Hosoya polynomials of twisted toroidal polyhexes

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Abstract

The Hosoya polynomial of a graph G with vertex set $V(G)$ is defined as $H(G,x) = \sum_{\{u,v\}\subseteq V(G)} x^{d_G(u,v)}$ on variable x, where $d_G(u,v)$ is the distance between vertices u and v. A toroidal polyhex $H(p,q,t)$ is a cubic bipartite graph embedded on the torus such that each face is a hexagon, which can be described by a string (p,q,t) of three integers $(p \geqslant 1, q \geqslant 1, 0 \leqslant t \leqslant p-1)$. In this paper, we give an analytical formulae for calculating the Hosoya polynomial of $H(p,q,t)$ for $t = 0$ or $p \leqslant 2q$ or $p \leqslant q + t$. Some early results in [2, 6, 26] are direct corollaries of our main results.

Keywords: Wiener index; Hosoya polynomial; toroidal polyhex.

1 Introduction

The *Hosoya polynomial* in variable x of a graph G with vertex set $V(G)$, introduced by Hosoya [9], 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* between vertices u and v of G (i.e., the length of a shortest path connecting u and v) (the subscript is omitted when there is no risk of confusion). Note that there is no constant term, while the definition contains the number of vertices as constant term in some literatures.

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The Hosoya polynomial of a graph not only contains more information concerning distance than any of the hitherto proposed distance-based topological indices, which were extensively studied in chemical graph theory, see for instance the surveys [15, 17], but also deduces some of them. For example, Wiener index $W(G)$ of graph G [22], the oldest and most well-studied topological index so far, is equal to the first derivative of the Hosoya polynomial at $x = 1$:

$$W(G) = \frac{\mathrm{d}}{\mathrm{d}x} H(G,x)\Big|_{x=1} . \tag{1}$$

Its chemical applications and mathematical properties are well documented [4, 5, 7, 8]. Moreover, the hyper-Wiener index $WW(G)$ [12], Tratch-Stankevitch-Zefirov index $TSZ(G)$ [21] can be deduced from $H(G,x)$ as follows:

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

$$TSZ(G) = \frac{1}{3!}\frac{\mathrm{d}^3}{\mathrm{d}x^3} x^2 H(G,x)\Big|_{x=1} . \tag{3}$$

To the best of our knowledge, the formulae (2) and (3) were first reported in [23] and [1], respectively. Two classes of more general structure descriptors $\frac{1}{k!}\frac{\mathrm{d}^k}{\mathrm{d}x^k} x^{k-1} H(G,x)\Big|_{x=1}$ and $\frac{1}{k!}\frac{\mathrm{d}^k}{\mathrm{d}x^k} H(G,x)\Big|_{x=1}$ for positive integer k were also studied [1, 13]. On the other hand, Brückler etc. [1] proposed a new class of distance-based molecular structure descriptors: Q-indices, which can reflect the fact that any kind of interaction between physical objects (in particular, between atoms in a molecule) decreases with increasing distance, and showed that Q-indices are equal to the Hosoya polynomial. So the Hosoya polynomial and the quantities derived from it will play a significant role in QSAR and QSPR researches, and abundant literature appeared on this topic for the theoretical consideration [24, 25] and computation [6, 23].

In this paper we focus on the Hosoya polynomial of a toroidal polyhex $H(p,q,t)$ which is described by a string (p,q,t) of three integers $p \geqslant 1, q \geqslant 1, 0 \leqslant t \leqslant p-1$ (see the next section for details on the definition) and give an analytical formula for calculating the Hosoya polynomial of $H(p,q,t)$ under the condition:

$$\text{either } t = 0 \text{ or } p \leqslant 2q \text{ or } p \leqslant q + t. \tag{4}$$

As corollaries, we can easily obtain Hosoya polynomials of two special classes of toroidal polyhexes [2, 6]. As another corollaries, Some distance-based topological indices, such as the Wiener index, Hyper-Wiener index, TSZ index, of $H(p,q,t)$ under Condition (4) can be obtained [26].

2 Some Preliminaries

A *toroidal polyhex* $H(p,q,t)$ [16, 19], described by three parameters p, q and t, is a 3-regular (cubic or trivalent) bipartite graph embedded on the torus such that each face is a hexagon and represented by a $p\times q$-parallelogram M in the plane (equipped with the regular hexagonal lattice L) with the usual boundary identification (see Fig. 1): each side of M connects the centers of two hexagons, and is perpendicular to an edge-direction of L, both top and bottom sides pass through p vertical edges of L; while two lateral sides pass through q edges. First identify its two lateral sides, then rotate the top cycle t hexagons ($0 \leqslant t \leqslant p-1$), finally identify the top and bottom at their corresponding points. If we only carry out the lateral boundary identification, then we obtain a *tubule*, denoted by $T(p,q)$. Toroidal polyhexes have been recently experimentally detected [14]. Various researches on toroidal polyhexes appeared in both chemical and mathematical literatures, such as theoretical background [18, 20], the enumeration of Kekulé structures [10, 11] and k-resonance [19, 27], etc.

Theorem 2.1. *[16, 20] $H(p,q,t)$ is a vertex-transitive graph.*

In the sequel G means the graph $H(p,q,t)$. In order to compute the Hosoya polynomial of G, let $H_v(G,x)$ denote the contribution of a given vertex v of G to the Hosoya polynomial of G. By Theorem 2.1, the Hosoya polynomial of G can be expressed as

$$H(G,x) = pqH_v(G,x). \tag{5}$$

Note that the number of vertices of G is $2pq$. So our main object is to compute $H_v(G,x)$ for any given vertex v.

Similar to the notations in [19, 27], we label vertices of G. In a given parallelogram embedding M of G defined above, we denote by *layer* $0,1,2,\cdots,q-1$ horizontal zig-zag lines in M from bottom to top, we denote vertices on layer k by $v_{0,k}, v_{1,k}, \cdots, v_{2p-1,k}$ (in the sense that the first subscript modules $2p$) from left to right ($0 \leqslant k \leqslant q-1$). For a concrete and strict definition, we refer the reader to Ref. [19, 27]. In G, $v_{0,k}$ and $v_{2p-1,k}$ are adjacent for $0 \leqslant k \leqslant q-1$ and $v_{i,0}$ and $v_{i+2t+1,q-1}$ are adjacent for all even i. In a 2-coloring of $V(G)$, $v_{i,j}$ is colored white or black according to the parity of i (see Fig. 1). However tubule $T(p,q)$ can also be obtained from G by deleting all edges passing through the bottom side of M.

In the following we define some notations. For a given vertex v of G, $0 \leqslant l \leqslant 2p-1$, $0 \leqslant k \leqslant q-1$, the sequence of distances from v to the vertices in layer k started at $v_{l,k}$ is defined:

$$S_G(l,k;v) := \big(d_G(v_{l,k},v), d_G(v_{l+1,k},v), \cdots, d_G(v_{l+2p-1,k},v)\big),$$

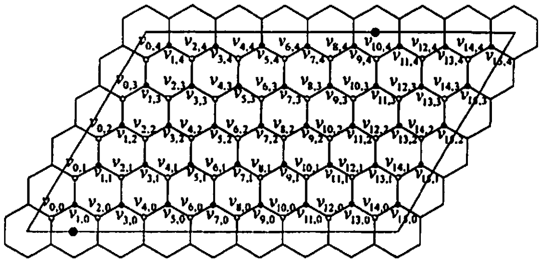

Fig. 1. A toroidal polyhex $H(p,q,t)$ for $p=8, q=5$ and $t=4$ and the labelling of vertices.

and $S_G(k;v)$ is the cyclic sequence of $S_G(l,k;v)$. For convenience, for non-negative integers m, n and s we define three sequences of integers as follows.

$$\begin{aligned} m,\nearrow,n &:= (m, m+1, m+2, \cdots, n); && (m \leqslant n)\\ m,\searrow,n &:= (m, m-1, m-2, \cdots, n); && (m \geqslant n)\\ m, \leftrightsquigarrow 2s, n &:= \overbrace{m,n,m,n,\cdots,m,n}^{2s\text{ terms}}; && (m \neq n). \end{aligned}$$

3 Calculating $H(H(p,q,t),x)$

Zhang et al. [26] have obtained the cyclic sequence of the distance sequence from vertex $v_{0,0}$ to vertices in layer k in G under Condition (4), i.e., Section 3.2 in [26], in which there are five cases and the fifth case contains six subcases. For example, the first case: $p \leqslant \frac{q}{2}$, the cyclic sequence of the distance sequence from $v_{0,0}$ to vertices in layer k is

$$S_G(k;v_{0,0}) = \begin{cases} (2k,\nearrow,p+k,\searrow,2k,\leftrightsquigarrow 2k, 2k+1), & 0 \leqslant k \leqslant p-1,\\ (2k,\leftrightsquigarrow 2p, 2k+1), & p \leqslant k \leqslant \frac{q-1}{2},\\ (2(q-k),\leftrightsquigarrow 2p, 2(q-k)-1), & \frac{q-1}{2} \leqslant k \leqslant q-p-1,\\ (2(q-k)-1,\leftrightsquigarrow 2(q-k), 2(q-k), & \\ \nearrow, p+q-k,\searrow, 2(q-k)), & q-p \leqslant k \leqslant q-1. \end{cases}$$

From above case 1, using software package MATHEMATICA 8.0, the contribution $H_{v_{0,0}}(G,x)$ of $v_{0,0}$ to Hosoya polynomial $H(G,x)$ can be obtained as follows:

$$H_{v_{0,0}}(G,x) = \frac{3x-(x+1)^2x^p + x^{2p+1} + p(x^2-1)x^q}{(x-1)^2}.$$

In view of the complicated expressions about the cyclic sequence of the distance sequence in the other cases, we don't list the other cases here. Similar to Case 1, we can obtain $H_{v_{0,0}}(G,x)$ in the other cases. By Eq. (5), we obtain $H(G,x)$ under Condition (4) as follows.

Theorem 3.1. *Let $H(p,q,t)$ be a twisted toroidal polyhex under the condition $t=0$ or $p \leqslant 2q$ or $p \leqslant q+t$. Then we have*

$$H(H(p,q,t),x) =$$
$$\begin{cases} \frac{pq(3x-(x+1)^2x^p+x^{2p+1}+p(x^2-1)x^q)}{(x-1)^2}, & p \leqslant \frac{q}{2}; \\ \frac{pq(\Theta+3x-(x+1)^2x^p-(2(x+1)^2+(p-q)(x^2-1))x^q)}{(x-1)^2}, & \frac{q}{2} < p \leqslant \frac{q}{2}+\frac{t}{2}; \\ \frac{pq(\Theta+3x-(x^p+x^{2p-t}+x^q)(x+1)^2+((2p-q-t)x^{2p-t}+(p-t)x^q)(x^2-1))}{(x-1)^2}, & \frac{q}{2}+\frac{t}{2} < p \leqslant \frac{q}{2}+\frac{3}{4}t; \\ \frac{pq(3x-(x^p-x^{2p-t}+x^q)(x+1)^2+((q+2t-2p)x^{2p-t}+(p-t)x^q)(x^2-1)+x^{2q+2t-2p+1})}{(x-1)^2}, & \frac{q}{2}+\frac{3}{4}t < p \leqslant \frac{q}{2}+t; \\ \frac{pq(3x-(x^p+x^q-x^{q+t})(x+1)^2+(q+t-p+(2p-q-2t)x^t)(x^2-1)x^q+x^{2p-2t+1})}{(x-1)^2}, & \frac{q}{2}+t < p \leqslant \min\{\frac{q}{2}+\frac{3}{2}t, q+t\}; \\ \frac{pq(\Theta+3x-(x^p+x^q+x^{q+t})(x+1)^2+(q+t-p+tx^t)(x^2-1)x^q)}{(x-1)^2}, & \min\{\frac{q}{2}+\frac{3}{2}t, q+t\} < p \leqslant q+t; \\ \frac{pq(\Theta+3x-(x^{p-t}+x^p+x^{q+t})(x+1)^2+((p-q-t)x^{p-t}+tx^{q+t})(x^2-1))}{(x-1)^2}, & q+t < p \leqslant 2q; \\ \frac{pq(3x-(x+1)^2x^q+x^{2q+1}+q(x^2-1)x^p)}{(x-1)^2}, & t=0 \text{ and } 2q < p, \end{cases}$$

where

$$\Theta = \begin{cases} (2+5x+2x^2)\,x^{\frac{2(p+q)}{3}}, & p+q \equiv 0 \pmod 3), \\ (2+x)^2x^{\frac{2p+2q+1}{3}}, & p+q \equiv 1 \pmod 3), \\ (1+2x)^2x^{\frac{2p+2q-1}{3}}, & p+q \equiv 2 \pmod 3). \end{cases}$$

4 Some corollaries from Theorem 3.1

From Theorem 3.1, i.e., the explicit expression of Hosoya polynomial $H(G,x)$ of a toroidal polyhex $G = H(p,q,t)$ under Condition (4), we can obtain some distance-based topological indices. First, from Eq. (1), the first derivative of Hosoya polynomial $H(G,x)$ at $x=1$ leads to the Wiener index of G as follows.

Corollary 4.1. *[26] For either $t=0$ or $p \leqslant 2q$ or $p \leqslant q+t$, if let* $z = \begin{cases} 0, & q+p \equiv 0 \pmod 3), \\ 2, & q+p \equiv 1 \pmod 3), \\ -2, & q+p \equiv 2 \pmod 3), \end{cases}$ *Then we have*

$$W(H(p,q,t)) = \begin{cases} \frac{1}{3}p^2q(3q^2+2p^2-2), & p \leqslant \frac{q}{2}; \\ \frac{1}{9}pq(\Theta_1+z), & \frac{q}{2} < p \leqslant \frac{q}{2}+\frac{t}{2}; \\ \frac{1}{9}pq(\Theta_2+z), & \frac{q}{2}+\frac{t}{2} < p \leqslant \frac{q}{2}+\frac{3}{4}t; \\ \frac{1}{3}pq\Theta_3, & \frac{q}{2}+\frac{3}{4}t < p \leqslant \frac{q}{2}+t; \\ \frac{1}{3}pq\Theta_4, & \frac{q}{2}+t < p \leqslant \min\{\frac{q}{2}+\frac{3}{2}t, q+t\}; \\ \frac{1}{9}pq(\Theta_1-3t+3t^3+z), & \min\{\frac{q}{2}+\frac{3}{2}t, q+t\} < p \leqslant q+t; \\ \frac{1}{9}pq(\Theta_5+z), & q+t < p \leqslant 2q; \\ \frac{1}{3}q^2p(3p^2+2q^2-2), & t=0 \text{ and } 2q < p. \end{cases}$$

where

$\Theta_1 = -2p^3 - 3q + 12p^2q + 3pq^2 + q^3$,

$\Theta_2 = -6p + 22p^3 - 24p^2q + 21pq^2 - 2q^3 + 3t - 36p^2t + 36pqt - 9q^2t + 18pt^2 - 9qt^2 - 3t^3$,

$\Theta_3 = 2p - 14p^3 - 2q + 24p^2q - 9pq^2 + 2q^3 - 2t + 36p^2t - 36pqt + 9q^2t - 30pt^2 + 15qt^2 + 8t^3$,

$\Theta_4 = -2p + 2p^3 + 3pq^2 + 2t - 12p^2t + 12pqt - 3q^2t + 18pt^2 - 9qt^2 - 8t^3$,

$\Theta_5 = -3p + p^3 + 3p^2q + 12pq^2 - 2q^3 - 9p^2t + 18pqt - 9q^2t + 9pt^2 - 9qt^2$.

Secondly, from Eqs. (2) and (3), we easily obtain the hyper-Wiener index and the TSZ index of G under Condition (4). Considering the more complicated expression than $W(H(p,q,t))$, we have no intention to list them here.

Except that the Hosoya polynomial of $H(p,q,t)$ can deduce some distance-based topological indices, the polynomial can also deduce the Hosoya polynomials for the special cases. For example, M.V. Diudea [2], Mehdi Eliasi and Bijan Taeri [6] obtained Hosoya polynomials for two classes of toroidal polyhexes: $HC6\ c,n$ and $VC6\ c,n$ with $n \geqslant c$ and c,n are all even in notations of [2]; $HC(p,q)$ with even p,q in [6]. There are close relationships between two kinds of notations: $HC6\ c,n = HC(p,q)$ iff $c=p, n=q$, hence the condition $n \geqslant c$ is equivalent to $q \geqslant p$; $VC6\ c,n = HC(p,q)$ iff $c=q, n=p$, hence the condition $n \geqslant c$ is equivalent to $p \geqslant q$. We only discuss the relationships between Diudea's notations and the notation $H(p,q,t)$ in what follows.

In fact, $HC6\ c,n$ and $VC6\ c,n$ are precisely $H(\frac{c}{2}, n, -\frac{n}{2}(\text{mod } \frac{c}{2}))$ and $H(\frac{n}{2}, c, -\frac{c}{2}(\text{mod } \frac{n}{2}))$, respectively. For $H(\frac{c}{2}, n, -\frac{n}{2}(\text{mod } \frac{c}{2}))$, let $p=\frac{c}{2}, q=n, t \equiv -\frac{n}{2}(\text{mod } \frac{c}{2}) \equiv -\frac{q}{2}(\text{mod } p)$. The condition $n \geqslant c$ is equivalent to $p \leqslant \frac{q}{2}$, which is exactly the condition of Case 1 in Theorem 3.1. For $H(\frac{n}{2}, c, -\frac{c}{2}(\text{mod } \frac{n}{2}))$, let $p=\frac{n}{2}, q=c, t \equiv -\frac{c}{2}(\text{mod } \frac{n}{2}) \equiv -\frac{q}{2}(\text{mod } p)$. The condition $n \geqslant c$ is equivalent to $p \geqslant \frac{q}{2}$. Hence $t = p - \frac{q}{2}$, i.e., $p = \frac{q}{2}+t$, which is contained in the condition $\frac{q}{2}+t \leqslant p \leqslant \min\{\frac{q}{2}+\frac{3}{2}t, q+t\}$, corresponding to Case 5 in Theorem 3.1. In fact, $HC6\ c,n$ and $VC6\ c,n$ with $n \geqslant c$ are precisely $H(p,q,-\frac{q}{2}(\text{mod } p))$ with $p \leqslant \frac{q}{2}$ and $p \geqslant \frac{q}{2}$ together with $p = \frac{q}{2}+t$, respectively. Hence from Theorem 3.1, we can obtain

Corollary 4.1. *[2, 6] Let n, c be even positive integers with $n \geqslant c$. Then*

$$H(HC6\ c, n,\ x) = \frac{cn\left(6x - 2x^{\frac{c}{2}} - 4x^{1+\frac{c}{2}} - 2x^{2+\frac{c}{2}} + 2x^{1+c} - cx^{n} + cx^{2+n}\right)}{4(x-1)^2};$$

$$H(VC6\ c, n,\ x) = \frac{cn\left(3x + x^{c+1} + \frac{1}{2}cx^{c}\left(x^2 - 1\right) - (1+x)^2(x^{c} + x^{\frac{n}{2}} - x^{\frac{c+n}{2}})\right)}{2(x-1)^2}.$$

Combined Corollary 4.1 and Eq. (1), we can obtain the Wiener indices of $HC6\ c, n$ and $VC6\ c, n$ as follows.

Corollary 4.2. *[2] Let n, c be even positive integers with $n \geqslant c$.*

$$W(HC6\ c, n) = \frac{1}{24}c^2 n\left(6n^2 + c^2 - 4\right);$$

$$W(VC6\ c, n) = \frac{1}{24}c^2 n\left(3n^2 + 3cn + c^2 - 4\right).$$

Similarly, we can obtain the hyper-Wiener indices and the TSZ indices as follows.

Corollary 4.3. *Let n, c be even positive integers with $n \geqslant c$.*

$$WW(HC6\ c, n) = \frac{1}{192}c^2 n\left(3c^3 + 4c^2 - 12c + 8\left(2n^3 + 3n^2 + n - 1\right)\right);$$

$$WW(VC6\ c, n) = \frac{c^2 n\left(5c^3 + 4c^2(n+1) + 2c(3n^2 + 6n - 10)\right)}{192} + \frac{4c^2 n(n^3 + 3n^2 + 4n - 4)}{192}.$$

Corollary 4.4. *Let n, c be even positive integers with $n \geqslant c$.*

$$TSZ(HC6\ c, n) = \frac{c^2 n\left(7c^4 - 30c^3 + 120c + 8\left(5n^4 - 20n^3 + 25n^2 - 10n - 14\right)\right)}{1920};$$

$$TSZ(VC6\ c, n) = \frac{c^2 n}{1920}(5n(n^3 + 8n^2 + 24n + 32) + 17c^4 + 5c^3(n+10) + 10c^2(n^2 + 4n - 4) + 10c(n^3 + 6n^2 + 12n - 20) - 112).$$

Usually, toroidal polyhexes have other notations, such as Kirby's notation $TPH(a, b, d)$ [10] and Diudea's notation VH$t[c, n]$ [3], which correspond to $H(a, d, b - d)$ and $H(\frac{c}{2}, n, \frac{t-n}{2})$, respectively.

5 discussion

In this paper we give the Hosoya polynomial of a twisted toroidal polyhex $H(p, q, t)$ under Condition (4), from which some existed results are obtained. As a future work, the Hosoya polynomial of a twisted toroidal polyhex $H(p, q, t)$ without any restriction on three parameters p, q, t can be studied.

6 Acknowledgements

We thank anonymous referees for careful check and valuable suggestions. The work is partially supported by NSFC (grant Nos. 11001113, 61202315).

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