Hosoya polynomials of the capped zig-zag nanotubes *

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Abstract

The Hosoya polynomial of a graph G is defined as $H(G,x) = \sum_{k \geqslant 0} d(G,k)x^k$, where $d(G,k)$ is the number of the vertex pairs at distance k in G. The calculation of Hosoya polynomials of molecular graphs is a significant topic because some important molecular topological indices such as Wiener index, hyper-Wiener index, and Wiener vector, can be obtained from Hosoya polynomials. Hosoya polynomials of zig-zag open-ended nanotubes have been given by Xu and Zhang et al. A capped zig-zag nanotube $T(p,q)[C,D;a]$ consists of a zig-zag open-ended nanotube $T(p,q)$ and two caps C and D with the relative position a between C and D. In this paper, we give a general formula for calculating Hosoya polynomial of any capped zig-zag nanotube. By the formula, Hosoya polynomial of any capped zig-zag nanotube can be deduced. Furthermore, it is also shown that any two non-isomorphic capped zig-zag nanotube $T(p,q)[C,D;a_1]$, $T(p,q)[C,D;a_2]$ with $q \geq q^* \geq p+1$ have the same Hosoya polynomial, where q^* is a integer which depends on structures of C and D.

K-words: Hosoya polynomial, Wiener index, capped zig-zag nanotubes.

* The project supported by NSFC(10831001)), NSFC (11171279),NSFC (11001113) and the Natural Science Foundation of Fujian Province of China (No. 2010J01008) and FJCEF(JA11163).

1 Introduction

The Wiener index was first introduced by Wiener [28] in 1947 for approximating the boiling points of alkanes. The *Wiener index* of a graph G is defined as:

$$W(G) = \sum_{\{u,v\}\subseteq V(G)} d_G(u,v).$$

where $d_G(u,v)$ is the distance between a pair of vertices u and v of G.

The Wiener index was originally defined for acyclic structures only, and the definition was later extended to general graphs by Hosoya (as the sum of distances); and in another maybe more natural way by Gutman (called Szeged index) [9]. Since then, Wiener index has been shown to correlate with many other properties of molecules [3, 4, 12, 13, 14, 15, 20, 28].

The hyper-Wiener index of an acyclic structure was first introduced by Randić [25], and was extended by Klein [22] so as to be applicable for any (cycle-containing) structure. For a graph G, the *hyper-Wiener index* $R(G)$ of G is defined as:

$$R(G) = R = \frac{1}{2} \sum_{\{u,v\}\subseteq V(G)} (d_G(u,v) + d_G^2(u,v)).$$

The *Wiener vector* of a graph G is introduced by Guo et al. [17] as follows:

For a connected graph G, let $W_k = \sum_{\{u,v\}\subseteq V(G),\ d_G(u,v)=k} d_G(u,v)$, $k = 1, 2, \cdots$. The vector $(W_1, W_2, \cdots)$ is called the Wiener vector of G, denoted by $WV(G)$.

Clearly, the sum of all components of the Wiener vector of G is just equal to the Wiener index of G, and Wiener vectors have higher discrimination than do Wiener indices.

The *Hosoya polynomial* of a connected graph G, introduced by Hosoya [18], is defined as:

$$H(G,x) = \sum_{k\geqslant 0} d(G,k)x^k,$$

where $d(G,k)$ is the number of vertex pairs at distance k in G.

Hosoya polynomials are also called Wiener polynomials, Wiener-Hosoya [8] and Hosoya-Wiener polynomials [34], because Wiener index, hyper-Wiener index, and Wiener vector of a graph G can be obtained from Hosoya polynomial $H(G)$ of G.

It was shown in Refs. [2, 17, 18, 27, 33] that $W(G) = H'(G,1)$, $R(G) = H'(G,1) + \frac{1}{2}H''G,1)$, and the Wiener vector $WV(G) = (W_1, W_2, ...)$ consists of the coefficients of the derivative $H'(G,x)$ of the Hosoya polynomial, where W_k is equal to the coefficient $kd(G,k)$ of x^{k-1} in $H'(G,x)$.

Hosoya polynomial of a graph contains more information about distance in the graph than any of the hitherto proposed distance-based topological indices, not only these, but some celebrated topological indices of a graph are often obtained directly from its Hosoya polynomial [1, 21, 24, 26]. So Hosoya polynomial and the quantities derived from it will play a significant role in QSAR/QSPR studies, and abundant literature appeared on this topic for the theoretical consideration [10, 11] and computation [15, 16, 23, 25, 27, 30, 31, 32, 33].

In ref. [27, 32, 33], Sagan, Yang, Yeh, Yan et al. computed some Hosoya polynomials for some common graphs, and a dendrimer (a certain highly regular tree of interest to chemists), and certain graphs of chemical interest. Gutman et al. [16] gave Hosoya polynomials of some benzenoid graphs. Diudea [6] gave analytical formulas for calculating Hosoya polynomials in several classes of toroidal nets. Xu, Zhang, and Diudea [30, 31] gave Hosoya polynomials of open-ended nanotubes and benzenoid chains.

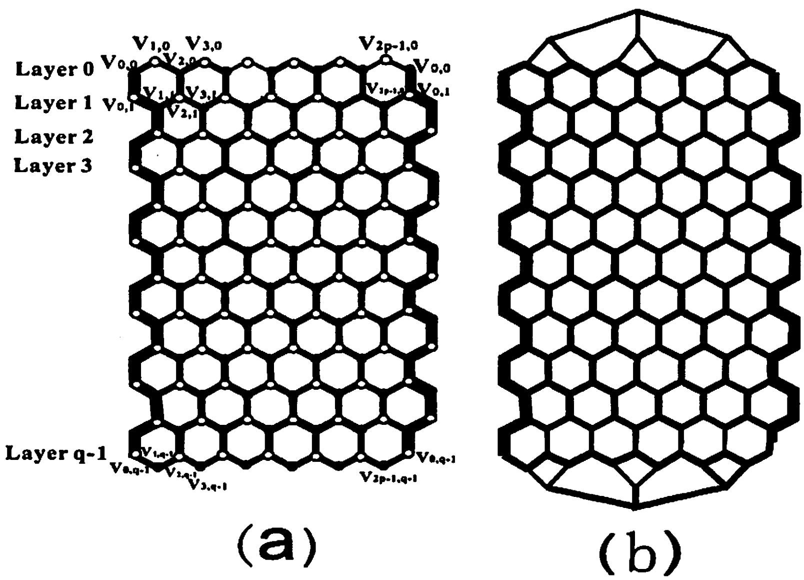

Fig. 1: (a). A zig-zag open-ended nanotube $T(p,q)$ with $p = 6$ and $q = 12$ in a planar mode; (b). A capped zig-zag nanotube in a planar mode.

A *zig-zag open-ended nanotube* [5, 30] is a finite section of a polyhex cylinder, described by two parameters p and q, denoted by $T(p,q)$ [23], which can be denoted in a planar mode as shown in Fig. 1(a), where the axis of $T(p,q)$ is vertical and the left bold boundary is identical with the right bold boundary with cutting off the nanotube $T(p,q)$.

A capped zig-zag nanotube [23, 29], denoted by $T(p,q)[C,D;a]$, is constructed by adding two suitable caps C and D to the upper open end and lower open end of a zig-zag open-ended nanotube $T(p,q)$ respectively, where a denotes the relative position between C and D (see Fig. 1(b)). Since $T(p,q)$ is symmetric round its axis, a cap, say D, may be arbitrarily fixed to the lower open end of $T(p,q)$, and then the other cap C may have $2p$ different positions corresponding to D for adding C to the upper open end of $T(p,q)$. Let $a = 0,1,2,\cdots,p-1;\ p,p+1,p+2,\cdots,2p-1$ denote the $2p$ different position of C corresponding to D, let $T(p,q)[C,D;0]$ be such a capped zig-zag nanotube, let $T(p,q)[C,D;p]$ be the capped zig-zag nanotube obtained from $T(p,q)[C,D;0]$ by overturning the cap C round a horizontal axis, and let $T(p,q)[C,D;a^*]$ (resp. $T(p,q)[C,D;p+a^*]$) denote the capped zig-zag nanotube obtained from $T(p,q)[C,D;0]$ (resp. $T(p,q)[C,D;p]$) by rotating the cap C $\frac{a^*}{p}$ circle round the axis of $T(p,q)$ anticlockwise where $a^* \in \{0,1,2,\cdots,p-1\}$.

Note that if one of C and D has a rotation automorphism of order p round the axis of $T(p,q)$ and one of C and D has a reflection automorphism about a plane passing through the axis of $T(p,q)$), then the $2p$ capped zig-zag nanotubes $T(p,q)[C,D;a]$ for $a = 1,2,\cdots,2p-1$ are pairwise isomorphic. In the case, we also simply denote the $2p$ isomorphic capped zig-zag nanotubes by $T(p,q)[C,D]$. If each of two caps has no reflection automorphism and no rotation automorphism of order p round the axis of $T(p,q)$, then either the $2p$ capped nanotubes are pairwise not isomorphic or some (not all) of the $2p$ capped nanotubes might be isomorphic. However, we shall show that any two non-isomorphic capped zig-zag nanotubes $T(p,q)[C,D;a_1]$, $T(p,q)[C,D;a_2]$ with $q \geq q^* \geq p+1$ have the same Hosoya polynomial (where q^* is defined in Definition 1 in the next section).

Recently, Xu and Zhang [30] obtained the Hosoya polynomial of the zig-zag open-ended nanotubes $T(p,q)$ as follows:

Theorem 1.1 *[Xu and Zhang [30]] (1) If* $q \leqslant \frac{p}{2}$,
$H(T(p,q),x) = 2pq + p\sum_{i=1}^{2q-1}(-i^2+3qi)x^i + 2pq^2\sum_{i=2q}^{p-1}x^i + pq(2q-1)x^p + 2p\sum_{i=p+1}^{p+q-1}(p+q-i)^2x^i$.

(2) *If* $\frac{p}{2} < q \leqslant p$, $H(T(p,q),x) = 2pq + p\sum_{i=1}^{p-1}(-i^2+3qi)x^i + p(3pq - p^2 - q)x^p + p\sum_{i=p+1}^{2q-1}(2p^2+4pq+i^2-4pi-qi)x^i + 2p\sum_{i=2q}^{p+q-1}(p+q-i)^2x^i$.

(3) *If* $q \geqslant p+1$, $H(T(p,q),x) = 2pq + p\sum_{i=1}^{p-1}(-i^2+3qi)x^i + p(3pq - p^2 - q)x^p + p\sum_{i=p+1}^{2p-1}(2p^2+4pq+i^2-4pi-qi)x^i + p^2\sum_{i=2p}^{2q-1}(2q-i)x^i$.

For a capped zig-zag nanotube $T(p,q)[C,D;a]$ consisting of an zig-zag open-ended nanotube $T(p,q)$ and two caps C and D, because of the variety of caps and that two vertices in $T(p,q)$ might have the distance in $T(p,q)$ different from the distance in $T(p,q)[C,D;a]$, the calculation of Hosoya polynomials of capped zig-zag nanotubes is more difficult than zig-zag open-ended nanotubes.

In this paper, we focus on Hosoya polynomials of capped zig-zag nanotubes. In order to calculate Hosoya polynomial of a capped zig-zag nanotube, we divide the capped zig-zag nanotube into three parts so that any two vertices in a part have the same distance in both the part and whole capped zig-zag nanotube, and then obtain a general formula for calculating Hosoya polynomial of any capped zig-zag nanotube from Hosoya polynomials of their three parts and from some other terms between the three parts. By the formula, the Hosoya polynomial of any capped zig-zag nanotube can be deduced. Furthermore, it is shown that any two non-isomorphic capped zig-zag nanotube $T(p,q)[C,D;a_1]$, $T(p,q)[C,D;a_2]$ with $q^* \geq p+1$ have the same Hosoya polynomial.

2 Hosoya polynomials of capped zig-zag nanotubes

Note that a zig-zag open-ended nanotube $T(p,q)$ is bipartite, its vertices can be colored such that every vertical edge connects a black top vertex with a white bottom vertex. For convenience, we denote by *layer* $0,1,\cdots,q-1$, the horizontal zig-zag lines in the planar mode of $T(p,q)$ from top to bottom, respectively. The layer k corresponds to a cycle C_k of length $2p$, $C_k = v_{0,k}v_{1,k}\cdots v_{2p-1,k}v_{0,k}$ where $v_{0,k}$ corresponds to the leftmost vertex in planar mode of $T(p,q)$ (see Fig. 1(a)). The cycles C_0 and C_{q-1} are called the upper boundary and the lower boundary of $T(p,q)$ respectively.

If two suitable caps C and D are added to $T(p,q)$ to obtain a caped zig-zag nanotube $T(p,q)[C,D;a]$, then the boundary $B(C)$ of C (resp. the boundary $B(D)$ of D) is identified with the boundary C_0 (resp. C_{q-1}) of $T(p,q)$.

For any two vertices in a cap C (resp. D), we need to investigate under what condition the distance between u and v in $T(p,q)$, denoted by $d_{T(p,q)}(u,v)$, is equal to the distance $d_{T(p,q)[C,D;a]}(u,v)$ in $T(p,q)[C,D;a]$.

Lemma 2.1 *Let $T(p,q)[C,D;a]$ be a caped zig-zag nanotube, and let u and v be any two vertices in a cap C (or D). If $q \geq \frac{1}{4}(p-1)$, then the distance between u and v in $T(p,q)$ is equal to the distance in $T(p,q)[C,D;a]$, that is, $d_{T(p,q)}(u,v) = d_{T(p,q)[C,D;a]}(u,v)$.*

Proof. Clearly, $d_{T(p,q)[C,D;a]}(u,v) \leq d_{T(p,q)}(u,v)$.

Assume that $q \geq \frac{1}{4}(p-1)$ but $d_{T(p,q)[C,D;a]}(u,v) < d_{T(p,q)}(u,v)$. Then there is a shortest path $P(u,v)$ in $T(p,q)[C,D;a]$ whose length $l(P(u,v))$

is less than $d_{T(p,q)}(u,v)$. Hence, $P(u,v)$ must contain some edges not in C. Let u' and v' be the vertices on $P(u,v)$ such that the path $P(u,u')$ and the path $P(v',v)$ on $P(u,v)$ are contained in C, and the path $P(u',v')$ on $P(u,v)$ has the end edges not in C. Let $P_{B(C)}(u',v')$ be a path on the boundary of C with length less or equal to p. Then $P(u,u') \cup P_{B(C)}(u',v') \cup P(v',v)$ contains a path in C with end vertices u and v, say $P_C(u,v)$. Thus we have that $l(P(u,u')) + l(P_{B(C)}(u',v')) + l(P(v',v)) \geq l(P_C(u,v)) \geq d_{T(p,q)}(u,v) > l(P(u,v)) = l(P(u-u')) + l(P(u',v')) + l(P(v'-v))$, and so $l(P(u',v')) < l(P_{B(C)}(u',v')) \leq p$.

Moreover, $P(u',v')$ must contain some edges in D which are not on the boundary $B(D)$ of D. Otherwise, $P(u',v')$ is contained in $T(p,q)$, and so $l(P_{B(C)}(u',v')) \geq l(P(u',v'))$, a contradiction. Let u'' and v'' be the vertices on $P(u',v')$ such that the path $P(u',u'')$ and the path $P(v'',v')$ on $P(u',v')$ are contained in $T(p,q)$, and the path $P(u'',v'')$ on $P(u',v')$ has the end edges in D which are not on $B(D)$. Then $l(P(u',u'')) = l(P(v'',v')) = 2q$ and $l(P(u'',v'')) \geq 1$. Therefore, $p > l(P(u',v')) \geq 4q+1$, that is, $q < \frac{1}{4}(p-1)$, again a contradiction. □

In the paper, we shall only consider longer caped zig-zag nanotubes $T(p,q)[C,D;a]$ with $q \geq \frac{1}{4}(p-1)$. By the above lemma, for any two vertices in a cap, their distance in the cap is the same with the distance in $T(p,q)[C,D;a]$. However, for two vertices in $T(p,q)$, their distance in $T(p,q)$ may be different from the distance in $T(p,q)[C,D;a]$. For example, for two vertices v_i and v_j on the common boundary of $T(p,q)$ and C, if $d_C(v_i,v_j) < d_{B(C)}(v_i,v_j)$, then $d_{T(p,q)}(v_i,v_j) > d_{T(p,q)[C,D;a]}(v_i,v_j)$.

For a cap C of a caped zig-zag nanotube $T(p,q)[C,D;a]$, a vertex on the boundary $B(C)$ of C is said to be an attachment vertex of C if it is adjacent to a vertex in $T(p,q)[C,D;a] - V(C)$. Let $V_a(C)$ be the set of attachment vertices of C, and let

$$m = \max\{d_{B(C)}(v_i,v_j) - d_C(v_i,v_j) \mid v_i,v_j \in V_a(C)\}.$$

We will show that, for $t \geq \lceil \frac{m+2}{2} \rceil$, any two vertices on the cycle C_t (the layer t) in $T(p,q)$ have the same distance in both C_t and $T(p,q)[C,D;a]$.

Theorem 2.2 *Let $T(p,q)[C,D;a]$ be a caped zig-zag nanotube, and $m = \max\{d_{B(C)}(v_i,v_j) - d_C(v_i,v_j) \mid v_i,v_j \in V_a(C)\} \geq 0$. If $t \geq \lceil \frac{m+2}{2} \rceil$, then any two vertices on the cycle C_t in $T(p,q)$ have the same distance in both C_t and $T(p,q)[C,D;a]$.*

Proof. By contradiction.

Assume that there are two vertices v_i and v_j on C_t such that $d_{C_t}(v_i,v_j) - d_{T(p,q)[C,D;a]}(v_i,v_j) > 0$ and it has the maximum value. Let

P be a shortest $(v_i - v_j)$-path on C_t, and Q a shortest $(v_i - v_j)$-path in $T(p,q)[C,D;a]$. Then Q must pass through some vertices in $C - B(C)$. Let $Q_C = Q \cap C$, and u_i and u_j the end vertices of the path Q_C. Let P_C be the shortest (u_i, u_j)-path on $C_0 = B(C)$. Denote by $l(P)$ the length of a path P. Then $l(P_C) + 2t \geq l(P) = d_{C_t}(v_i, v_j) > d_{T(p,q)[C,D;a]}(v_i, v_j) = l(Q) \geq 2(2t-1) + l(Q_C)$, and so $m \geq l(P_C) - l(Q_C) > 2t - 2$, that is, $t < \frac{m+2}{2}$. This contradicts that $t \geq \lceil \frac{m+2}{2} \rceil$. □

By Theorem 2.2, we can extend the cap C in $T(p,q)[C,D;a]$ to C^* such that the boundary $B(C^*)$ of C^* is C_t, where $t = \lceil \frac{m}{2} \rceil$. Note that if $m = 0$ then $C^* = C$. Similarly, let

$$m' = \max\{d_{B(D)}(v_i, v_j) - d_D(v_i, v_j) \mid v_i, v_j \in V_a(D)\},$$

we extend the cap D to D^* such that $B(D^*) = C_{t'}$, where $t' = q - 1 - \lceil \frac{m'}{2} \rceil$. Then $T(p,q)[C,D;a]$ can be also denoted as the caped zig-zag nanotube $T(p,q^*)[C^*,D^*;a]$ where $q^* = q - \lceil \frac{m}{2} \rceil - \lceil \frac{m'}{2} \rceil$ and the layer k of $T(p,q^*)$, denoted by C_k^*, is just the layer $k+t$, C_{k+t}. $T(p,q^*)[C^*,D^*;a]$ can be divided to three parts C^*, D^*, and $T(p,q^*-2) = T(p,q^*)[C^*,D^*;a] - V(C^*) - V(D^*)$ so that any two vertices in a part have the same distance in both the part and $T(p,q^*)[C^*,D^*;a]$.

Definition 1. Let $T(p,q)[C,D;a]$ be a capped zig-zag nanotube, let $t = \lceil \frac{m}{2} \rceil$ and $t' = q - 1 - \lceil \frac{m'}{2} \rceil$, and let C^* and D^* be the extended caps such that layer L_t of $T(p,q)$ is $B(C^*)$ and layer $L_{t'}$ of $T(p,q)$ is $B(D^*)$. Let $T(p,q^*)$ be the reduced zig-zag open-ended nanotube whose layer 0 is just L_t of $T(p,q)$ and layer q^*-1 is just $L_{t'}$ of $T(p,q)$, and so $q^* = q - \lceil \frac{m}{2} \rceil - \lceil \frac{m'}{2} \rceil$. Then $T(p,q^*)[C^*,D^*;a]$ is called the associated capped zig-zag nanotube of $T(p,q)[C,D;a]$.

Definition 2. Let G be a connected graph, and let A and B be disjoint vertex-induced subgraphs of G. Let $d(A,B,k)$ denote the number of the pairs $\{a_i, b_j\}$ of vertices with distance k for $a_i \in V(A)$, $b_j \in V(B)$. Then the Hosoya polynomial $H(A,B,x)$ between A and B is defined as $H(A,B,x) = \sum_{k>0} d(A,B,k)x^k$.

Now we can obtain Hosoya polynomial of a capped zig-zag nanotube $T(p,q)[C,D;a]$ from Hosoya polynomials of C^*, D^*, and $T(p,q^*-2)$, together with other terms corresponding to the distances between pairs of vertices in different parts.

By definition of the Hosoya polynomial and the above partition of $T(p,q)[C,D;a]$ to C^*, D^*, and $T(p,q^*-2)$, the Hosoya polynomial of $T(p,q)[C,D;a] = T(p,q^*)[C^*,D^*;a]$ can be denoted as follows:
$H(T(p,q)[C,D;a],x) = H(T(p,q^*)[C^*,D^*;a],x)$
$= \sum_{u,v \in V(C^*)} x^{d_{C^*}(u,v)} + \sum_{u,v \in V(D^*)} x^{d_{D^*}(u,v)}$

$+\sum_{u,v\in V(T(p,q^*-2))} x^{d_{T(p,q^*-2)}(u,v)}$
$+\sum_{u\in V(C^*),v\in V(T(p,q^*-2))} x^{d_{T(p,q^*)[C^*,D^*;a]}(u,v)}$
$+\sum_{u\in V(D^*),v\in V(T(p,q^*-2))} x^{d_{T(p,q^*)[C^*,D^*;a]}(u,v)}$
$+\sum_{u\in V(C^*),v\in V(D^*)} x^{d_{T(p,q^*)[C^*,D^*;a]}(u,v)}.$

Hence we have the following theorem.

Theorem 2.3 *Let $T(p,q)[C,D;a]$ be a capped zig-zag nanotube, and $T(p,q^*)[C^*,D^*;a]$ the associated caped zig-zag nanotube. Then* $H(T(p,q)[C,D;a],x) = H(T(p,q^*)[C^*,D^*;a],x) = H(C^*,x) + H(D^*,x) + H(T(p,q^*-2),x) + H(C^*,T(p,q^*-2),x) + H(D^*,T(p,q^*-2),x) + H(C^*,D^*,x)$.

The Hosoya polynomial $H(T(p,q^*-2),x)$ can be obtained by Theorem 1.1. The Hosoya polynomials $H(C^*,x)$ and $H(D^*,x)$ can be calculated directly. To obtain $H(T(p,q)[C,D;a],x)$, we need to give the methods for calculating $H(C^*,T(p,q^*-2),x)$, $H(D^*,T(p,q^*-2),x)$, and $H(C^*,D^*,x)$.

Definition 3. Let $T(p,q)[C,D;a]$ be a caped zig-zag nanotube, and $T(p,q^*)[C^*,D^*;a]$ the associated caped zig-zag nanotube. Let $V_a(C^*)$ (resp. $V_a(D^*)$) be the set of attachment vertices of the cap C^* (resp. D^*). For any vertex v_i in C^*, let $d_{C^*}(v_i,V_a(C^*))$ denote the minimum distance in C^* from v_i to a vertex in $V_a(C^*)$. Then the Hosoya polynomial $H(C^*,V_a(C^*),x)$ from C^* to $V_a(C^*)$ is defined as $H(C^*,V_a(C^*),x) = \sum_{v_i\in V(C^*)} x^{d_{C^*}(v_i,V_a(C^*))}$. Similarly, $H(D^*,V_a(D^*),x) = \sum_{v_i\in V(D^*)} x^{d_{D^*}(v_i,V_a(D^*))}$.

Definition 4. Let $T(p,q)[C,D;a]$ be a caped zig-zag nanotube, and $G = T(p,q^*)[C^*,D^*;a]$ the associated caped zig-zag nanotube. For a vertex u_i in C^* and the vertex sequence of $V_a(C^*)$, $(v_{0,0},v_{2,0},\cdots,v_{2p-2,0})$, let $S^b_{u_i,0} = (d_{C^*}(u_i,v_{0,0}),d_{C^*}(u_i,v_{2,0}),\cdots,d_{C^*}(u_i,v_{2p-2,0}))$ denote the distance sequence from u_i to attachment vertices of C^*. For $s = 1,2,\cdots$, let $S^b_{u_i,2s} = (d_G(u_i,v_{0,2s}),d_G(u_i,v_{2,2s}),\cdots,d_G(u_i,v_{2p-2,2s}))$ (resp. $S^w_{u_i,2s} = (d_G(u_i,v_{1,2s}),d_G(u_i,v_{3,2s}),\cdots,d_G(u_i,v_{2p-1,2s}))$) denote the distance sequence from u_i to the black (resp. white) vertices on layer $2s$ of $T(p,q^*)$, and let $S^w_{u_i,2s-1} = (d_G(u_i,v_{0,2s-1}),d_G(u_i,v_{2,2s-1}),\cdots,d_G(u_i,v_{2p-2,2s-1}))$ (resp. $S^b_{u_i,2s-1} = (d_G(u_i,v_{1,2s-1}),d_G(u_i,v_{3,2s-1}),\cdots,d_G(u_i,v_{2p-1,2s-1})))$ denote the distance sequence from u_i to the white (resp. black) vertices on layer $2s-1$ of $T(p,q^*)$. The Hosoya polynomial from u_i to layer k of $T(p,q^*)$ is denoted by $H(u_i,C^*_k,x) = \sum_{j=0,1,2,\cdots,2p-1} x^{d_G(u_i,v_{j,k})}$.

Lemma 2.4 *Let $G = T(p,q)[C,D;a]$ be a caped zig-zag nanotube, and $G = T(p,q^*)[C^*,D^*;a]$ the associated caped zig-zag nanotube with*

$q^* \geq p+1$. Let $S^b_{u_i,0} = (d_{C^*}(u_i, v_{0,0}), d_{C^*}(u_i, v_{2,0}), \cdots, d_{C^*}(u_i, v_{2p-2,0}))$ be the distance sequence from a vertex u_i in C^* to attachment vertices of C^*, and $d_{C^*}(u_i, V_a(C^*)) = c_{u_i}$. Then, for $s = 1, 2, \cdots$,

(i) $S^w_{u_i,2s-1} = S^b_{u_i,2s-2} + (1, 1, \cdots, 1)$
$= (d_G(u_i, v_{0,2s-2}) + 1,\ d_G(u_i, v_{2,2s-2}) + 1,\ \cdots,\ d_G(u_i, v_{2p-2,2s-2}) + 1)$;
$S^b_{u_i,2s-1} = (min\{d_G(u_i, v_{0,2s-1}), d_G(u_i, v_{2,2s-1})\} + 1,\ min\{d_G(u_i, v_{2,2s-1}), d_G(u_i, v_{4,2s-1})\} + 1, \cdots,\ min\{d_G(u_i, v_{2p-2,2s-1}, d_G(u_i, v_{0,2s-1}\} + 1))$;

(ii) $S^w_{u_i,2s} = S^b_{u_i,2s-1} + (1, 1, \cdots, 1)$
$= (d_G(u_i, v_{1,2s-1}) + 1,\ d_G(u_i, v_{3,2s-1}) + 1,\ \cdots,\ d_G(u_i, v_{2p-1,2s-1}) + 1)$;
$S^b_{u_i,2s} = (min\{d_G(u_i, v_{2p-1,2s}), d_G(u_i, v_{1,2s})\} + 1,\ min\{d_G(u_i, v_{1,2s}), d_G(u_i, v_{3,2s})\} + 1, \cdots,\ min\{d_G(u_i, v_{2p-3,2s}, d_G(u_i, v_{2p-1,2s}\} + 1))$;

(iii) *if $k \geq p$, then* $S^w_{u_i,k} = (2k-1+c_{u_i}, 2k-1+c_{u_i}, \cdots, 2k-1+c_{u_i})$, $S^b_{u_i,k} = (2k + c_{u_i}, 2k + c_{u_i}, \cdots, 2k + c_{u_i})$.

Proof. (i) and (ii) are obvious. (iii) Let $d_{C^*}(u_i, v_{2j,0}) = c_{u_i}$. If $d_{C^*}(u_i, v_{2j,0})$ is a unique minimum element in $S^b_{u_i,0}$, then, by (i) and (ii), in $S^b_{u_i,k}$ there are exactly $k+1$ minimum elements for $k < p$. Particularly, if $k = p-1$, then in $S^w_{u_i,k}$ there are exactly $p-1$ minimum elements, and every element in $S^b_{u_i,p-1}$ have a same value, and so if $k \geq p$

$$S^w_{u_i,k} = (2k-1+c_{u_i}, 2k-1+c_{u_i}, \cdots, 2k-1+c_{u_i}),$$

$$S^b_{u_i,k} = (2k + c_{u_i}, 2k + c_{u_i}, \cdots, 2k + c_{u_i}).$$

If $d_{C^*}(u_i, v_{2j,0})$ is not a unique minimum element in $S^b_{u_i,0}$, then there is a $r < p$ such that every element in $S^w_{u_i,r}$ (resp. $S^b_{u_i,r}$) have the same value, and for $k \geq p > r$ the conclusion of (iii) also holds. □

By Lemma 2.4, we can divide $T(p, q^* - 2)$ to two vertex disjoint nanotubes T_1 and T_2 in which T_1 consists of layers $1, 2, \cdots, p-1$ in $T(p, q^*)$ and T_2 consists of layers $p, p+1, \cdots, q^*-2$ in $T(p, q^*)$ so that $H(C^*, T(p, q^* - 2), x) = H(C^*, T_1, x) + H(C^*, T_2, x)$. Similarly, $T(p, q^* - 2)$ can be divided as two vertex disjoint nanotubes T_1' and T_2' in which T_1' consists of layers $q^* - p - 1, \cdots, q^* - 2$ in $T(p, q^*)$ and T_2' consists of layers $1, 2, \cdots, q^* - p - 2$ in $T(p, q^*)$ so that $H(D^*, T(p, q^* - 2), x) = H(D^*, T_1', x) + H(D^*, T_2', x)$. By Lemma 2.4, we have the following.

Theorem 2.5 *Let $T(p, q)[C, D; a]$ be a capped zig-zag nanotube, and $T(p, q^*)[C^*, D^*; a]$ the associated caped zig-zag nanotube with $q^* \geq p+1$. Then* $H(C^*, T_1, x) = \sum_{u_i \in V(C^*)} \sum_{k=1}^{p-1} H(u_i, C_k^*, x)$;
$H(C^*, T_2, x) = H(C^*, V_a(C^*), x) \cdot \sum_{k=p}^{q^*-2} p(1+x)x^{2k-1}$;
$H(C^*, T(p, q^* - 2), x) = H(C^*, T_1, x) + H(C^*, T_2, x)$
$= \sum_{u_i \in V(C^*)} \sum_{k=1}^{p-1} H(u_i, C_k^*, x) + H(C^*, V_a(C^*), x) \cdot \sum_{k=p}^{q^*-2} p(1+x)x^{2k-1}$;

$H(D^*, T_1', x) = \sum_{u_i \in V(D^*)} \sum_{k=q^*-p-1}^{q^*-2} H(u_i, C_k^*, x)$;
$H(D^*, T_2', x) = H(D^*, V_a(D^*), x) \cdot \sum_{k=p}^{q^*-2} p(1+x)x^{2k-1}$;
$H(D^*, T(p, q^* - 2), x) = H(D^*, T_1', x) + H(D^*, T_2', x)$
$= \sum_{u_i \in V(D^*)} \sum_{k=q^*-p-1}^{q^*-2} H(u_i, C_k^*, x)$
$+ H(D^*, V_a(D^*), x) \cdot \sum_{k=p}^{q^*-2} p(1+x)x^{2k-1}$.

Now we consider $H(C^*, D^*, x)$. By Lemma 2.4(iii), for $u_i \in V(C^*)$, if $q^* \geq p$, then $S^w_{u_i, q^*-1} = (2q^* - 3 + c_{u_i}, 2q^* - 3 + c_{u_i}, \cdots, 2q^* - 3 + c_{u_i})$, that is, the distance from u_i to any white vertex on layer $q^* - 1$, an attachment vertex of D^*, is equal to $d_{C^*}(u_i, V_a(C^*)) + 2q^* - 3$. So, for $v_j \in V(D^*)$, $d_{T(p,q^*)[C^*,D^*;a]}(u_i, v_j) = d_{C^*}(u_i, V_a(C^*)) + 2q^* - 3 + d_{D^*}(v_j, V_a(D^*))$. Therefore, we have the following.

Theorem 2.6 *Let $T(p,q)[C,D;a]$ be a capped zig-zag nanotube, and $T(p,q^*)[C^*,D^*;a]$ the associated caped zig-zag nanotube. Then*

$H(C^*, D^*, x) = x^{2q^*-3} H(C^*, V_a(C^*), x) \cdot H(D^*, V_a(D^*), x)$.

Theorem 2.7 *Let $T(p,q)[C,D;a]$ be a capped zig-zag nanotube, and $T(p,q^*)[C^*,D^*;a]$ the associated caped zig-zag nanotube with $q^* \geq p+1$. Then*

$H(T(p,q)[C,D;a], x) = H(T(p,q^*)[C^*,D^*;a], x)$
$= H(C^*, x) + H(D^*, x) + H(T(p, q^* - 2), x)$
$+ \sum_{u_i \in V(C^*)} \sum_{k=1}^{p-1} H(u_i, C_k, x)$
$+ H(C^*, V_a(C^*), x) \cdot \sum_{k=p}^{q^*-2} p(1+x)x^{2k-1}$
$+ \sum_{u_i \in V(D^*)} \sum_{k=q^*-p-1}^{q^*-2} H(u_i, C_k, x)$
$+ H(D^*, V_a(D^*), x) \cdot \sum_{k=p}^{q^*-2} p(1+x)x^{2k-1}$
$+ x^{2q^*-3} H(C^*, V_a(C^*), x) \cdot H(D^*, V_a(D^*), x)$.

Corollary 2.8 *Let $T(p,q)[C,C;a]$ be a capped zig-zag nanotube, and $T(p,q^*)[C^*,C^*;a]$ the associated caped zig-zag nanotube with $q^* \geq p+1$. Then*

$H(T(p,q)[C,C;a], x) = H(T(p,q^*)[C^*,C^*;a], x)$
$= 2H(C^*, x) + H(T(p, q^* - 2), x) + 2\sum_{u_i \in V(C^*)} \sum_{k=1}^{p-1} H(u_i, C_k, x)$
$+ 2H(C^*, V_a(C^*), x) \cdot \sum_{k=p}^{q^*-2} p(1+x)x^{2k-1} + x^{2q^*-3}(H(C^*, V_a(C^*), x))^2$.

From Theorem 2.7, it is not difficult to see that every term in $H(T(p,q)[C,D;a], x)$ is not related to the position a of C according to D. So we have the following.

Theorem 2.9 *Let $T(p,q)[C,D;a_1]$ and $T(p,q)[C,D;a_2]$ be any two non-isomorphic capped zig-zag nanotubes, and $T(p,q^*)[C^*,D^*;a_1]$ and $T(p,q^*)[C^*,D^*;a_2]$ the associated caped zig-zag nanotubes with $q^* \geq p+1$. Then $H(T(p,q)[C,D;a_1]) = H(T(p,q)[C,D;a_2])$.*

By Theorem 2.9, for any two non-isomorphic capped zig-zag nanotubes $T(p,q)[C,D;a_1]$, $T(p,q)[C,D;a_2]$ and their associated caped zig-zag nanotubes $T(p,q^*)[C^*,D^*;a_1]$ and $T(p,q^*)[C^*,D^*;a_2]$ with $q^* \geq p+1$, they have the same Hosoya polynomial. Therefore their Hosoya polynomial can be simply denoted by $H(T(p,q)[C,D])$ and $H(T(p,q^*)[C^*,D^*])$.

3 Discussion and Application

To calculate Hosoya polynomials of graphs by directly calculating distances of every pair of vertices in graphs is tedious, although it can be done so. A good method for calculating Hosoya polynomials of graphs is to deduce formulae for special classes of graphs.

In the above section, for any capped zig-zag nanotube $T(p,q)[C,D]$, we give a general formula for calculating Hosoya polynomial of $T(p,q)[C,D]$, in which the terms $H(C^*,x) + H(D^*,x)$, $\sum_{u_i \in V(C^*)} \sum_{k=1}^{p-1} H(u_i, C_k, x)$, $\sum_{u_i \in V(D^*)} \sum_{k=q^*-p-1}^{q^*-2} H(u_i, C_k, x)$, $H(C^*, V_a(C^*), x)$, $H(D^*, V_a(D^*), x)$ depend on the structures of caps C and D. However, for a much longer capped zig-zag nanotube (that is, q is much large), p and the numbers of vertices of caps C and D are much smaller than q, so the terms can be easily and directly calculated, and then Hosoya polynomial of the capped zig-zag nanotube can be easily deduced. We can conclude that the method in the present paper is more efficient for calculating Hosoya polynomials of much longer capped zig-zag nanotubes.

In the follows, we will show how to apply the previous theorems to deduce the Hosoya polynomials of two capped zig-zag nanotubes.

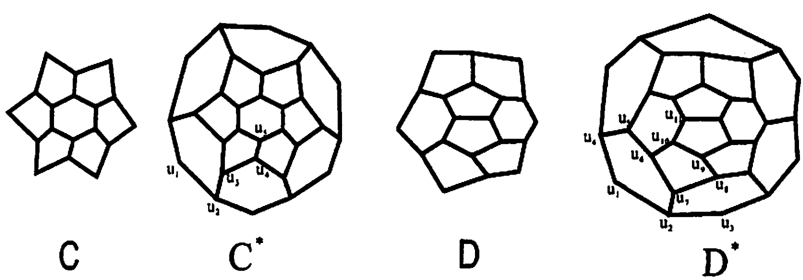

Fig. 2: Two caps C, D and the extended caps C^*, D^*.

Example 1. Let $T(6,q)[C,D]$ be a caped zig-zag nanotube with $q \geqslant 11$ and with caps C and D shown in Fig.2, and $T(6,q^*)[C^*,D^*]$ the associated caped zig-zag nanotube. Then

$H(T(6,q)[C,D],x) = H(T(6,q^*)[C^*,D^*],x) = 12q^* + 38 + 99x + 210x^2 + 303x^3 + 395x^4 + 465x^5 + 505x^6 + 506x^7 + 482x^8 + 450x^9 + 432x^{10} + 324x^{11} + 228x^{12} + 156x^{13} + 84x^{14} + 12x^{15} + 6\sum_{k=1}^{5}(3q^* - 6 - k)kx^k + 6(17q^* - 70)x^6 + 6\sum_{k=7}^{11}(24(q^*+1) - (q^*+22)k + k^2)x^k + 36\sum_{k=12}^{2q^*-5}(2q^* - 4 - k)x^k + 12(6 + 6x + 6x^2 + 6x^3 + 6x^4 + x^5)\sum_{k=6}^{q^*-2}(1+x)x^{2k-1} + 12(3 + 6x + 9x^2 + 12x^3 + 15x^4 + 13x^5 + 10x^6 + 7x^7 + 4x^8 + x^9)x^{2q^*-3}$.

Proof. For the caps C and D, we have $m = m' = 1$, $t = t' = \lceil \frac{m}{2} \rceil = 1$, $q^* = q - 2$, and the extended caps C^* and D^* are as shown in Fig. 2.

$H(C^*,x)$, $H(D^*,x)$, $H(C^*,V_a(C^*),x)$, $H(D^*,V_a(D^*),x)$ can be calculated directly.

$$H(C^*,x) = 30 + 42x + 78x^2 + 93x^3 + 96x^4 + 75x^5 + 39x^6 + 12x^7.$$

$$H(D^*,x) = 32 + 45x + 84x^2 + 102x^3 + 107x^4 + 90x^5 + 54x^6 + 14x^7.$$

$$H(C^*,V_a(C^*),x) = 6(1 + x + x^2 + x^3 + x^4).$$

$$H(D^*,V_a(D^*),x) = 2(3 + 3x + 3x^2 + 3x^3 + 3x^4 + x^5).$$

In order to calculate $H(C^*,T_1,x)$, we divide vertices of C^* to symmetry equivalence classes such that any two vertices in a same class are in symmetric position in C^*. Clearly, there are 5 symmetry equivalence classes in C^* each of which has 6 vertices. Take a representative u_i in the ith class, $i = 1,2,3,4,5$. It is easy to calculate that $S^b_{u_1,0} = (0,2,4,6,4,2)$, $S^b_{u_2,0} = (1,1,3,5,5,3)$, $S^b_{u_3,0} = (2,2,4,6,6,4)$, $S^b_{u_4,0} = (3,3,3,5,7,5)$, $S^b_{u_5,0} = (4,4,4,5,6,5)$. Hence, by Lemma 2.4, the Hosoya polynomial $H(u_i,C_k^*,x)$ from u_i to layer k of $T(p,q^*)$, where $i = 1,2,3,4,5$ and $k = 1,2,\cdots,p-1$, can be calculated easily, and it follows from Theorem 2.5 that

$H(C^*,T_1,x) = 6\sum_{u_i \in \{u_1,u_2,\cdots,u_5\}}\sum_{k=1}^{5} H(u_i,C_k,x) = 6(x + 4x^2 + 9x^3 + 16x^4 + 25x^5 + 34x^6 + 39x^7 + 39x^8 + 36x^9 + 35x^{10} + 26x^{11} + 18x^{12} + 12x^{13} + 6x^{14})$,

$H(C^*,T_2,x) = 36(1 + x + x^2 + x^3 + x^4)\sum_{k=6}^{q^*-2}(1+x)x^{2k-1}$.

Similarly, we have

$H(D^*,T_1',x) = 2(3x + 12x^2 + 27x^3 + 48x^4 + 75x^5 + 104x^6 + 123x^7 + 124x^8 + 117x^9 + 111x^{10} + 84x^{11} + 60x^{12} + 42x^{13} + 24x^{14} + 6x^{15})$,

$H(D^*,T_2',x) = 12(3 + 3x + 3x^2 + 3x^3 + 3x^4 + x^5)\sum_{k=6}^{q^*-2}(1+x)x^{2k-1}$.

By Theorems 1.1 and 2.6,

$H(T(6,q^*-2),x) = 12(q^*-2) + 6\sum_{k=1}^{5}(3q^* - 6 - k)kx^k + 6(17q^* - 70)x^6$

$+6\sum_{k=7}^{11}(24(q^*+1)-(q^*+22)k+k^2)x^k+36\sum_{k=12}^{2q^*-5}(2q^*-4-k)x^k$,
$H(C^*,D^*,x)=12(3+6x+9x^2+12x^3+15x^4+13x^5+10x^6+7x^7+4x^8+x^9)x^{2q^*-3}$.

Now, by Theorem 2.7, $H(T(6,q)[C,D],x) = H(T(6,q^*)[C^*,D^*]$ can be given by the above calculating results. □

Example 2. Let $T(10,q)[C,D]$ be a caped zig-zag nanotube with $q \geqslant 13$ and with caps $C \cong D$ shown in Fig. 3, and $T(6,q^*)[C^*,D^*]$ the associated caped zig-zag nanotube. Then

$H(T(10,q)[C,D],x) = H(T(10,q^*)[C^*,D^*],x) = 20q^*-80+190x+400x^2+600x^3+820x^4+1000x^5+1180x^6+1330x^7+1460x^8+1570x^9+1640x^{10}+1650x^{11}+1610x^{12}+1540x^{13}+1500x^{14}+1440x^{15}+1410x^{16}+1350x^{17}+1310x^{18}+1040x^{19}+800x^{20}+600x^{21}+400x^{22}+200x^{23}+100x^{24}$
$+10\sum_{k=1}^{9}(3(q^*-2)-k)kx^k+10(29q^*-158)x^{10}+10\sum_{k=11}^{19}(40q^*+120-(q^*+38)k+k^2)x^k+100\sum_{k=20}^{2q^*-5}(2q^*-4-k)x^k+100(2+2x+2x^2+2x^3+2x^4+x^5+x^6)\sum_{k=10}^{q^*-2}(1+x)x^{2k-1}+25(2+2x+2x^2+2x^3+2x^4+x^5+x^6)^2x^{2q^*-3}$.

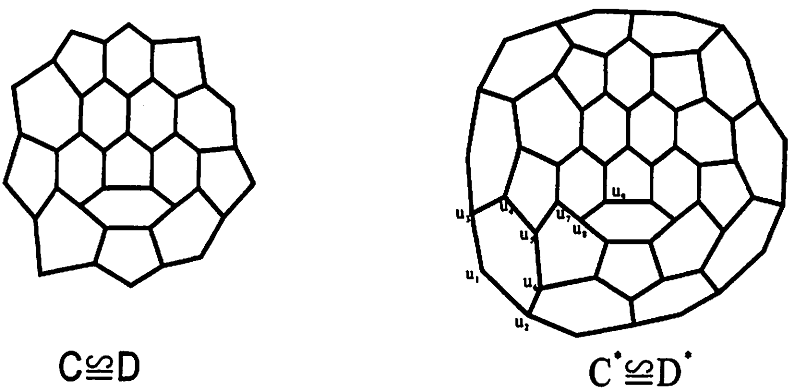

Fig. 3: Caps $C \cong D$ and the extended caps $C^* \cong D^*$.

Proof. For the caps $C \cong D$, we have $m = m' = 2$, $t = t' = \lceil \frac{m}{2} \rceil = 1$, $q^* = q - 2$, and the extended caps C^* and D^* are as shown in Fig. 3.

Similarly, we have

$H(C^*,x) = H(D^*,x) = 5(12+17x+32x^2+42x^3+50x^4+50x^5+48x^6+42x^7+32x^8+24x^9+13x^{10}+4x^{11})$.

$H(C^*,V_a(C^*),x) = H(D^*,V_a(D^*),x) = 5(2+2x+2x^2+2x^3+2x^4+x^5+x^6)$

$H(C^*,T_1,x) = H(D^*,T_1',x) = 5(2x+8x^2+18x^3+32x^4+50x^5+70x^6+91x^7+114x^8+133x^9+151x^{10}+161x^{11}+161x^{12}+154x^{13}+150x^{14}+144x^{15}+141x^{16}+135x^{17}+131x^{18}+104x^{19}+80x^{20}+60x^{21}+40x^{22}+20x^{23}+10x^{24})$.

$H(C^*, T_2, x) = H(D^*, T_2', x) = 50(2 + 2x + 2x^2 + 2x^3 + 2x^4 + x^5 + x^6) \sum_{k=10}^{q^*-2}(1 + x)x^{2k-1}$.

$H(T(10, q^* - 2), x) = 20(q^* - 2) + 10\sum_{k=1}^{9}(3(q^* - 2) - k)kx^k + 10(29q^* - 158)x^{10} + 10\sum_{k=11}^{19}(40q^* + 120 - (q^* + 38)k + k^2)x^k + 100\sum_{k=20}^{2q^*-5}(2q^* - 4 - k)x^k$.

$H(C^*, D^*, x) = 25(2 + 2x + 2x^2 + 2x^3 + 2x^4 + x^5 + x^6)^2 x^{2q^*-3}$.

By Corollary 2.8. the conclusion holds.

Acknowledgement

The authors would like to thank the referees for their helpful and careful comments.

References

[1] F. Buckley and F. Harary, Distance in Graphs, Addison-Wesley, Redwood, CA, 1990.

[2] G. G. Cash, Relationship Between the Hosoya Polynomial and the Hyper-Wiener Index, Appl. Math. Lett. 15 (2002) 893-895.

[3] A. A. Dobrynin, R. Entringer, I. Gutman, Wiener index of trees: Theory and applications, *Acta Appl. Math.* **66** (2001) 211-249.

[4] A. A. Dobrynin, I. Gutman, S. Klavžar and P. Žigert, Wiener index of hexagonal systems, *Acta Appl. Math.* **72** (2002) 247-294.

[5] M. S. Dresselhaus, G. Dresselhaus and P. Avonris, *Carbon Nanotubes Synthesis, Structure, Properties and Applications,* Springer-Verlag, Berlin, 2001.

[6] M. V. Diudea, Hosoya polynomial in tori, *MATCH Commun. Math. Comput. Chem.* **45**(2002) 109-122.

[7] M. Endo, S. Iijima and M. S. Dresselhaus, *Carbon nanotubes*, Pergamon, 1996. *Croat. Chem. Acta* **73** (2000) 383-403.

[8] E. Estrada. Novel strategies in the search of topological indices, *Topologic Indices and Related Descriptors in QSAR and QSPR Gordon and Breach* (1999) 403-453.

[9] I. Gutman, A. A. Dobrynin, The Szeged index - a success story, *Graph Theory Notes N. Y.* **34** (1998) 37-44.

[10] I. Gutman, Some properties of the Wiener polynomial, *Graph Theory Notes* **25** (1993) 13-18.

[11] I. Gutman, E. Estrada and O. Ivanciuc, Some properties of the Hosoya polynomial of trees, *Graph Theory Notes* (New York) **36** (1999) 7-13.

[12] I. Gutman and O. Polansky, Mathematical Concepts in Organic Chemistry, Sping-Verlag, Germany, 1986.

[13] I. Gutman, S. Klavžar and B. Mohar (eds.), *Fifty years of the Wiener index, MATCH Commun. Math. Comput. Chem.*, Vol. **35** (1997) 1-259.

[14] I. Gutman, S. Klavžar and B. Mohar (eds.), *Fiftieth anniversary of the Wiener index, Discrete Appl. Math.* **80** (1997) 73-81.

[15] I. Gutman, S. Klavžar, M. Petkovšek and P. Žigert, On Hosoya polynomials of benzenoid graphs, *MATCH Commun. Math. Comput. Chem.* **43** (2001) 49-66.

[16] I. Gutman, S. Klavžar, M. Petkovšek and P. Žigert, On Hosoya polynomials of benzenoid graphs[J], *MATCH Commun. Math. Comput. Chem.* **43** (2001) 49-66.

[17] X. Guo, D. J. Klein, W. G. Yan, Y. N. Yeh, Hyper-Wiener vector, Wiener matrix sequence, and Wiener polynomial sequence of a graph, *Int. J. Quantum Chem.* **106(8)** (2006) 1756-1761.

[18] H. Hosoya, On some counting polynomials in chemistry, *Discrete Appl. Math.* **19** (1988) 239-257.

[19] H. Hosoya, Topological index. A newly proposed quantity characterizing the topological nature of structural isomers of saturated hydrocarbons, *Bull. Chem. Soc. Jpn.* (1971) 2332-2339.

[20] D. J, Klein, D. Mihalić, D. Plavšić, N. Trinajstić, Molecular topological index: A relation with the Wiener index, J. Chem. Int. Comput. Sci 32 (1992) 304-305.

[21] E. V. Konstantinova and M. V. Diudea, The Wiener polynomial derivatives and other topological indices in chemical research, *Croat. Chem. Acta* **73** (2000) 383-403.

[22] D. J. Klein, I. Lukovits, and I. Gutman, On the Definition of the Hyper-Wiener Index for Cycle-Containing Structures, J. Chem. Inf. Comput. Sci. 35 (1995) 50-52.

[23] J. G. Qian, F. J. Zhang, On the number of Kekulé structures in the capped zig-zag nanotubes, *Journal of Mathematical Chemistry* **38** (2005) 233-246.

[24] M. Randić, Novel molecular descriptor for structure-property studies, *Chem. Phys. Lett.* **211** (1993) 478-483.

[25] M. Randić, Novel Molecular Description for Structure-Property Studies, Chem. Phys. Lett. 211 (1993) 478-483.

[26] M. Randić, J. Zupan, On interpretation of well-known topological indices. J. Chem. Int-comput. Sci. 41 (2001) 550-560.

[27] B. E. Sagan, Y. N. Yeh and P. Zhang, The Wiener polynomial of a graph, *Int. J. Quantum Chem.* **60** (1996) 959-969.

[28] H. Wiener, Structural determination of paraffin boiling points, *J. Amer. Chem. Soc.* **69** (1947) 17-20.

[29] E. W. Wong, P. E. Sheehan, and C. M. Lieber, Nanobeam mechanics: Elasticity, strength, and toughness of nanorods and nanotubes, *Science* **277** (1997) 1971-1975.

[30] S. Xu, H. Zhang and M. V. Diudea, Hosoya polynomials of zig-zag open-ended nanotubes, *MATCH Commun. Math. Comput. Chem.* 57 (2007) 443-456.

[31] S. Xu, H. Zhang, M. V. Diudea, Hosoya polynomials of armchair open-ended nanotubes, *Int. J. Quantum Chem.* **107** (2007) 586-596.

[32] W. G. Yan, B. Y. Yang and Y. N. Yeh, The behavior of Wiener indices and polynomials of graphs under five graph decorations [J], *Applied Mathematics Letters* **20** (2007) 290-295.

[33] B. Y. Yang and Y. N. Yeh, Wiener polynomials of some chemically interesting graphs, *Int. J. Quantum Chem.* **99** (2004) 80-91.

[34] B. Zmazek, J. Zerovnik, On the generalization of the Hosoya-wiener polynomial, *MATCH Commun. Math. Comput. Chem.* **55** (2006) 359-362.