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Hosoya Polynomials of Hexagonal Triangles and Trapeziums

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Abstract

The Hosoya polynomial of a graph G with vertex set $V(G)$ is defined as $H(G,x) = \sum_{\{u,v\}\subseteq V(G)} x^{d_G(u,v)}$ in variable x, where the sum is over all unordered pairs $\{u,v\}$ of vertices in G, $d_G(u,v)$ is the distance of two vertices u,v in G. In this paper, we investigate Hosoya polynomials of hexagonal trapeziums, tessellations of congruent regular hexagons shaped like trapeziums and give their explicit analytical expressions. As a special case, Hosoya polynomials of hexagonal triangles are obtained. Also, the three well-studied topological indices: Wiener index, hyper-Wiener index and Tratch-Stankevitch-Zefirov index, of hexagonal trapeziums can be easily obtained.

1 Introduction

A molecular graph (or chemical graph) is a representation of the structural formula of a chemical compound in terms of graph theory. Specifically, a *molecular graph* is a simple graph whose vertices correspond to the atoms of the compound and edges correspond to chemical bonds.

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Let G be a molecular graph with vertex set $V(G)$, $d_G(u,v)$ be the *topological distance* between vertices u and v in G, i.e., the length of a shortest path connecting u and v in G. The *Hosoya polynomial* in variable x of G, introduced by Hosoya [7], is defined as

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

where the sum is taken over all unordered pairs of (not necessarily distinct) vertices in G. Hence the polynomial contains the number of vertices as the constant term.

The Hosoya polynomial not only contains more information concerning distance in the molecular graph than any of the hitherto proposed distance-based molecular structure descriptors, which were extensively studied in chemical graph theory, see for instance the surveys [10, 11], but also deduces some of them. For example, Wiener index $W(G)$ of a molecular graph G [16], the oldest and most well-studied molecular structure descriptor so far, is equal to the first derivative of the Hosoya polynomial in $x = 1$:

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

Its chemical applications and mathematical properties are well documented [2, 3, 5, 6]. Moreover, hyper-Wiener index $WW(G)$ [9], Tratch-Stankevitch-Zefirov index $TSZ(G)$ [15] can be deduced from $H(G,x)$ as follows:

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

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

In this paper, we shall give Hosoya polynomials of hexagonal trapeziums $T_{m,n}$ (see Fig. 1) and Hosoya polynomials of hexagonal triangles T_m (see Fig. 2). The rest of the paper is organized as follows. In Section 2, we shall give definitions of hexagonal trapeziums and hexagonal triangles and some lemmas about distances. In Section 3, we give and prove explicit analytical expressions of Hosoya polynomials of hexagonal trapeziums and hexagonal triangles and, as corollaries, give formulae of three their well-studied topological indices: Wiener index, hyper-Wiener index, Tratch-Stankevitch-Zefirov index.

2 Preliminaries

Given two positive integers m and n, let us construct a parallelogram hexagon system of size (m,n), denoted by $P(m,n)$, in the plane equipped with the regular hexagonal lattice

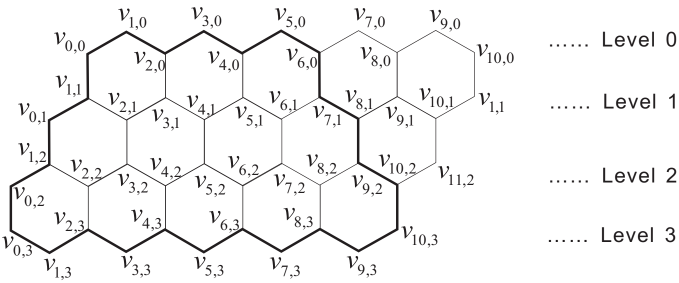

Fig. 1: The graph $P(5,3)$ with labellings of vertices; the embedding of hexagonal trapezoid $T_{5,3}$ represented by the bold line and its interior.

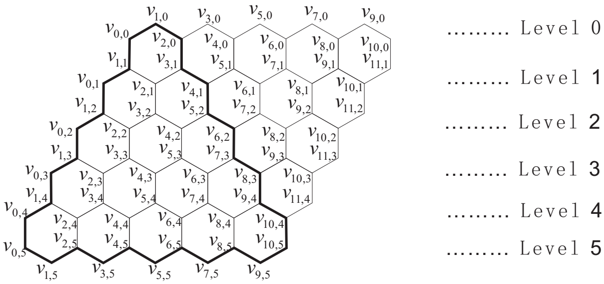

Fig. 2: The graph $P(5,5)$ and the embedding of hexagonal triangle T_5 represented by the bold line and its interior.

(see Fig. 1): there are $n+1$ horizontal levels marked from 0 to n and, for $1 \leqslant i \leqslant n-1$, level i contains $2m+2$ vertices lying as a zigzag path, denoted by $v_{0,i}, v_{1,i}, \cdots, v_{2m+1,i}$ from left to right, for $i \in \{0, n\}$, level i contains $2m+1$ vertices, denoted by $v_{0,i}, v_{1,i}, \cdots, v_{2m,i}$ in the similar way.

A hexagonal trapezium, denoted by $T_{m,n}$ for some positive integers m, n, can be considered as a subgraph of $P(m,n)$, which is illustrated by bold lines and its interior in Fig. 1 and inherits the labels of vertices. In particular, if $m = n$, then $T_{m,n}$ is called a *hexagonal triangle* (see Fig. 2), denoted simply by T_m.

Lemma 2.1. *[14] Let $T_{m,n}$ be a hexagonal trapezium considered as a subgraph of $P(m,n)$. Then*

$$d_{T_{m,n}}(u,v) = d_{P(m,n)}(u,v),$$

for any pairs of vertices u and v in $T_{m,n}$.

By the construction of $T_{m,n}$, we have the sequence consisting of vertices of $T_{m,n}$ on level k is,

if $0 \le k \le n-1$,

$$(v_{0,k}, v_{1,k}, \cdots, v_{2m-2n+2k+2,k}),$$

if $k = n$,

$$(v_{0,n}, v_{1,n}, \cdots, v_{2m,n}).$$

In the following we make some preparations for calculating the Hosoya polynomials of hexagonal trapeziums $T_{m,n}$.

In $P(m,n)$, we define a distance sequence from $v_{i,0}$ to every vertex of level k in $P(m,n)$: If $k = 0$ or $k = n$,

$$S_{P(m,n)}(i,k) := (d(v_{0,k}, v_{i,0}), d(v_{1,k}, v_{i,0}), \cdots, d(v_{2m,k}, v_{i,0}));$$

If $1 \le k \le n-1$,

$$S_{P(m,n)}(i,k) := (d(v_{0,k}, v_{i,0}), d(v_{1,k}, v_{i,0}), \cdots, d(v_{2m+1,k}, v_{i,0})).$$

Also, we can define a distance sequence from $v_{i,0}$ to every vertex of level k in $T_{m,n}$: If $0 \le k \le n-1$,

$$S_{T_{m,n}}(i,k) := (d(v_{0,k}, v_{i,0}), d(v_{1,k}, v_{i,0}), \cdots, d(v_{2m-2n+2k+2,k}, v_{i,0})); \quad (4)$$

If $k = n$,

$$S_{T_{m,n}}(i,n) := (d(v_{0,n}, v_{i,0}), d(v_{1,n}, v_{i,0}), \cdots, d(v_{2m,n}, v_{i,0})). \quad (5)$$

For a concise description of $S_{P(m,n)}(i,k)$, we define the following notations. Given nonnegative integers l, r, s, we define

$$l, \nearrow, r := l, l+1, l+2, ..., r \qquad (l \le r);$$
$$l, \searrow, r := l, l-1, l-2, ..., r \qquad (l \ge r);$$
$$l, \leftrightsquigarrow 2s, r := \overbrace{l, r, l, r, ..., l, r}^{2s} \qquad (l \ne r).$$

Lemma 2.2. *[8] Let $0 \leq i \leq m-n+1$ and $0 \leq k \leq n$. Then if i is odd,*

$$S_{P(m,n)}(i,k) = \begin{cases} (i, \searrow, 0, \nearrow, 2m-i), & k=0; \\ (2k+i, \searrow, 2k, \leftrightsquigarrow 2k+2, 2k+1, \nearrow, 2m-i+1), & 1 \leq k \leq n-1; \\ (2n+i-1, \searrow, 2n, \leftrightsquigarrow 2n+2, 2n+1, \nearrow, 2m-i+1), & k=n. \end{cases}$$

if i is even,

$$S_{P(m,n)}(i,k) = \begin{cases} (i, \searrow, 0, \nearrow, 2m-i), & k=0; \\ (2k+i, \searrow, 2k-1, \leftrightsquigarrow 2k, 2k, \nearrow, 2m-i+1), & 1 \leq k \leq n-1; \\ (2n+i-1, \searrow, 2n-1, \leftrightsquigarrow 2n, 2n, \nearrow, 2m-i+1), & k=n. \end{cases}$$

By Lemmas 2.1, 2.2 and the sequences (4), (5), we can give the distance sequence $S_{T_{m,n}}(i,k)$ from $v_{i,0}$ to vertices on level k.

Theorem 2.3. *Let $0 \leq i \leq m-n+1$, for $0 \leq k \leq n$,*

if i is odd, then

$$S_{T_{m,n}}(i,k) = \begin{cases} (2k+i, \searrow, 2k, \leftrightsquigarrow 2k+2, 2k+1, \nearrow, 2m-2n+2k-i+2), & 0 \leq k \leq n-1; \\ (2n+i-1, \searrow, 2n, \leftrightsquigarrow 2n+2, 2n+1, \nearrow, 2m-i+1), & k=n; \end{cases}$$

if i is even, then

$$S_{T_{m,n}}(i,k) = \begin{cases} (i, \searrow, 0, \nearrow, 2m-2n+2k-i+2), & k=0; \\ (2k+i, \searrow, 2k-1, \leftrightsquigarrow 2k, 2k, \nearrow, 2m-2n+2k-i+2), & 1 \leq k \leq n-1; \\ (2n+i-1, \searrow, 2n-1, \leftrightsquigarrow 2n, 2n, \nearrow, 2m-i+1), & k=n. \end{cases}$$

3 Hosoya polynomials of hexagonal trapeziums $T_{m,n}$

Note that $T_{m,1}$ is exactly the linear hexagonal chain L_m with m hexagons.

Lemma 3.1. *[13]*

$$H(T_{m,1},x) = 2 + x + \frac{m(x^2-x-4)(x^2+1)}{x-1} + \frac{2x^2(x+1)(x^{2m}-1)}{(x-1)^2}.$$

For the simplicity, we define one notation as follows:

$$H_i(T_{m,n},x) = \sum_{u \in V(T_{m,n})} x^{d(u,v_{i,0})}, \tag{6}$$

i.e., the contribution of the vertex $v_{i,0}$ to the Hosoya polynomial $H(T_{m,n},x)$ of $T_{m,n}$. By Theorem 2.3 and Eq. (6), we have

Lemma 3.2. *If i is odd,*

$$H_i(T_{m,n},x) = \frac{1+x+x^2-x^{i+1}-x^{2m-i+2}+x^{2m-i+3}+x^{2m-i+4}-x^{2m-2n-i+3}}{(x-1)^2(x+1)}$$
$$-\frac{(2+n)x^{2n+2}+x^{2n+3}-nx^{2n+4}+x^{2n+i}-x^{2n+i+1}-x^{2n+i+2}}{(x-1)^2(x+1)};$$

If i is even,

$$H_i(T_{m,n},x) = \frac{1+2x-x^{i+1}-x^{2m-i+2}+x^{2m-i+3}+x^{2m-i+4}-x^{2m-2n-i+3}}{(x-1)^2(x+1)}$$
$$-\frac{(1+n)x^{2n+1}+x^{2n+2}-(n-1)x^{2n+3}+x^{2n+i}-x^{2n+i+1}-x^{2n+i+2}}{(x-1)^2(x+1)}.$$

Let $Hb(T_{m,n},x)$ be the contribution of $2m-2n+3$ vertices $v_{0,0}, v_{1,0}, \cdots, v_{2m-2n+2,0}$ lying on level 0 of $T_{m,n}$ to the Hosoya polynomial of $T_{m,n}$. Among these $2m-2n+3$ vertices, $v_{0,0}, v_{1,0}, \cdots, v_{m-n,0}$ have two isomorphic images (including itself), and $v_{m-n+1,0}$ has exactly one isomorphic image, i.e., itself.

Lemma 3.3.

$$Hb(T_{m,n},x) = 2\sum_{i=0}^{m-n} H_i(T_{m,n},x) + H_{m-n+1}(T_{m,n},x) - \left(\frac{2(m-n+1)x}{1-x} - \frac{x^2-x^{2m-2n+4}}{(1-x)^2}\right). \tag{7}$$

Note that the occurrence of the last term in the right-hand side of Eq. (7) is because we have counted twice the contribution of pairs of distinct vertices among $v_{0,0}, v_{1,0}, \cdots,$ $v_{2m-2n+2,0}$ in the first two terms of the right-hand side of Eq. (7).

Substituting equations in Lemma 3.2 for Eq. (7), we have

Lemma 3.4.

$$Hb(T_{m,n},x) = \frac{(2m-2n+3)(x^2+1)}{(x-1)^2} + \frac{(2+m-n)x+x^2+(n-m-1)x^3}{(x+1)(x-1)^3}$$
$$-\frac{(x^2+1)x^{2m-2n+4}-2(x^2+x-1)x^{2m+3}-[2+(m+n+mn-n^2)x]x^{2n}}{(x+1)(x-1)^3}$$
$$+\frac{[2m-3n+(2n^2-m-2n-2mn-1)x]x^{2n+2}}{(x+1)(x-1)^3}$$
$$+\frac{[3n-2m-3-n(n-m-1)x]x^{2n+4}}{(x+1)(x-1)^3}.$$

Since $T_{m,n-1}$ is an isometric subgraph of $T_{m,n}$ and can be obtained by deleting vertices lying on level 0 of $T_{m,n}$, so we can recursively obtain

$$H(T_{m,n},x) = H(T_{m,1},x) + \sum_{i=2}^{n} Hb(T_{m,i},x). \tag{8}$$

By Lemmas 3.1 and 3.4 and Eq. (8), we have

Theorem 3.5. *Let $T_{m,n}$ be a hexagonal trapezium, then*

$$\begin{aligned}H(T_{m,n},x) &= \frac{1+2(n+m+mn)-n^2+x^{2(m-2n+2)}(x^2+1)+x^{2m+2}(1+2nx)}{(x+1)^2(x-1)^4}\\ &+\frac{[4nx^2-(6+4n)]x^{2m+4}+[n^2-4-3n-2m(2+n)](x+2x^2)+(8+4n)x^3}{2(x+1)^2(x-1)^4}\\ &+\frac{[4m(1+n)-2n^2]x^3+2[4-(1+2m)n+n^2]x^4+[2-(1+2m)n+n^2]x^5}{2(x+1)^2(x-1)^4}\\ &+\frac{(3+2m-n)(1+n)x^6+2(x^2-2)nx^{2m+5}+[2+(2m+mn-n^2)x]x^{2n+2}}{(x+1)^2(x-1)^4}\\ &+\frac{[(2m-3n-3)x-n]x^{2n+3}+[2n^2-2m(1+n)-3]x^{2n+5}}{(x+1)^2(x-1)^4}\\ &+\frac{[(3n-2m-3)-n(n-m-1)x]x^{2n+6}}{(x+1)^2(x-1)^4}.\end{aligned}$$

We can obtain the Hosoya polynomial of the hexagonal triangle T_m by setting $n=m$ in Theorem 3.5 as follows.

Theorem 3.6. *Let $H(T_m,x)$ be the Hosoya polynomial of the hexagonal triangle T_m, then*

$$\begin{aligned}H(T_m,x) &= \frac{m[m(x^2-1)(2x^2-x+2)+6x^{2m+3}(x^2+x-1)+x^2(8x^2-x+6)+7x-8]}{2(x-1)^3(x+1)}\\ &+\frac{1-2x-4x^2+4x^3+5x^4+x^5+4x^6+3x^{2m+2}(1-2x^2-x^3-x^4)}{(x-1)^4(x+1)^2}.\end{aligned}$$

From Theorems 3.5, 3.6 and, Eqs. (1)-(3), we can get some related topological indices.

Corollary 3.7. *[17] Let $W(T_{m,n})$ be the Wiener index of hexagonal trapezium $T_{m,n}$, then*

$$\begin{aligned}W(T_{m,n}) &= \frac{1}{3}[4m^3(1+n)^2+2m^2(3+11n+6n^2-2n^3)]+\frac{1}{30}[n(28+45n-35n^2-8n^4)\\ &+20m(1+9n+6n^2-4n^3+n^4)].\end{aligned}$$

Corollary 3.8.

$$\begin{aligned}WW(T_{m,n}) &= \frac{1}{360}[240m^4(1+n)^2-80m^3(4n^3-15n^2-28n-9)+60m^2(4n^4-20n^3+\\ &37n^2+60n+11)+n(414+575n-390n^2+185n^3-384n^4-40n^5)-\\ &4m(12n^5-210n^4+265n^3-525n^2-607n-45)];\\ TSZ(T_{m,n}) &= \frac{1}{2520}[672m^5(1+n)^2-560m^4(2n^3-9n^2-17n-6)+280m^3(21+90n+\\ &53n^2-24n^3+4n^4)+28m^2(150+1109n+765n^2-530n^3+180n^4-24n^5)\\ &+n(3546+4641n-2674n^2+2835n^3-4396n^4-1176n^5-256n^6)\\ &+28m(36+669n+665n^2-285n^3+435n^4-12n^5+16n^6)].\end{aligned}$$

Corollary 3.9. *[17, 18] Let $W(T_m)$ be the Wiener index of hexagonal triangle T_m, then*

$$W(T_m) = \frac{m(4m^4 + 40m^3 + 115m^2 + 95m + 16)}{10}.$$

Corollary 3.10.

$$WW(T_m) = \frac{m(8m^5 + 104m^4 + 425m^3 + 670m^2 + 407m + 66)}{40};$$
$$TSZ(T_m) = 384m(64m^6 + 1064m^5 + 5992m^4 + 14945m^3 + 17626m^2 + 9191m + 1518).$$

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