. A nanostructure is an object of intermediate size between microscopic and molecular structures. It is a product derived through engineering at molecular scale. Carbon nanotubes have exhibited unusual properties in experimental sciences. They have noteworthy applications in engineering sciences, material sciences and optics. Diudea was the first chemist who considered the matter of computing topological indices of nanostructures.[2-7] In the present article, we continue our works on computing some topological indices of nanostructures.[8-12]

Now, we introduce some notation and terminology. A graph G consist of a set of vertices $V(G)$ and a set of edges $E(G)$. The number of vertices and edges in a graph will be denoted by $|V(G)|$ and $|E(G)|$, respectively. The *degree*, $deg(u)$ of a vertex $u \in V(G)$ is the number of vertices of G adjacent to u. 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:

$$d(v,x) = d(v,y) + 1 = d(u,x) + 1 = d(u,y).$$

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 $C(e) := \{f \in E(G);\ f\ co\ e\}$ 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 $C_1, C_2, \dots, C_k$ form a partition of $E(G)$:

$$E(G) = C_1 \cup C_2 \cup \dots \cup C_k,\ C_i \cap C_j = \emptyset \text{ for } i \neq j \text{ and } i,j = 1,2,\dots,k.$$

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.

Omega and its related counting polynomials:

Four counting polynomials have been defined on the ground of *qoc* strips:

$$\Omega(G,x) = \sum_c m(G,c).x^c \qquad (1)$$

$$\Theta(G,x) = \sum_c m(G,c).c.x^c \qquad (2)$$

$$Sd(G,x) = \sum_c m(G,c).x^{|E(G)|-c} \qquad (3)$$

$$\Pi(G,x) = \sum_c m(G,c).c.x^{|E(G)|-c} \qquad (4)$$

with $m(G,c)$ being the number of strips of length c. For more study, see papers.[13-15] $\Omega(G,x)$ and $\Theta(G,x)$ polynomials count equidistant edges in G while $Sd(G,x)$ and $\Pi(G,x)$, non-equidistant edges.

Some topological indices:

The first derivative (computed at $x = 1$) of these counting polynomials give interesting inter-relations and valuable information on the graph

$$\Theta'(G,1) = \sum_c m(G,c).c^2 = \Theta(G) \qquad (5)$$

$$Sd'(G,1) = \sum_c m(G,c).(|E(G)| - c) = Sd(G) \qquad (6)$$

$$\Pi'(G,1)=\sum_{c} m(G,c).c.(|E(G)|-c)=\Pi(G) \quad (7)$$

We encourage the interested readers to consult papers[16-18] and references therein for more information on Theta index (Θ), Sadhana index (Sd) and Pi index (Π) and its computational techniques. The first Zagreb index have been introduced more than thirty years ago in 1972 by Gutman and Trinajstić.[19] Recently, the Hyper Zagreb index (HM) and Forgotten Zagreb index (F), have been introduced by Shirdel et al.[20] and Furtula and Gutman[21] as the revised version of the first Zagreb index. In fact, they are defined as:

$$HM(G)=\sum_{uv\in E(G)} [deg(u)+deg(v)]^2 \qquad (8)$$

$$F(G)=\sum_{uv\in E(G)} [deg(u)^2+deg(v)^2] \qquad (9)$$

Results and Discussion

Nanostructures of polycyclic aromatic hydrocarbon (PAH) derivatives are potential candidates for improving the performance of nanoelectronics, optoelectronics, and photovoltaic cells.[22-24] Tetracene is the four-ringed member of the series of acenes. Tetracene has several advantages as a fission material. Figure 1 shows the linear [n]-Tetracene.

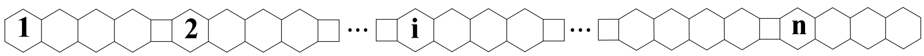

Figure 1. The linear [n]-Tetracene.

Now we compute the closed formula for Omega, Theta, Sadhana, Pi polynomials for linear [n]-Tetracene in the following theorems. To do it, at first, we should consider the following examples.

Example 1. Consider the graph $T = T[2]$, shown in Figure 2. One can see this graph has exactly 3 strips e_1, e_2 and e_3. On the other hand $|C(e_1)| = 10$, $|C(e_2)| = 2$ and $|C(e_3)| = 2$. Hence,

$$\Omega(T, x) = x^{10} + 17x^2,$$
$$\Theta(T, x) = 10x^{10} + 34x^2.$$

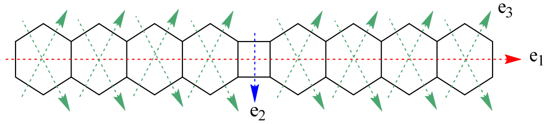

Figure 2. The linear [n]-Tetracene, n=2.

Example 2. Consider the graph $T = T[3]$, shown in Figure 3. One can see this graph has exactly 3 strips e_1, e_2 and e_3. On the other hand $|C(e_1)| = 15$, $|C(e_2)| = 2$ and $|C(e_3)| = 2$. Hence,

$$\Omega(T, x) = x^{15} + 26x^2,$$
$$\Theta(T, x) = 15x^{15} + 52x^2.$$

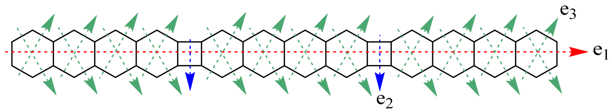

Figure 3. The linear [n]-Tetracene, n=3.

By continuing this method we achieve the graph of linear [n]-Tetracene. Hence, by computing the number of strips of equal size and substitute in the equation (1)-(4) the following theorem can be deduced:

Theorem 1. *Consider the linear [n]-Tetracene (denoted by $T = T[n]$, Figure 1). Then, the Omega and its related polynomials of $T[n]$ are computed as follows:*

$$\Omega(T, x) = x^{5n} + (9n - 1)x^2,$$
$$\Theta(T, x) = 5nx^{5n} + (18n - 2)x^2,$$
$$Sd(T, x) = (9n - 1)x^{23n-4} + x^{18n-2},$$
$$\Pi(T, x) = (18n - 2)x^{23n-4} + 5nx^{18n-2}.$$

Proof. To compute the omega and theta polynomials of $T[n]$, it is enough to calculate *C(e)* for every e in $E(T)$. By Figure 2 and Figure 3, one can see that, there are three distinct cases of *qoc* strips. We denote the corresponding edges by e_1, e_2 and e_3. By continuing method it is easy to check that $|C(e_1)| = 5n$, $|C(e_2)| = 2$ and $|C(e_3)| = 2$. On the other hand, there are $1, n-1$ and $8n$ similar edges for each of edges e_1, e_2 and e_3, respectively.

So, we have

$$\Omega(T,x) = \sum_c m(T,c).x^c$$
$$= (1 \times x^{5n}) + \left((n-1) \times x^2\right) + (8n \times x^2)$$
$$= x^{5n} + (9n-1)x^2.$$

Also,

$$\Theta(T,x) = \sum_c m(T,c).c.x^c$$
$$= (1 \times 5n \times x^{5n}) + \left((n-1) \times 2 \times x^2\right) + (8n \times 2 \times x^2)$$
$$= 5nx^{5n} + (18n-2)x^2.$$

Since, first derivative of omega polynomial (in *x=1*), equals the number of edges in the graph. We have

$$\Omega'(T,1) = |E(T)| = 23n - 2.$$

Thus, we have

$$Sd(T,x) = \sum_c m(T,c).x^{|E(T)|-c}$$
$$= \left(1 \times x^{|E(T)|-5n}\right) + \left((n-1) \times x^{|E(T)|-2}\right) + \left(8n \times x^{|E(T)|-2}\right)$$
$$= (9n-1)x^{23n-4} + x^{18n-2}.$$

Also,

$$\Pi(T,x) = \sum_c m(T,c).c.x^{|E(T)|-c}$$
$$= \left(1 \times 5n \times x^{|E(T)|-5n}\right) + \left((n-1) \times 2 \times x^{|E(T)|-2}\right)$$
$$+ \left(8n \times 2 \times x^{|E(T)|-2}\right)$$
$$= (18n-2)x^{23n-4} + 5nx^{18n-2}.$$

Theorem 2. *The Theta index, Sadhana index and Pi index of the linear [n]-Tetracene are computed as:*

$\Theta(T) = 25n^2 + 36n - 4,$

$Sd(T) = 207n^2 - 41n + 2,$

$\Pi(T) = 504n^2 - 128n + 8.$

Proof. By using equations (5)-(7) and proof of Theorem 1, we are done.

Now, we consider the vertical Tetracenic nanotube and denote by $G = G[p,q]$. For other related research and historical details, see the paper series. [25,26]

Theorem 3. *Let* $p,q \in N$. *Then, the Omega and its related polynomials of* $G[p,q]$ $(\forall p,q > 1;\ 4p \geq q-1)$ *are given by:*

$$\Omega(G,x) = qx^{5p} + (q-1)x^{4p} + 4\sum_{i=1}^{q-1} x^{2i} + (9p-2q+2)x^{2q},$$

$$\Theta(G,x) = 5pqx^{5p} + 4p(q-1)x^{4p} + 4\sum_{i=1}^{q-1} 2ix^{2i}$$
$$+ (18pq - 4q^2 + 4q)x^{2q},$$

$$Sd(G,x) = qx^{27pq-9p} + (q-1)x^{27pq-8p} + 4\sum_{i=1}^{q-1} x^{(27pq-4p)-2i}$$
$$+ (9p-2q+2)x^{27pq-4p-2q},$$

$$\Pi(G,x) = 5pqx^{27pq-9p} + 4p(q-1)x^{27pq-8p} + 4\sum_{i=1}^{q-1} 2ix^{(27pq-4p)-2i} + (18pq - 4q^2 + 4q)x^{27pq-4p-2q}.$$

Proof. Let $G = G[p,q]$ be the V-Tetracenic nanotube, with $18pq$ vertices (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 compute Omega polynomial. By using the cut method and Figure 4, there are some distinct cases of *qoc* strips. We denote the corresponding edges by $e_1, e_2, e_3, \dots, c_q$.

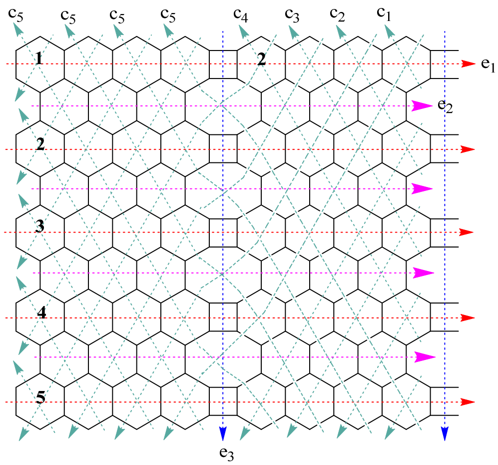

Figure 4. The *qoc* strips of edges $e_1, e_2, e_3, c_1, c_2, c_3, c_4$ and c_5 in graph of $G[2,5]$.

Table 1. The number of co-distant edges of V-Tetracenic nanotube.

Type of Edges	$\lvert C(e)\rvert$	m
e_1	$5p$	q
e_2	$4p$	$q-1$
e_3	$2q$	p
c_i	$2i$	4
$\forall i = 1,2,\dots,q-1$		
c_q	$2q$	$8p-2q+2$

Now, we apply the formula of Omega polynomial to compute this polynomial for G. Since

$$\Omega(G,x) = \sum_{c} m(G,c).x^{c},$$

by using Table 1, we have

$$\Omega(G,x) = qx^{5p} + (q-1)x^{4p} + px^{2q} + \sum_{i=1}^{q-1} 4x^{2i} + (8p-2q+2)x^{2q}.$$

Also, since

$$\Theta(G,x) = \sum_{c} m(G,c).c.x^{c},$$

we get

$$\Theta(G,x) = 5pqx^{5p} + 4p(q-1)x^{4p} + 2pqx^{2q} + \sum_{i=1}^{q-1} 4 \times 2ix^{2i}$$
$$+ (16pq - 4q^2 + 4q)x^{2q}.$$

The first derivative (computed at $x = 1$) of Omega polynomial is equal to the number of edges. Therefore, $|E(G)| = 27pq - 4p$. From equations (1)-(4), one can obtain the Sadhana polynomial and Pi polynomial by replacing x^{c} with $x^{|E(G)|-c}$ in Omega polynomial and Theta polynomial. This completes our proof.

Theorem 4. *The Theta index, Sadhana index and Pi index of the V-Tetracenic nanotube are computed as:*

$$\Theta(G) = 41p^2q + 36pq^2 - 16p^2 - \frac{8}{3}q^3 + \frac{8}{3}q,$$

$$Sd(G) = 243p^2q + 108pq^2 - 36p^2 - 124pq + 16p,$$

$$\Pi(G) = 729p^2q^2 - 257p^2q + 32p^2 - 36pq^2 + \frac{8}{3}q^3 - \frac{8}{3}q.$$

Proof. By using Table 1 and equations (5)-(7), we are done.

In following, we consider the horizontal Tetracenic nanotube and denote by $H = H[p,q]$ (Figure 5). The various types of quasi-orthogonal cuts are drawn by arrows.

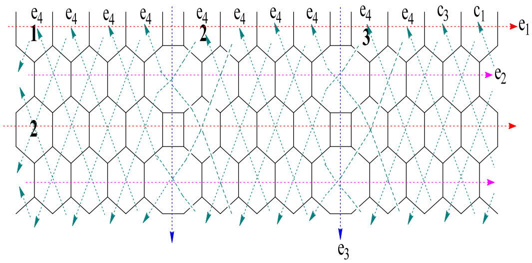

Figure 5. The *qoc* strips of edges e_1, e_2, e_3, e_4, c_1 and c_3 in graph of $H[3,2]$.

Theorem 5. *Let $p, q \in N$. Then, the Omega and its related polynomials of $H[p,q]$ $(\forall p,q > 1; 4p \geq q)$ are given by:*

$$\Omega(H,x) = qx^{5p} + qx^{4p} + 4\sum_{\substack{i=1 \\ i\ is\ odd}}^{2q-1} x^i + (9p-2q-1)x^{2q},$$

$$\Theta(H,x) = 5pqx^{5p} + 4pqx^{4p} + 4\sum_{\substack{i=1 \\ i\ is\ odd}}^{2q-1} ix^i + (18pq-4q^2-2q)x^{2q},$$

$$Sd(H,x) = qx^{27pq-2q-5p} + qx^{27pq-2q-4p} + 4\sum_{\substack{i=1 \\ i\ is\ odd}}^{2q-1} x^{(27pq-2q)-i} + (9p-2q-1)x^{27pq-4q},$$

$$\Pi(H,x) = 5pqx^{27pq-2q-5p} + 4pqx^{27pq-2q-4p} + 4\sum_{\substack{i=1 \\ i\ is\ odd}}^{2q-1} ix^{(27pq-2q)-i} + (18pq-4q^2-2q)x^{27pq-4q}.$$

Proof. Let $H = H[p,q]$ be the H-Tetracenic nanotube, with $18pq$ vertices and $27pq - 2q$ edges (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, see Figure 5). By using the cut method and computing the number of co-distant edges of $H = H[p, q]$, we can fill the Table 2.

Table 2. The number of co-distant edges of H-Tetracenic nanotube.

Type of Edges	$\|C(e)\|$	m
e_1	$5p$	q
e_2	$4p$	q
e_3	$2q$	$p-1$
c_i , i is odd. $\forall i = 1, 3, \ldots, 2q-1$	i	4
e_4	$2q$	$8p-2q$

By using these calculations, equations (1)-(4), the theorem is proved.

Theorem 6. *The Theta index, Sadhana index and Pi index of the H-Tetracenic nanotube are computed as:*

$$\Theta(H) = 41p^2q + 36pq^2 - 4q^2 - \frac{8}{3}q^3 - \frac{4}{3}q,$$

$$Sd(H) = 243p^2q + 108pq^2 - 8q^2 - 72pq + 4q,$$

$$\Pi(H) = 729p^2q^2 - 144pq^2 - 41p^2q + \frac{8}{3}q^3 + 8q^2 + \frac{4}{3}q.$$

Proof. By using Table 2 and equations (5)-(7), we are done.

Now, we are ready to compute the Omega and its related counting polynomials of Tetracenic nanotori $K = K[p, q]$, depicted in Figure 6. The various types of quasi-orthogonal cuts are drawn by arrows.

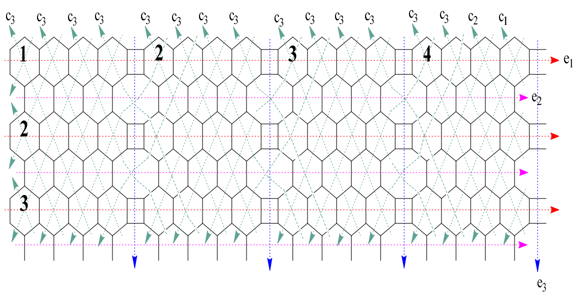

Figure 6. The *qoc* strips of edges e_1, e_2, e_3, c_1, c_2 and c_3 in graph of $[4, 3]$.

Theorem 7. *Let* $p, q \in N$. *Then, the Omega and its related polynomials of* $K[p,q]$ $(\forall p, q > 1; 4p \geq q-1)$ *are given by:*

$$\Omega(K,x) = qx^{5p} + qx^{4p} + 4\sum_{i=1}^{q-1} x^{2i} + (9p - 2q + 2)x^{2q},$$

$$\Theta(K,x) = 5pqx^{5p} + 4pqx^{4p} + 4\sum_{i=1}^{q-1} 2ix^{2i} + (18pq - 4q^2 + 4q)x^{2q},$$

$$Sd(K,x) = qx^{27pq-9p} + qx^{27pq-8p} + 4\sum_{i=1}^{q-1} x^{(27pq-4p)-2i} + (9p - 2q + 2)x^{27pq-4p-2q},$$

$$\Pi(K,x) = 5pqx^{27pq-9p} + 4pqx^{27pq-8p} + 4\sum_{i=1}^{q-1} 2ix^{(27pq-4p)-2i} + (18pq - 4q^2 + 4q)x^{27pq-4p-2q}.$$

Proof. Let $K = K[p,q]$ be the Tetracenic nanotori, with $18pq$ vertices and $27pq$ edges. The proof can be done in the same way as in the proof of Theorem 3.

Table 3. The number of co-distant edges of Tetracenic nanotori.

Type of Edges	$\lvert C(e)\rvert$	m
e_1	$5p$	q
e_2	$4p$	q
e_3	$2q$	p
c_i $\forall i = 1,2,\dots,q-1$	$2i$	4
c_q	$2q$	$8p - 2q + 2$

The results of the above theorem can be summarized as follows:

Theorem 8. *The Theta index, Sadhana index and Pi index of the Tetracenic nanotori are computed as:*

$$\Theta(K) = 41p^2q + 36pq^2 - \frac{8}{3}q^3 + \frac{8}{3}q,$$

$$Sd(K) = 243p^2q + 108pq^2 - 81pq,$$

$$\Pi(K) = 729p^2q^2 - 41p^2q - 36pq^2 + \frac{8}{3}q^3 - \frac{8}{3}q.$$

Finally, we calculate the Hyper Zagreb index and forgotten Zagreb index of nanostructures by use an algebraic method.

Theorem 9. *The Hyper Zagreb index and forgotten Zagreb index of nanostructures are computed as:*

Nanostructure	HM	F
G	$972pq - 320p$	$486pq - 152p$
H	$972pq - 124q$	$486pq - 76q$
K	$972pq$	$486pq$

Proof. For computing the Hyper Zagreb index and forgotten Zagreb index of nanostructures ($G[p,q], H[p,q]$ and $K[p,q]$) we consider three type edges, (a) edge E_1 with ended vertices of degree 2 and 2, (b) edge E_2 with ended vertices of degree 2 and 3, (c) edge E_3 with ended vertices of degree 3 and 3. The obtained data is arranged in Table 4.

Table 4. Computing the number of edges in nanostructures.

Nanostructure	$\lvert E_1\rvert$	$\lvert E_2\rvert$	$\lvert E_3\rvert$
G	0	$16p$	$27pq - 20p$
H	$2q$	$4q$	$27pq - 8q$
K	0	0	$27pq$

Using the data given by Table 4, the Hyper Zagreb and forgotten Zagreb indices are calculated.

Examples

In this section, we give some examples in the following tables. In fact, we obtain some topological indices of nanostructures by replacing different number of p and q.

Table 5. Some values of the topological indices of V-Tetracenic nanotube.

p	q	$Sd(G)$	$\Theta(G)$	$\Pi(G)$	$HM(G)$	$F(G)$
2	2	2200	536	9464	3248	1640
2	3	4004	1012	22704	5192	2612
2	4	6240	1584	41680	7136	3584
2	5	8908	2236	66408	9080	4556

Table 6. Some values of the topological indices of H-Tetracenic nanotube.

p	q	$Sd(H)$	$\Theta(H)$	$\Pi(H)$	$HM(H)$	$F(H)$
3	2	5214	1130	23834	5584	2764
3	3	8769	1967	54202	8376	4146
3	4	12956	2964	96892	11168	5528
3	5	17775	4105	151920	13960	6910

Table 7. Some values of the topological indices of Tetracenic nanotori.

p	q	$Sd(K)$	$\Theta(K)$	$\Pi(K)$	$HM(K)$	$F(K)$
4	2	8856	1872	44784	7776	3888
4	3	14580	3200	101776	11664	5832
4	4	21168	4768	181856	15552	7776
4	5	28620	6560	285040	19440	9720

Conclusions

In theoretical chemistry, molecular structure descriptors are used to compute properties of chemical compounds. Among topological descriptors, topological indices play significant roles in anticipating chemical phenomena. This article is the continuation of the work[26], which were provided general partitions of co-distant edges of nanostructures. We used these partitions to computed topological indices of linear [n]-Tetracene, vertical and horizontal Tetracenic nanotube and nanotori.

Acknowledgements

The authors would like to thank the anonymous referee for his/her helpful comments that have improved the presentation of results in this article.

References

1. Todeschini, R.; Consonni, V. Handbook of Molecular Descriptors, *Weinheim, Wiley-VCH*, 2000.
2. Diudea, M. V.; Graovac, A. Generation and graph-theoretical properties of c_4-tori, Commun. Math. Comput. Chem. **2001**, *44*, 93-102.
3. Diudea, M. V.; Silaghi-Dumitrescu, I.; Parv, B. Toranes versus torenes. *Commun. Math. Comput. Chem*. **2001**, *44*, 117-133.
4. Diudea, M. V.; John, P. E. Covering polyhedral tori. *MATCH Commun. Math. Comput. Chem*. **2001**, *44*, 103-116.
5. Diudea, M. V. Toroidal graphenes from 4-valent tori. *Bull. Chem. Soc. Jpn*. **2002**, *75*, 487-492.
6. Diudea, M. V. Hosoya polynomial in tori. *Commun. Math. Comput. Chem*. **2002**, *45*, 109-122.
7. Diudea, M. V. Omega Polynomial in All *R*[8] Lattices. *Iranian Journal of Mathematical Chemistry*, **2010**, *1(1)*, 69-77.

8. Soleimani, N.; Nikmehr, M. J.; Tavallaee, H. A. Theoretical study of nanostructures using topological indices. *Studia Universitatis Babes-Bolyai, Chemia*. **2014**, *59(4)*, 139-148.

9. Nikmehr, M. J.; Veylaki, M.; Soleimani, N. Some topological indices of V-Phenylenic nanotube and nanotori. *Optoelectron. Adv. Mater.-Rapid Comm*. **2015**, *9(9)*, 1147-1149.

10. Nikmehr, M. J.; Soleimani, N.; Tavallaee, H. A. Computing some topological indices of carbon nanotubes. *Proceedings of the Institute of Applied Mathematics*. **2015**, *4(1)*, 20-25.

11. Soleimani, N.; Mohseni, E.; Maleki, N. Connectivity indices of some famous dendrimers. *Journal of Chemical and Pharmaceutical Research*. **2016**, *8(8)*, 229-235.

12. Soleimani, N.; Mohseni, E.; Helalbin, S. Theoretical study of nanostar dendrimers. *Studia Universitatis Babes-Bolyai, Chemia*. **2016**, *61(1)*, 127-140.

13. Diudea, M. V. Omega polynomial, *Carpath. J. Math*. **2006**, *22*, 43-47.

14. Diudea, M. V.; Cighera, S.; Johnb, P. E. Omega and Related Counting Polynomials, *MATCH Commun. Math. Comput. Chem*. **2008**, *60*, 237-250.

15. Ashrafi, A. R.; Ghorbani, M.; Jalali, M. Computing sadhana polynomial of V-phenylenic nanotubes and nanotori. *Ind. J. Chem*. **2008**, *47A*, 535-537.

16. Khadikar, P. V.; Mandoli, D.; Karmakar, S. Sadhana(Sd): A New Cyclic Index: QSPR/QSAR Studies of Linear Polyacenes. *Bioinformatics Trends*. **2006**, *1*, 51-63.

17. Khadikar, P. V.; Joshi, S.; Bajaj, A. V.; Mandloi, D. Correlations between the Benzene Character of Acenes or Helicenes and Simple Molecular Descriptors. *Bioorg. Med. Chem. Lett*. **2004**, *14*, 1187-1191.

18. Khadikar, P. V.; Singh, S.; Jaiswal, M.; Mandoli, D. Topological Estimation of Electronic Absorption Bands: Arene Absorption Spectra as a Tool for Modeling Their Toxicity Environmental Pollution. *Bioorg. Med. Chem. Lett*. **2004**, *14*: 4795-4801.

19. Gutman, I.; Trinajstić, N. Graph theory and molecular orbitals, Total π-electron energy of alternant hydrocarbons. *Chem. Phys. Lett.* **1972**, *17*, 535-538.

20. Shirdel, G. H.; Rezapour, H.; Sayadi, A. M. The Hyper-Zagreb Index of Graph Operations. *Iranian Journal of Mathematical Chemistry*. **2013**, *4(2)*, 213-220.

21. Furtula, B.; Gutman, I. A forgotten topological index, *J. Math. Chem.* **2015**, *53*, 1184-1190.

22. Feng, X. L.; Liu, M. Y.; Pisula, W.; Takase, M.; Müllen, K. Supramolecular Organization and Photovoltaics for Triangle-shaped discotics with swallow-tails. *Adv. Mater*. **2008**, *14*, 2684-2689.

23. Hietschold, M.; Lackinger, M.; Griessl, S.; Heckl, W. M.; Gopakumar, T. G.; Flynn, G. W. Molecular structures on crystalline metallic surfaces–From STM images to molecular electronics. *Microelect. Engineer*. **2005**, *82*, 207-214.

24. Schmidt-Mende, L.; Fechtenkotter, A.; Müllen, K.; Moons, E.; Friend, R. H.; Mackenzie, J. D. Self-organized discotic liquid crystals for high-efficiency organic photovoltaics. *Science*. **2001**, *293*, 1119-1122.

25. Diudea, M. V. Phenylenic and naphthylenic tori. *Fullerenes, Nanotubes Carbon Nanostruct*. **2002**, *10*, 273-292.

26. Soleimani, N.; Nikmehr, M. J.; Tavallaee, H. A. Computation of the different topological indices of nanostructures. *Journal of the national science foundation of Sri Lanka*. **2015**, *43(2)*, 127-133.