J Math Chem (2009) 45:488–502
DOI 10.1007/s10910-008-9422-3

ORIGINAL PAPER

Hosoya polynomials of $TUC_4C_8(S)$ nanotubes

Shoujun Xu · Heping Zhang

Published online: 30 August 2008

Abstract The Hosoya polynomial of a chemical graph G is $H(G, x) = \sum_{\{u,v\}\subseteq V(G)} x^{d_G(u,v)}$, where $d_G(u, v)$ denotes the distance between vertices u and v. In this paper, we obtain analytical expressions for Hosoya polynomials of $TUC_4C_8(S)$ nanotubes. Accordingly, the Wiener index, obtained by Diudea et al. (*MATCH Commun. Math. Comput. Chem.* **50**, 133–144, (2004)), and the hyper-Wiener index are derived.

Keywords Hosoya polynomial · Wiener index · Hyper-Wiener index · $TUC_4C_8(S)$ nanotube

1 Introduction

Carbon nanotubes, one-dimensional carbon allotropes, were first discovered in 1991 by Iijima [13] and next in 1993 by the Iijima's group [14] and the Bethune's group [2]. Diudea et al. [4,20] recently constructed TUC_4C_8 nanotubes, tubules tessellated by square C_4 and octagon C_8 in different ways. Among them, there is one highly symmetric special case of interest: $TUC_4C_8(S)$ nanotube. About mathematical aspects related to the counting of distance sums of the special case (i.e., Wiener index defined below) we can refer to [20].

This work is supported by the Fundamental Research Fund for Physics and Mathematic of Lanzhou University (Grant No. LZULL200809).

S. Xu (✉) · H. Zhang
School of Mathematics and Statistics, Lanzhou University, Lanzhou, Gansu 730000, People's Republic of China
e-mail: shjxu@lzu.edu.cn

H. Zhang
e-mail: zhanghp@lzu.edu.cn

The *Hosoya polynomial* of a connected graph G is defined as:

$$H(G, x) := \sum_{\{u,v\}\subseteq V(G)} x^{d_G(u,v)},$$

where $d_G(u, v)$ is the distance (i.e., the number of edges in a shortest path) between a pair of vertices u and v of G (Subscript G is omitted when the graph is clear from the context). The polynomial was introduced by Hosoya [12], who named it the *Wiener polynomial* because the well-known *Wiener index* $W(G)$, introduced originally for alkanes by Wiener [21] as the sum of distances between all pairs of vertices in G [11], is equal to the first derivative of the polynomial in $x = 1$:

$$W(G) = \frac{dH(G, x)}{dx}\Big|_{x=1}. \tag{1}$$

Similarly, from the Hosoya polynomial, another topological index $WW(G)$ of G [16], called as *hyper-Wiener index*, may be obtained [25]:

$$WW(G) = \frac{1}{2}\frac{d^2(xH(G, x))}{dx^2}\Big|_{x=1}. \tag{2}$$

The Wiener index is one of the oldest graph-based structure descriptors and extensively studied since the middle of 1970s. For the researches on the Wiener index we can refer to two special issues [8,9], whereas chemical applications and the computation of the hyper-Wiener index are referred to [1,15,18].

The Hosoya polynomial has many applications [5,10,17]. Abundant literature appeared on this topic for the theoretical consideration [6,7,22] and computation [3,10,19,23–26].

In this paper, we focus on $TUC_4C_8(S)$ nanotubes, proposing a recursive method for calculating the Hosoya polynomial H in the corresponding graph, which is similar to that developed in Refs. [24,25]. By means of this method, explicit expressions for H are obtained (i.e., Theorem 4.3). Finally, according to relations (1) and (2) we give explicit formulae for the Wiener index and the hyper-Wiener index of $TUC_4C_8(S)$ nanotubes.

2 Distance from the reference vertex v_0

A $TUC_4C_8(S)$ *nanotube* is a finite section of a cylinder tessellated alternately by squares and octagons, described by two parameters $p(\geqslant 1)$ and $q(\geqslant 2)$ and simply denoted by $T(p, q)$, and drawn in the plane (equipped with alternately horizontal regular square-octagon lattice) using the representation of a cylinder by a rectangular R with the vertical boundary identification (see Fig. 1), such that there are p squares in each horizontal row and the total number $p(q - 1)$ of squares. Of course, there is the other method by which $T(p, q)$ is obtained [20]. For convenience, in the plane representation of $T(p, q)$, we denote by *level* $0, 1, 2, \ldots, q - 1$ horizontal armchair lines from top to bottom, respectively. Note that each level is exactly a $4p$-length cycle.

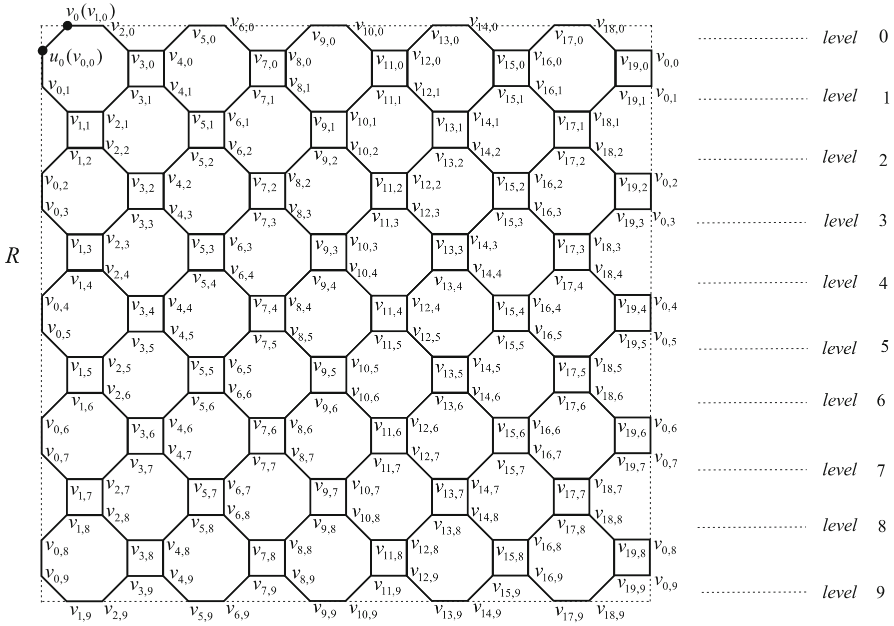

Fig. 1 A $TUC_4C_8(S)$ nanotube $T(p, q)$ with $p = 5, q = 10$, labeling for vertices and its two special vertices v_0 and u_0. Note that the vertices with the same label are identified

We denote by $v_{0,k}, v_{1,k}, v_{2,k}, \ldots, v_{4p-1,k}$ all vertices lying at the level k from left to right (in the sense that the first subscript modules $4p$). We specify two vertices $v_{0,0}$ and $v_{1,0}$ as u_0 and v_0, respectively (see Fig. 1).

Let H be a connected subgraph of a graph G. Then $d_H(u, v) \geqslant d_G(u, v)$ for any pair of vertices u and v of H. H is a *convex subgraph* of G if any shortest path of G joining two vertices of H is already in H. Hence if H is convex, then $d_H(u, v) = d_G(u, v)$.

For $2 \leqslant r \leqslant q-1$, $T(p, r)$ can be considered as a subgraph of $T(p, q)$ induced by r consecutive levels in $T(p, q)$. For convenience, we denote by $T(p, 1)$ the induced subgraph of $T(p, q)$ by one level, i.e., isomorphic to the $4p$-length cycle C_{4p}, by $T(p, 0)$ the null graph, i.e., the graph with no vertices and no edges. Similar to the proof of Lemma 2.1 in Ref. [27], we get

Lemma 2.1 *For any integer* r *with* $1 \leqslant r \leqslant q-1$, $T(p, r)$ *is a convex subgraph of* $T(p, q)$.

Given an octagon O of $T(p, q)$. All vertices on O lying at levels k and $k+1$ are denoted by $v_{m,k}, v_{m+1,k}, v_{m+2,k}, v_{m+3,k}$ and $v_{m,k+1}, v_{m+1,k+1}, v_{m+2,k+1}, v_{m+3,k+1}$ for some even m, respectively.

Lemma 2.2 *Let* $a_1 := \min\{d(v_{m,k}, v_0), d(v_{m+3,k}, v_0)\}$ *and* $a_2 := \min\{d(v_{m+1,k}, v_0), d(v_{m+2,k}, v_0)\}$.

(1) *If* $a_1 < a_2$, *then*

$$d(v_{m+i,k+1}, v_0) = d(v_{m+i,k}, v_0) + 1, \quad \textit{for} \quad 0 \leqslant i \leqslant 3.$$

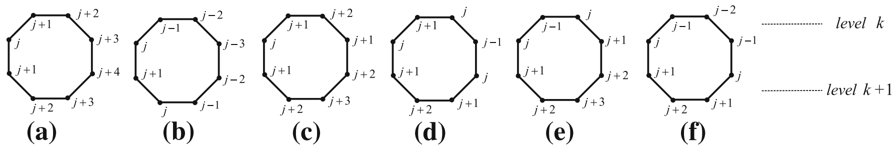

Fig. 2 Illustration for the proof of Lemma 2.2. The labeling on vertices represent the distance from the vertex v_0. The cases (**a**), (**b**), (**c**) and (**d**) satisfy the condition $a_1 < a_2$, while the cases (**e**) and (**f**) satisfy the condition $a_1 > a_2$

(2) *If* $a_1 > a_2$, *then*

$$d(v_{m+i,k+1}, v_0) = \begin{cases} d(v_{m+i,k}, v_0) + 1, & i = 0, 3; \\ d(v_{m+i,k}, v_0) + 3, & i = 1, 2. \end{cases}$$

Proof By Lemma 2.1, we have

$$d(v_{m+i,k+1}, v_0) = d(v_{m+i,k}, v_0) + 1 \quad \text{for } i = 0, 3, \tag{3}$$

$$d(v_{m+1,k+1}, v_0) = \min\{d(v_{m,k+1}, v_0) + 1, d(v_{m+3,k+1}, v_0) + 2\} \tag{4}$$

and

$$d(v_{m+2,k+1}, v_0) = \min\{d(v_{m,k+1}, v_0) + 2, d(v_{m+3,k+1}, v_0) + 1\}. \tag{5}$$

Let $j := d(v_{m,k}, v_0)$. If $a_1 \neq a_2$, then $\big(d(v_{m,k}, v_0), d(v_{m+1,k}, v_0), d(v_{m+2,k}, v_0), d(v_{m+3,k}, v_0)\big)$ has six possible cases: $(j, j+1, j+2, j+3)$, $(j, j-1, j-2, j-3)$, $(j, j+1, j+2, j+1)$, $(j, j+1, j, j-1)$, $(j, j-1, j, j+1)$ and $(j, j-1, j-2, j-1)$ (see Fig. 2). Combining Eqs. (3)–(5), we obtain the distances $d(v_{m+i,k+1}, v_0)$ for $0 \leqslant i \leqslant 3$ shown as in Fig. 2. After simple examinations, we obtain the assertions.

For convenience, for nonnegative integers m, n, s and t, where s and t have different parities, we define four sequences as follows:

$$\begin{aligned} &m, \nearrow, n := (m, m+1, m+2, \ldots, n), \quad (m \leqslant n); \\ &m, \searrow, n := (m, m-1, m-2, \ldots, n), \quad (m \geqslant n); \\ &s, \upuparrows, t := (s, s+1, s, s+1, s+2, s+3, s+2, s+3, \ldots, t-1, \\ &t, t-1, t), \quad (s < t); \\ &s, \downdownarrows, t := (s, s-1, s, s-1, s-2, s-3, s-2, s-3, \ldots, t+1, \\ &t, t+1, t), \quad (s > t). \end{aligned}$$

In $T(p, q)$, we define a series of sequences about distance from the reference vertex v_0 to vertices, respectively, lying at levels $k = 0, 1, 2, \ldots, q-1$ (note that for convenience of description in the following, the first term of the sequence is $d(v_{1,k}, v_0)$ instead of $d(v_{0,k}, v_0)$):

$$S_k = \big(d(v_{1,k}, v_0), d(v_{2,k}, v_0), \ldots, d(v_{4p-1,k}, v_0), d(v_{0,k}, v_0)\big), \quad \text{for } 0 \leqslant k \leqslant q-1.$$

Lemma 2.3 (1) *If* $0 \leqslant k \leqslant p-1$, *then*

$$S_k = \begin{cases} (2k, 2k+1, 2k+2, \upuparrows, 3k+1, \nearrow, 2p+k, \searrow, 3k, \downdownarrows, 2k+1), & k \text{ even}; \\ (2k+1, \upuparrows, 3k+1, \nearrow, 2p+k, \searrow, 3k, \downdownarrows, 2k+2, 2k+1, 2k), & \text{otherwise}. \end{cases}$$

(2) *If* $p \leqslant k \leqslant q-1$, *then*

$$S_k = \begin{cases} (2k, 2k+1, 2k+2, \upuparrows, p+2k-1, p+2k, & p \text{ and } k \text{ both even}; \\ p+2k+1, p+2k, \downdownarrows, 2k+1), & \\ (2k+1, \upuparrows, p+2k, p+2k+1, & p \text{ even and } k \text{ odd}; \\ p+2k, p+2k-1, \downdownarrows, 2k+2, 2k+1, 2k), & \\ (2k, 2k+1, 2k+2, \upuparrows, p+2k, p+2k+1, & p \text{ odd and } k \text{ even}; \\ p+2k, p+2k-1, \downdownarrows, 2k+1), & \\ (2k+1, \upuparrows, p+2k-1, p+2k, p+2k+1, & \text{otherwise}. \\ p+2k, \downdownarrows, 2k+2, 2k+1, 2k), & \end{cases}$$

Proof We use induction on k. The assertion is easily obtained when $k = 0$. Suppose that $k > 0$ and the assertions hold for S_k. In what follows we prove that the assertions hold for S_{k+1}. We only give the proof when k is even and for the other case we can give the similar proof. The induced subgraph by levels k and $k+1$ of $T(p, q)$ is shown as Fig. 3. Obviously, for any $0 \leqslant i \leqslant p-1$, the vertices $v_{4i,k}, v_{4i+1,k}, v_{4i+2,k}$ and $v_{4i+3,k}$ lying at level k and the vertices $v_{4i,k+1}, v_{4i+1,k+1}, v_{4i+2,k+1}$ and $v_{4i+3,k+1}$ lying at level $k+1$ are exactly belong to some octagon of $T(p, q)$. Let

$$a_{1i} := \min\{d(v_{4i,k}, v_0), d(v_{4i+3,k}, v_0)\},$$
$$a_{2i} := \min\{d(v_{4i+1,k}, v_0), d(v_{4i+2,k}, v_0)\}.$$

In the following we distinguish two cases to discuss.

Case 1. $0 \leqslant k \leqslant p-1$.
From S_k, we know, for $0 \leqslant i \leqslant \frac{k}{2}$,

$$\big(d(v_{4i,k}, v_0), d(v_{4i+1,k}, v_0), d(v_{4i+2,k}, v_0), d(v_{4i+3,k}, v_0)\big)$$
$$= (2k+2i+1, 2k+2i, 2k+2i+1, 2k+2i+2),$$

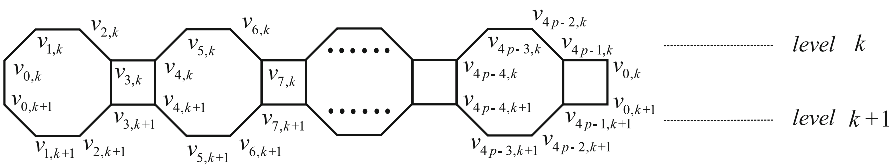

Fig. 3 The induced subgraph of $T(p, q)$ by levels k and $k+1$

then $a_{1i} > a_{2i}$. By Lemma 2.2, we obtain

$$d(v_{4i+j,k+1}, v_0) = \begin{cases} d(v_{4i+j,k}, v_0) + 1, & j = 0, 3; \\ d(v_{4i+j,k}, v_0) + 3, & j = 1, 2. \end{cases}$$

So

$$\big(d(v_{4i,k+1}, v_0), d(v_{4i+1,k+1}, v_0), d(v_{4i+2,k+1}, v_0), d(v_{4i+3,k+1}, v_0)\big)$$
$$= (2k + 2i + 2, 2k + 2i + 3, 2k + 2i + 4, 2k + 2i + 3).$$

We further obtain

$$\big(d(v_{0,k+1}, v_0), d(v_{1,k+1}, v_0), \ldots, d(v_{2k,k+1}, v_0), d(v_{2k+1,k+1}, v_0), d(v_{2k+2,k+1}, v_0), d(v_{2k+3,k+1}, v_0)\big) = (2k + 2, 2k + 3, \upuparrows, 3k + 2, 3k + 3, 3k + 4, 3k + 3). \tag{6}$$

Similarly, we can obtain, for $p - \frac{k}{2} \leqslant i \leqslant p - 1$,

$$\big(d(v_{4i,k+1}, v_0), d(v_{4i+1,k+1}, v_0), d(v_{4i+2,k+1}, v_0), d(v_{4i+3,k+1}, v_0)\big)$$
$$= (2p + 2k - 2i + 2, 2p + 2k - 2i + 3, 2p + 2k - 2i + 2, 2p + 2k - 2i + 1).$$

(Note that in this case $\big(d(v_{4i,k}, v_0), d(v_{4i+1,k}, v_0), d(v_{4i+2,k}, v_0), d(v_{4i+3,k}, v_0)\big) = (2p + 2k - 2i + 1, 2p + 2k - 2i, 2p + 2k - 2i - 1, 2p + 2k - 2i)$ and $a_{1i} > a_{2i}$.) So

$$\big(d(v_{4p-2k,k+1}, v_0), d(v_{4p-2k+1,k+1}, v_0), d(v_{4p-2k+2,k+1}, v_0), d(v_{4p-2k+3,k+1}, v_0), \ldots, d(v_{4p-2,k+1}, v_0), d(v_{4p-1,k+1}, v_0)\big)$$
$$= (3k + 2, 3k + 3, 3k + 2, 3k + 1, \downdownarrows, 2k + 4, 2k + 3). \tag{7}$$

Similar to the above discussions, for $\frac{k}{2} + 1 \leqslant i \leqslant p - \frac{k}{2} - 1$, we get $a_{1i} < a_{2i}$. By Lemma 2.2, then, for $0 \leqslant j \leqslant 3$,

$$d(v_{4i+j,k+1}, v_0) = d(v_{4i+j,k}, v_0) + 1.$$

Since

$$\big(d(v_{2k+4,k}, v_0), d(v_{2k+5,k}, v_0), \ldots, d(v_{4p-2k-1,k}, v_0)\big)$$
$$= (3k + 3, \nearrow, 2p + k, \searrow, 3k + 2),$$

$$\big(d(v_{2k+4,k+1}, v_0), d(v_{2k+5,k+1}, v_0), \ldots, d(v_{4p-2k-1,k+1}, v_0)\big)$$
$$= (3k + 4, \nearrow, 2p + k + 1, \searrow, 3k + 3). \tag{8}$$

Combining Eqs. (6)–(8), we obtain the sequence S_{k+1}.

Case 2. $p \leqslant k \leqslant q-1$.

From S_k, regardless of the parity of p, for any $0 \leqslant i \leqslant p-1$, we have $a_{1i} > a_{2i}$. So, by Lemma 2.2,

$$d(v_{4i+j,k+1}, v_0) = \begin{cases} d(v_{4i+j,k}, v_0)+1, & j=0,3; \\ d(v_{4i+j,k}, v_0)+3, & j=1,2. \end{cases}$$

After simple examinations, we obtain the sequence S_{k+1}.

3 The partial Hosoya polynomial of $T(p,q)$

Let G be a graph with vertex set $V(G)$. We define the *partial Hosoya polynomial* of G associated with a vertex $v \in V(G)$ as

$$H_G(v) := \sum_{u \in V(G)} x^{d(u,v)}.$$

Lemma 3.1

$$H_{T(p,q)}(v_0) = \begin{cases} \frac{(x+1)(x^q-1)\left((x^2+x+1)x^{2p}-(x^2+1)(x^q+1)+x^{2q+1}\right)}{(x-1)(x^3-1)}, & \text{if } 1 \leqslant q \leqslant p; \\ \frac{(x+1)(x^p-1)\left((x^2+x+1)x^{2q}-(x^2+1)(x^p+1)+x^{2p+1}\right)}{(x-1)(x^3-1)}, & \text{otherwise.} \end{cases} \quad (9)$$

Proof If $1 \leqslant q \leqslant p$, by Lemma 2.3(1), we have

$$\begin{aligned} &H_{T(p,q)}(v_0) \\ &= \sum_{k=0}^{q-1}\left(x^{2k} - x^{2k+1} + 4\sum_{i=2k+1}^{3k+1} x^i - x^{3k+1} + 2\sum_{i=3k+2}^{2p+k} x^i - x^{2p+k}\right) \\ &= -\frac{x^{2q}-1}{x+1} + 4\sum_{k=0}^{q-1}\sum_{i=2k+1}^{3k+1} x^i - \frac{x(x^{3q}-1)}{x^3-1} + 2\sum_{k=0}^{q-1}\sum_{i=3k+2}^{2p+k} x^i - \frac{x^{2p}(x^q-1)}{x-1} \\ &= -\frac{x^{2q}-1}{x+1} - \frac{x(x^{3q}-1)}{x^3-1} - \frac{x^{2p}(x^q-1)}{x-1} + 4\left(\sum_{i=1}^{3q-2}\sum_{k=\lceil\frac{i-1}{3}\rceil}^{q-1} x^i - \sum_{i=1}^{2q-1}\sum_{k=\lceil\frac{i}{2}\rceil}^{q-1} x^i\right) \\ &\quad + 2\left(\sum_{i=2}^{2p}\sum_{k=0}^{q-1} x^i + \sum_{i=2p+1}^{2p+q-1}\sum_{k=i-2p}^{q-1} x^i - \sum_{i=2}^{3q-2}\sum_{k=\lceil\frac{i-1}{3}\rceil}^{q-1} x^i\right) \end{aligned}$$

$$
\begin{aligned}
&= -\frac{x^{2q}-1}{x+1} - \frac{x(x^{3q}-1)}{x^3-1} - \frac{x^{2p}(x^q-1)}{x-1} + 4\sum_{i=1}^{3q-2}\left(q-\left\lceil\frac{i-1}{3}\right\rceil\right)x^i \\
&\quad -4\sum_{i=1}^{2q-1}\left(q-\left\lceil\frac{i}{2}\right\rceil\right)x^i + 2q\sum_{i=2}^{2p}x^i + 2\sum_{i=2p+1}^{2p+q-1}(2p+q-i)x^i \\
&\quad -2\sum_{i=2}^{3q-2}\left(q-\left\lceil\frac{i-1}{3}\right\rceil\right)x^i \\
&= -\frac{x^{2q}-1}{x+1} - \frac{x(x^{3q}-1)}{x^3-1} - \frac{x^{2p}(x^q-1)}{x-1} - 2\sum_{i=1}^{3q-2}\left\lceil\frac{i-1}{3}\right\rceil x^i + 4\sum_{i=1}^{2q-1}\left\lceil\frac{i}{2}\right\rceil x^i \\
&\quad +4q\sum_{i=2q}^{3q-2}x^i + 2q\sum_{i=3q-1}^{2p+q-1}x^i + 2\sum_{i=2p+1}^{2p+q-1}(2p-i)x^i \\
&= -\frac{x^{2q}-1}{x+1} - \frac{x(x^{3q}-1)}{x^3-1} - \frac{x^{2p}(x^q-1)}{x-1} \\
&\quad -\frac{2}{3}\left(\sum_{i=1}^{3q-2} ix^i - \sum_{\substack{i=1\\ i\equiv 1 \pmod 3}}^{3q-2} x^i + \sum_{\substack{i=1\\ i\equiv 2 \pmod 3}}^{3q-2} x^i\right) + 4\left(\sum_{i=1}^{2q-1}\frac{i+1}{2}x^i - \sum_{\substack{i=1\\ i \text{ even}}}^{2q-1}\frac{1}{2}x^i\right) \\
&\quad +\frac{4q(x^{3q-1}-x^{2q})}{x-1} + \frac{2q(x^{2p+q}-x^{3q-1})}{x-1} + 2\left(\frac{x^{2p+1}(x^q-1)}{(x-1)^2} - \frac{qx^{2p+q}}{x-1}\right) \\
&= -\frac{x^{2q}-1}{x+1} - \frac{x(x^{3q}-1)}{x^3-1} + \frac{(x+1)x^{2p}(x^q-1)}{(x-1)^2} \\
&\quad -\frac{2}{3}\left(\frac{(3qx^{3q+1}-2x^{3q+1}+x^{3q}+x^2)}{x(x-1)^2} - \frac{x(x^{3q}-1)}{x^3-1} + \frac{x^2(x^{3q-3}-1)}{x^3-1}\right) \\
&\quad +4\left(\frac{qx^{2q}}{x-1} - \frac{x(x^{2q}-1)}{(x+1)(x-1)^2}\right) + \frac{2qx^{3q-1}}{x-1} - \frac{4qx^{2q}}{x-1} \\
&= -\left(\frac{x^{2q}-1}{x+1} + \frac{4x(x^{2q}-1)}{(x+1)(x-1)^2}\right) + \frac{(x+1)x^{2p}(x^q-1)}{(x-1)^2} \\
&\quad -\left(\frac{2(3qx^{3q+1}-2x^{3q+1}+x^{3q}+x^2)}{3x(x-1)^2}\right. \\
&\quad \left. +\frac{x(x^{3q}-1)}{3(x^3-1)} + \frac{2x^2(x^{3q-3}-1)}{3(x^3-1)}\right) + \frac{2qx^{3q-1}}{x-1} \\
&= -\frac{(x+1)(x^{2q}-1)}{(x-1)^2} + \frac{(x+1)x^{2p}(x^q-1)}{(x-1)^2} \\
&\quad -\left(\frac{2qx^{3q-1}}{x-1} - \frac{x(x+1)(x^{3q}-1)}{(x-1)(x^3-1)}\right) + \frac{2qx^{3q-1}}{x-1} \\
&= \frac{(x+1)(x^q-1)}{(x-1)(x^3-1)}\big((x^2+x+1)x^{2p} - (x^2+1)(x^q+1) + x^{2q+1}\big). \qquad (10)
\end{aligned}
$$

If $q > p$, by Lemma 2.3(2), regardless of parities of p and k , we always have

$$
\begin{aligned}
&H_{T(p,q)}(v_0)\\
&= H_{T(p,p)}(v_0) + \sum_{k=p}^{q-1}\left(x^{2k} - x^{2k+1} + 4\sum_{i=2k+1}^{p+2k} x^i - x^{p+2k} + x^{2p+k+1}\right)\\
&= H_{T(p,p)}(v_0) - \frac{x^{2p}(x^{2q-2p}-1)}{x+1} + 4\left(\sum_{i=2p+1}^{3p}(q-p)x^i\right.\\
&\quad \left. + \sum_{i=3p+1}^{p+2q-2}\left(q - \left\lceil\frac{i-p}{2}\right\rceil\right)x^i - \sum_{i=2p+1}^{2q-2}\left(q - \left\lceil\frac{i}{2}\right\rceil\right)x^i\right) + \frac{x^{3p}(x^{2q-2p}-1)}{x+1}\\
&= H_{T(p,p)}(v_0) + \frac{x^{2p}(x^p-1)(x^{2q-2p}-1)}{x+1} + \frac{4(q-p)x^{2p+1}(x^p-1)}{x-1}\\
&\quad + 4\left(\sum_{i=3p+1}^{p+2q-2}\left(q - \frac{i-p}{2}\right)x^i - \sum_{\substack{i=3p+1\\ i-p\equiv 1 (\mathrm{mod}\ 2)}}^{p+2q-2}\frac{1}{2}x^i\right)\\
&\quad - 4\left(\sum_{i=2p+1}^{2q-2}\left(q - \frac{i}{2}\right)x^i - \sum_{\substack{i=2p+1\\ i\,\mathrm{odd}}}^{2q-2}\frac{1}{2}x^i\right)\\
&= H_{T(p,p)}(v_0) + \frac{x^{2p}(x^p-1)(x^{2q-2p}-1)}{x+1} + \frac{4(q-p)x^{2p+1}(x^p-1)}{x-1}\\
&\quad + \left(\frac{2(2q+p)x^{3p+1}(x^{2q-2p-2}-1)}{x-1} - 2\sum_{i=3p+1}^{p+2q-2} ix^i - \frac{2x^{3p+1}(x^{2q-2p-2}-1)}{x^2-1}\right)\\
&\quad - \left(\frac{4qx^{2p+1}(x^{2q-2p-2}-1)}{x-1} - 2\sum_{i=2p+1}^{2q-2} ix^i - \frac{2x^{2p+1}(x^{2q-2p-2}-1)}{x^2-1}\right)\\
&= H_{T(p,p)}(v_0) + \frac{x^{2p}(x^p-1)(x^{2q-2p}-1)}{x+1} + \frac{4(q-p)x^{2p+1}(x^p-1)}{x-1}\\
&\quad + \frac{2(2q+p)x^{3p+1}(x^{2q-2p-2}-1)}{x-1} - \frac{2x^{2p+1}(x^p-1)(x^{2q-2p-2}-1)}{x^2-1}\\
&\quad - \frac{4qx^{2p+1}(x^{2q-2p-2}-1)}{x-1} - 2\left(\sum_{i=3p+1}^{p+2q-2} ix^i - \sum_{i=2p+1}^{2q-2} ix^i\right)\\
&= H_{T(p,p)}(v_0) + \frac{x^{2p}(x^p-1)(x^{2q-2p}-1)}{x+1} + \frac{4(q-p)x^{2p+1}(x^p-1)}{x-1}\\
&\quad + \frac{4qx^{3p+1}(x^{2q-2p-2}-1)}{x-1} + \frac{2px^{3p+1}(x^{2q-2p-2}-1)}{x-1}
\end{aligned}
$$

$$
\begin{aligned}
&-\frac{2x^{2p+1}(x^p-1)(x^{2q-2p-2}-1)}{x^2-1}-\frac{4qx^{2p+1}(x^{2q-2p-2}-1)}{x-1}\\
&-2\Bigg(\frac{2px^{2p+1}(x^p-1)(x^{2q-2p-2}-1)}{x-1}-\frac{x^{2p+1}(x^p-1)(x^{2q-2p-2}-1)}{(x-1)^2}\\
&+\frac{px^{3p+1}(x^{2q-2p-2}-1)}{x-1}+\frac{2(q-p-1)x^{2q-1}(x^p-1)}{x-1}\Bigg)\\
=&H_{T(p,p)}(v_0)+\frac{x^{2p}(x^p-1)(x^{2q-2p}-1)}{x+1}+\Bigg(\frac{4(q-p)x^{2p+1}(x^p-1)}{x-1}\\
&-\frac{4(q-p-1)x^{2q-1}(x^p-1)}{x-1}\Bigg)+\Bigg(\frac{4qx^{3p+1}(x^{2q-2p-2}-1)}{x-1}\\
&-\frac{4qx^{2p+1}(x^{2q-2p-2}-1)}{x-1}\Bigg)\\
&+\Bigg(-\frac{2x^{2p+1}(x^p-1)(x^{2q-2p-2}-1)}{x^2-1}+\frac{2x^{2p+1}(x^p-1)(x^{2q-2p-2}-1)}{(x-1)^2}\Bigg)\\
&-\frac{4px^{2p+1}(x^p-1)(x^{2q-2p-2}-1)}{x-1}\\
=&H_{T(p,p)}(v_0)+\frac{x^{2p}(x^p-1)(x^{2q-2p}-1)}{x+1}\\
&-\frac{4(q-p)x^{2p+1}(x^p-1)(x^{2q-2p-2}-1)}{x-1}\\
&+\frac{4x^{2q-1}(x^p-1)}{x-1}+\frac{4qx^{2p+1}(x^p-1)(x^{2q-2p-2}-1)}{x-1}\\
&+\frac{4x^{2p+1}(x^p-1)(x^{2q-2p-2}-1)}{(x+1)(x-1)^2}-\frac{4px^{2p+1}(x^p-1)(x^{2q-2p-2}-1)}{x-1}\\
=&H_{T(p,p)}(v_0)+\frac{x^{2p}(x^p-1)(x^{2q-2p}-1)}{x+1}\\
&+\Bigg(\frac{4x^{2q-1}(x^p-1)}{x-1}+\frac{4x^{2p+1}(x^p-1)(x^{2q-2p-2}-1)}{(x+1)(x-1)^2}\Bigg)\\
=&H_{T(p,p)}(v_0)+\frac{x^{2p}(x^p-1)(x^{2q-2p}-1)}{x+1}+\frac{4x^{2p+1}(x^p-1)(x^{2q-2p}-1)}{(x+1)(x-1)^2}\\
=&H_{T(p,p)}(v_0)+\frac{(x+1)(x^p-1)(x^{2q}-x^{2p})}{(x-1)^2}. \qquad (11)
\end{aligned}
$$

By substituting Eq. (10) into Eq. (11), we obtain explicit expression of $H_{T(p,q)}(v_0)$ as Eq. (9) in the case $q > p$. □

4 Main results

In this section, we are ready to calculate the Hosoya polynomial of $T(p, q)$, simply denoted by $H(p, q, x)$. Firstly, for $q \geqslant 2$, we consider the corresponding *difference* *polynomial*:

$$\Delta H(p, q, x) := H(p, q, x) - H(p, q-1, x).$$

For convenience, we set $\Delta H(p, 1, x) = H(p, 1, x)$. Then

Lemma 4.1

$$H(p, q, x) = \sum_{j=1}^{q} \Delta H(p, j, x).$$

From the above lemma, our aim is changed into calculating $\Delta H(p, q, x)$. By Lemma 2.1, $T(p, q-1)$ can be considered as the induced convex subgraph of $T(p, q)$ by deleting all vertices of level 0, so $\Delta H(p, q, x)$ is equal to the contribution of vertices lying at level 0 to $H(p, q, x)$. By the structure of $T(p, q)$, we know the status of all $2p$ vertices with degree 2 in layer 0 are equivalent, as well all $2p$ vertices with degree 3 in layer 0. So (Note that $H_{T(p,1)}(v_0) = H_{T(p,1)}(u_0)$ and $H(C_{4p}, x) = 2pH_{T(p,1)}(v_0) + 2p$.)

$$\Delta H(p, q, x) = 2pH_{T(p,q)}(v_0) + 2pH_{T(p,q)}(u_0) - \big(2pH_{T(p,1)}(u_0) - 2p\big). \quad (12)$$

The subtraction of the last term in the right-hand side of Eq. (12) is reasoned as follows: contribution of pairs of distinct vertices lying at level 0 to $H(p, q, x)$ is counted twice in the first two terms.

By Lemma 2.1, for any vertex v not lying at level 0, we get

$$d_{T(p,q)}(u_0, v) = d_{T(p,q)}(v_{0,1}, v) + 1,$$

so (for the unity of expression, we set $H_{T(p,0)}(v_0) = 0$.)

$$H_{T(p,q)}(u_0) = xH_{T(p,q-1)}(v_0) + H_{T(p,1)}(u_0). \quad (13)$$

By Eqs. (12) and (13), we obtain

Lemma 4.2

$$\Delta H(p, q, x) = 2p + 2pH_{T(p,q)}(v_0) + 2pxH_{T(p,q-1)}(v_0).$$

By Lemmas 3.1, 4.1 and 4.2, we get our main results, i.e., the Hosoya polynomial of $T(p, q)$, as follows.

Theorem 4.3 *In the case $q \leqslant p$,*

$$\begin{aligned}H(p,q,x) =& 2pq + \frac{4px^{2p+1}(x+1)(x^q-1)}{(x-1)^3}\\ &- \frac{2pq(x+1)^2\big((x^2+1)(x^{2p}-1)+x^{2p+1}\big)}{(x-1)(x^3-1)}\\ &+ \frac{2px(x+1)\big(x(x^2+1)(x^{3q}-1)-(x^2+x+1)^2(x^{2q}-1)\big)}{(x-1)(x^3-1)^2}.\end{aligned}$$

While in the case $q > p$,

$$\begin{aligned}H(p,q,x) =& 2pq + \frac{2px(x+1)(x^p-1)(x^{2q}+x^{2p}-x^p-1)}{(x-1)^3}\\ &+ \frac{2px^2(x+1)(x^2+1)(x^{3p}-1)}{(x-1)(x^3-1)^2}\\ &- \frac{2p(x+1)^2\big(q(x^p-1)((x^2+1)(x^p+1)-x^{2p+1})+px^{3p+1}\big)}{(x-1)(x^3-1)}.\end{aligned}$$

Proof If $q \leqslant p$, by Lemmas 3.1, 4.1 and 4.2, we get

$$\begin{aligned}&H(p,q,x)\\ &= \sum_{j=1}^{q} \Delta H(p,j,x) = \sum_{j=1}^{q} \big(2p + 2pH_{T(p,j)}(v_0) + 2pxH_{T(p,j-1)}(v_0)\big)\\ &= 2pq + 2p(x+1)\sum_{j=1}^{q} H_{T(p,j)}(v_0) - 2pxH_{T(p,q)}(v_0)\\ &= 2pq + \frac{2p(x+1)^2}{(x-1)(x^3-1)}\\ &\quad\times\left(\left(x^2+x+1\right)x^{2p}\left(\frac{x(x^q-1)}{x-1}-q\right)-(x^2+1)\left(\frac{x^2(x^{2q}-1)}{x^2-1}-q\right)\right.\\ &\quad\left.+\left(\frac{x^4(x^{3q}-1)}{x^3-1}-\frac{x^3(x^{2q}-1)}{x^2-1}\right)\right) - \Big(\frac{2px^{2p+1}(x+1)(x^2+x+1)(x^q-1)}{(x-1)(x^3-1)}\\ &\quad-\frac{2px(x+1)(x^2+1)(x^{2q}-1)}{(x-1)(x^3-1)}+\frac{2px(x+1)x^{2q+1}(x^q-1)}{(x-1)(x^3-1)}\Big)\\ &= 2pq + \frac{4px^{2p+1}(x+1)(x^q-1)}{(x-1)^3} - \frac{2pq(x+1)^2\big((x^2+1)(x^{2p}-1)+x^{2p+1}\big)}{(x-1)(x^3-1)}\\ &\quad+\frac{2px(x+1)\big(x(x^2+1)(x^{3q}-1)-(x^2+x+1)^2(x^{2q}-1)\big)}{(x-1)(x^3-1)^2}.\end{aligned}$$

Similarly, if $q > p$,

$$
\begin{aligned}
&H(p,q,x)\\
=&H(p,p,x)+\sum_{j=p+1}^{q}\Delta H(p,j,x)\\
=&H(p,p,x)+\sum_{j=p+1}^{q}\big(2p+2pH_{T(p,j)}(v_0)+2pxH_{T(p,j-1)}(v_0)\big)\\
=&H(p,p,x)+2(q-p)p+2p(x+1)\sum_{j=p+1}^{q}H_{T(p,j)}(v_0)\\
&+2px\big(H_{T(p,p)}(v_0)-H_{T(p,q)}(v_0)\big)\\
=&H(p,p,x)+2(q-p)p+\frac{2p(x+1)^2(x^p-1)}{(x-1)(x^3-1)}\\
&\left((x^2+x+1)\frac{x^2(x^{2q}-x^{2p})}{x^2-1}-(q-p)\left((x^2+1)(x^p+1)-x^{2p+1}\right)\right)\\
&+\frac{2px(x+1)(x^2+x+1)(x^p-1)(x^{2p}-x^{2q})}{(x-1)(x^3-1)}\\
=&\left(2p^2+\frac{4px^{2p+1}(x+1)(x^p-1)}{(x-1)^3}-\frac{2p^2(x+1)^2\big((x^2+1)(x^{2p}-1)+x^{2p+1}\big)}{(x-1)(x^3-1)}\right.\\
&\left.+\frac{2px(x+1)\big(x(x^2+1)(x^{3p}-1)-(x^2+x+1)^2(x^{2p}-1)\big)}{(x-1)(x^3-1)^2}\right)+2(q-p)p\\
&+\frac{2px(x+1)(x^p-1)(x^{2q}-x^{2p})}{(x-1)^3}\\
&-\frac{2pq(x+1)^2(x^p-1)\big((x^2+1)(x^p+1)-x^{2p+1}\big)}{(x-1)(x^3-1)}\\
&+\frac{2p^2(x+1)^2\big((x^2+1)(x^{2p}-1)+x^{2p+1}-x^{3p+1}\big)}{(x-1)(x^3-1)}\\
=&2pq+\frac{2px(x+1)(x^p-1)(x^{2q}+x^{2p})}{(x-1)^3}-\frac{2p^2(x+1)^2x^{3p+1}}{(x-1)(x^3-1)}\\
&+\frac{2px^2(x+1)(x^2+1)(x^{3p}-1)}{(x-1)(x^3-1)^2}-\frac{2px(x+1)(x^p-1)(x^p+1)}{(x-1)^3}\\
&-\frac{2pq(x+1)^2(x^p-1)\big((x^2+1)(x^p+1)-x^{2p+1}\big)}{(x-1)(x^3-1)}\\
=&2pq+\frac{2px(x+1)(x^p-1)(x^{2q}+x^{2p}-x^p-1)}{(x-1)^3}+\frac{2px^2(x+1)(x^2+1)(x^{3p}-1)}{(x-1)(x^3-1)^2}\\
&-\frac{2p(x+1)^2\big(q(x^p-1)((x^2+1)(x^p+1)-x^{2p+1})+px^{3p+1}\big)}{(x-1)(x^3-1)}.
\end{aligned}
$$

□

Corollary 4.4 ([20]) *In the case of short tubes, i.e., $q \leqslant p$,*

$$W(T(p,q)) = \frac{2}{3}pq\big(12qp^2 + (q^2-1)(4p+q)\big).$$

While in the case of long tubes, i.e., $q > p$,

$$W(T(p,q)) = \frac{2}{3}p^2\big(-p^3 + 4qp^2 + (6q^2+1)p + 8q^3 - 6q\big).$$

Corollary 4.5 *In the case of short tubes, i.e., $q \leqslant p$,*

$$\begin{aligned} WW(T(p,q)) = &\frac{pq}{15}\big(80qp^3 + 20(2q^2+3q-2)p^2 + 10(q^3+2q^2-2)p \\ &+ (q^2-1)(12q^2+5q+2)\big). \end{aligned}$$

While in the case of long tubes, i.e., $q > p$,

$$\begin{aligned} WW(T(p,q)) = &\frac{p^2}{15}\big(-18p^4 + 5(12q-1)p^3 + 20(q^2+q+1)p^2 \\ &+ 5(8q^3+6q^2-14q+1)p \\ &+ 40q^3(q+1) - 30q - 2\big). \end{aligned}$$

Remark Some computations in this paper can be performed by applying the Software package MATHEMATICA 5.2.

Acknowledgement We thank Professor Mircea V. Diudea for making some papers available to us.

References

1. R. Aringhieri, P. Hansen, F. Malucelli, A linear algorithm for the hyper-Wiener index of chemical trees. J. Chem. Inf. Comput. Sci. **41**, 958–963 (2001)
2. D.S. Bethune, C.H. Kiang, M.S. Devries, G. Gorman, R. Savoy, J. Vazquez , R. Beyers, Cobalt catalyzed growth of carbon nanotubes with single atomic layer walls, Nature **363**, 605–607 (1993)
3. M.V. Diudea, Hosoya polynomial in tori, MATCH Commun. Math. Comput. Chem. **45**, 109–122 (2002)
4. M.V. Diudea, Covering nanostructures, in *Nanostructures-Novel Architecture*, ed. by M.V. Diudea (NOVA, New York, 2005), pp. 203–242
5. E. Estrada, O. Ivanciuc, I. Gutman, A. Gutierrez, L. Rodriguez, Extended Wiener indices. A new set of descriptors for quantitative structure-property studies, New J. Chem. **22**, 819–822 (1998)
6. I. Gutman, Some properties of the Wiener polynomial, Graph Theory Notes **25**, 13–18 (1993)
7. I. Gutman, E. Estrada, O. Ivanciuc, Some properties of the Hosoya polynomial of trees, Graph Theory Notes **36**, 7–13 (1999)
8. I. Gutman, S. Klavžar, B. Mohar (eds.), Fifty years of the Wiener index. MATCH Commun. Math. Comput. Chem. **35**, 1997
9. I. Gutman, S. Klavžar, B. Mohar (eds.), Fiftieth anniversary of the Wiener index. Discrete Appl. Math. **80**, 1997
10. I. Gutman, S. Klavžar, M. Petkovšek, P. Žigert, On Hosoya polynomials of benzenoid graphs. MATCH Commun. Math. Comput. Chem. **43**, 49–66 (2001)

11. H. Hosoya, Topological index. A newly proposed quantity characterizing the topological nature of structural isomers of saturated hydrocarbons. Bull. Chem. Soc. Jpn. **44**, 2332–2339 (1971)
12. H. Hosoya, On some counting polynomials in chemistry. Discrete Appl. Math. **19**, 239–257 (1988)
13. S. Iijima, Helical microtubules of graphitic carbon. Nature **354**, 56–58 (1991)
14. S. Iijima, T. Ichihashi, Single shell carbon nanotubes of one nanometer diameter. Nature **363**, 603–605 (1993)
15. S. Klavžar, P. Žigert, I. Gutman, An algorithm for the calculation of the hyper-Wiener index of benzenoid hydrocarbons. Comput. Chem. **24**, 229–233 (2000)
16. D.J. Klein, I. Lukovits, I. Gutman, On the definition of the hyper-Wiener index for cycle-containing structures. J. Chem. Inf. Comput. Sci. **35**, 50–52 (1995)
17. E.V. Konstantinova, M.V. Diudea, The Wiener polynomial derivatives and other topological indices in chemical research. Croat. Chem. Acta **73**, 383–403 (2000)
18. M. Randić, Novel molecular descriptor for structure-property studies. Chem. Phys. Lett. **211**, 478–483 (1993)
19. B.E. Sagan, Y.-N. Yeh, P. Zhang, The Wiener polynomial of a graph. Int. J. Quantum Chem. **60**, 959–969 (1996)
20. M. Stefu, M.V. Diudea, Wiener index of C_4C_8 nanotubes. MATCH Commun. Math. Comput. Chem. **50**, 133–144 (2004)
21. H. Wiener, Structural determination of paraffin boiling points. J. Am. Chem. Soc. **69**, 17–20 (1947)
22. S. Xu, H. Zhang, The Hosoya polynomial decompositions for catacondensed benzenoid graphs. Discrete Appl. Math. (online)
23. S. Xu, H. Zhang, Hosoya polynomials under gated amalgamations. Discrete Appl. Math. (online)
24. S. Xu, H. Zhang, Hosoya polynomials of armchair open-ended nanotubes. Int. J. Quantum Chem. **107**, 586–596 (2007)
25. S. Xu, H. Zhang, M.V. Diudea, Hosoya polynomials of zig-zag open-ended nanotubes. MATCH Commun. Math. Comput. Chem. **57**, 443–456 (2007)
26. B.-Y. Yang, Y.-N. Yeh, Wiener polynomials of some chemically interesting graphs. Int. J. Quantum Chem. **99**, 80–91 (2004)
27. H. Zhang, S. Xu, Y. Yang, Wiener index of toroidal polyhexes. MATCH Commun. Math. Comput. Chem. **56**, 153–168 (2006)