MATCH
Communications in Mathematical and in Computer Chemistry

MATCH Commun. Math. Comput. Chem. **69** (2013) 755-763

ISSN 0340 - 6253

Hosoya Polynomials of Circumcoronene Series

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(Received March 29, 2012)

Abstract

The Hosoya polynomial (also called Wiener polynomial) of a graph G with the 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 the sum is over all unordered pairs $\{u,v\}$ of distinct vertices in G, $d_G(u,v)$ is the distance of two vertices u,v in G. In 2004, Yang and Yeh evaluated $H(G,x)$ for certain graphs of chemical interest, and posted an open problem for evaluating the Hosoya polynomial of the circumcoronene C_r of order r. In this paper, we solve this problem and give analytical expressions associated with r. The topological indices—Wiener index and hyper-Wiener index of C_r can also be obtained from $H(C_r,x)$ through this work.

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1 Introduction

The Wiener index was first introduced by Wiener [21] in 1947 for approximating the boiling points of alkanes. The effect of approximation was surprisingly good. Since then, the Wiener index has attracted the attention of chemists. Especially, since mathematical researchers participate in the field in 1970's, the Wiener index was extensively studied in the literature. About its mathematical properties and chemical applications, the reader can refer to Refs. [1, 17], two recent surveys [2, 3] and two special issues [9, 10] and references therein. Concretely, the *Wiener index* of a connected graph G with the vertex set $V(G)$ 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 in G.

The *Hosoya polynomial* of a connected graph G, introduced by Hosoya [13], is defined as:

$$H(G,x) = \sum_{\{u,v\}\subseteq V(G)} x^{d_G(u,v)}, \tag{1}$$

where the sum is over all unordered pairs $\{u,v\}$ (possibly identical) of vertices in G.

Wiener polynomial not only contains more information about distance in the graph than any of the hitherto proposed distance-based topological indices, but also evaluates some of them. For example, the Wiener index is equal to the first derivative of Hosoya polynomial in $x = 1$; another topological index—*hyper-Wiener index* [15, 18], which is defined as

$$WW(G) = \frac{1}{2} \sum_{\{u,v\}\subseteq V(G)} \left(d_G(u,v) + d_G^2(u,v)\right), \tag{2}$$

is equal to the half of the second derivative of the Hosoya polynomial multiplied by x in $x = 1$. Also the *Wiener vector* recently proposed by Guo *et al.* [12] is the coefficient sequence of the first derivative of the polynomial, etc. 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 [5, 7] and computation [11, 22, 23, 24, 25, 27, 28].

In 2004, Yang and Yeh [27] computed Hosoya polynomials of some interesting chemical graphs, such as polygonal chains made by hexagons, which are the abstractions of aromatic compound, and regular two-dimensional hexagonal patterns. In the same paper, they mentioned circumcoronene series C_r (see Fig. 1), which is a kind of graphs with chemical research interest. The Hosoya polynomial C_r is still intractable.

In this paper, we give analytical expressions of $H(C_r, x)$ by means of recursive skills and the isometric subgraph property in graph theory. As corollaries, the Wiener index and the hyper-Wiener index of C_r can be obtained from $H(C_r, x)$.

2 Preliminary

Given two positive integers p and q, let us construct a *rectangular hexagon system (RHS)* of size (p, q), denoted by $R(p, q)$, as follows. There are q horizontal levels marked from 0 to $q-1$ and each level contains $2p+1$ vertices lying as a zigzag path. In level $i (0 \leqslant i \leqslant q-1)$, we label the vertices $v_{-p,i}, v_{-(p-1),i}, \cdots, v_{p-1,i}, v_{p,i}$ from left to right. By linking edges vertically between two adjacent levels, we obtain $R(p, q)$ in honeycomb shape (also see Fig. 1). Because $R(p, q)$ is bipartite, we can color its vertices with black and white as in Fig. 1.

A *circumcoronene* of order r, denoted by C_r, is a benzenoid system consisting of one central hexagon, surrounded by $r-1$ layers of hexagonal cells, $r \geqslant 1$. Note that C_r is a molecular graph, corresponding to benzene ($r = 1$), coronene ($r = 2$), circumcoronene ($r = 3$), circumcircumcoronene ($r = 4$), etc [6]. Comparing with $R(p, q)$, C_r is a big regular hexagon such that r layers of hexagons wrap up together but not a big rectangle (see Fig. 1).

Here we embed C_r into $R(p, q)$ such that the bottom boundary of C_r contains the vertices $v_{0,0}, v_{1,0}, \cdots, v_{2r,0}$ of level 0. In this way, C_r lies on levels $0, 1, \cdots, 2r-1$, and the sequence of vertices of C_r on level k is

$$(v_{-k,k}, v_{-(k-1),k}, \cdots, v_{2r+k-1,k}, v_{2r+k,k}) \quad \text{if} \quad 0 \leqslant k \leqslant r-1; \tag{3}$$

$$(v_{k-2r+1,k}, v_{k-2r+2,k}, \cdots, v_{4r-k-2,k}, v_{4r-k-1,k}) \quad \text{if} \quad r \leqslant k \leqslant 2r-1. \tag{4}$$

Besides the bottom boundary, the top boundary of C_r lies on level $2r-1$. Between levels 0 and $2r-1$, each level has four vertices lying on the boundary of C_r. They are the first two and the last two vertices in the sequences in (3) and (4).

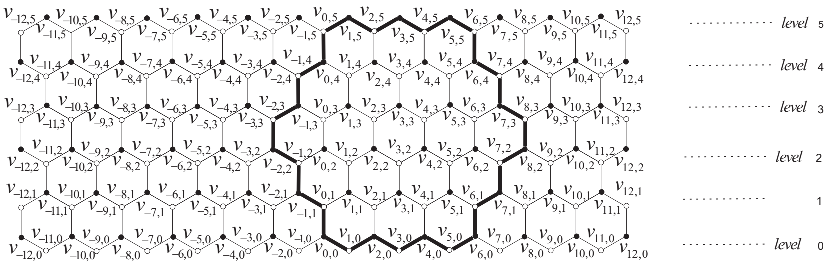

Fig. 1. An RHS with $p = 12$ and $q = 6$, labeling of vertices; the embedding of the circumcoronene C_3 represented by the bold line and its interior.

From [14], we know that this is an *isometric embedding* into $R(p, q)$, i.e.,

Lemma 2.1. *In the above embedding of C_r into $R(p, q)$ with $p \geq 3r, q \geq 2r$,*

$$d_{C_r}(u, v) = d_{R(p,q)}(u, v) \text{ for any pairs of vertices } u \text{ and } v \text{ in } C_r.$$

In the sequel, we assume that $p = 3r, q = 2r$.

In the following we make some preparation for calculating the Hosoya polynomials of the circumcoronene C_r.

In $R(3r, 2r)$, we define a distance sequence between $v_{i,0}$ and vertices in level k:

$$S_{R(3r,2r)}(i, k) := \big(d(v_{-3r,k}, v_{i,0}), d(v_{-(3r-1),k}, v_{i,0}), \cdots, d(v_{3r,k}, v_{i,0})\big). \tag{5}$$

To describe $S_{R(3r,2r)}(i, k)$ shortly, we define the following notations. Given nonnegative integers m, r and s, we define

$$m, \nearrow, n := m, m+1, m+2, \cdots, n \qquad (m \leqslant n);$$

$$m, \searrow, n := m, m-1, m-2, \cdots, n \qquad (m \geqslant n);$$

$$m, \leftrightsquigarrow 2s, n := \overbrace{m, n, m, n, \cdots, m, n}^{2s \text{ terms}} \qquad (m \neq n).$$

Lemma 2.2. *[29] Suppose that $-r \leq i \leq r$. Then for $0 \leq k \leq 2r - 1$,*

$$S_{R(3r,2r)}(i, k) = \begin{cases} (3r + k + i, \searrow, 2k, \leftrightsquigarrow 2k + 2, 2k + 1, \nearrow, 3r + k - i), & \text{if } i \text{ is odd;} \\ (3r + k + i, \searrow, 2k, 2k - 1, \leftrightsquigarrow 2k, 2k, \nearrow, 3r + k - i), & \text{if } i \text{ is even.} \end{cases} \tag{6}$$

Combining Lemmas 2.1, 2.2 and the sequences in (3) and (4), we can give the distance sequence $S_{C_r}(i,k)$ between $v_{i,0}$ and vertices of C_r on level k.

Lemma 2.3. *Let* $1 \leqslant i \leqslant r$. *If* i *is odd, then*

$$S_{C_r}(i,k) = \begin{cases} (2k+i, \searrow, 2k, \leftrightsquigarrow 2k+2, , 2k+1, \nearrow, 2r+2k-i), & 0 \leqslant k \leqslant r-1; \\ (2r+i-1, \searrow, 2k, \leftrightsquigarrow 2k+2, , 2k+1, \nearrow, 4r-i-1), & r \leqslant k < r+\frac{i-1}{2}; \\ (2k, \leftrightsquigarrow 2r+i+1, , 2k+1, \nearrow, 4r-i-1), & r+\frac{i-1}{2} \leqslant k < 2r-\frac{i+1}{2}; \\ (2k, \leftrightsquigarrow 6r-2k-2, 2k+1, 2k), & 2r-\frac{i+1}{2} \leqslant k \leqslant 2r-1. \end{cases}$$

If i *is even, then*

$$S_{C_r}(i,k) = \begin{cases} (2k+i, \searrow, 2k-1, \leftrightsquigarrow 2k, , 2k, \nearrow, 2r+2k-i), & 0 \leqslant k \leqslant r-1; \\ (2r+i-1, \searrow, 2k-1, \leftrightsquigarrow 2k, , 2k, \nearrow, 4r-i-1), & r \leqslant k < r+\frac{i}{2}; \\ (2k-1, \leftrightsquigarrow 2r+i, , 2k, \nearrow, 4r-i-1), & r+\frac{i}{2} \leqslant k < 2r-\frac{i}{2}; \\ (2k-1, \leftrightsquigarrow 6r-2k-2, 2k, 2k-1), & 2r-\frac{i}{2} \leqslant k \leqslant 2r-1. \end{cases}$$

Proof. By Lemma 2.1 and comparing Eq. (5), and also (3) and (4), $S_{C_r}(i,k)$ is substantially a part of $S_{R(p,q)}(i,k)$ by cutting off two useless ends. Concretely, in the case of odd i, when $k < r + \frac{i-1}{2}$, we can guarantee $2r+i-1 > 2k$ and easily $4r-i-1 > 2k+1$ (note $i \leqslant r$). When $2r - \frac{i+1}{2} \leqslant k$, we ensure $4r-i-1 > 2k+1$. We can similarly get the observations in the another case. □

In fact, Lemma 2.3 can be deduced from the distance function on brick walls in [20].

3 Calculating Hosoya polynomial of circumcoronene series

Denote by $H_{v_{i,0}}(C_r,x)$ the contribution of the vertex $v_{i,0}$ to the Hosoya polynomial of C_r. Denote by $Hb_{v_{i,0}}(C_r,x)$ the contribution of the distances between the vertex $v_{i,0}$ and the boundary vertices in C_r to the Hosoya polynomial of C_r. Using the software MATHEMATICA 5.2, by Lemma 2.3 we obtain

Lemma 3.1.

$$\begin{aligned}
&H_{v_{i,0}}(C_r,x)\\
=&\frac{2x+1}{(x-1)^2(x+1)}-\frac{(x+x^{2r})(x^i+x^{2r-i})}{(x-1)^2(x+1)}+\frac{\lfloor\frac{i}{2}\rfloor x^{2r+i}}{x-1}+\frac{(r-\lceil\frac{i}{2}\rceil)x^{4r-i}}{x-1}+\\
&\left(\frac{r}{x-1}+\frac{x}{(x-1)^2(x+1)}\right)x^{4r-1}+\frac{1-(-1)^i}{2}\left(\frac{x}{x-1}+(r+\frac{x}{x^2-1})\right)x^{4r-1};\\
&Hb_{v_{i,0}}(C_r,x)\\
=&-\frac{x+1}{x-1}+\left\lfloor\frac{i}{2}\right\rfloor(x+1)x^{2r+i-2}+(r-\left\lceil\frac{i}{2}\right\rceil)(x+1)x^{4r-i-2}\\
&+\frac{(rx-r+1)(x+1)}{x-1}x^{4r-3}+\frac{1-(-1)^i}{2}(rx^2+x-r+1)x^{4r-3}.
\end{aligned}$$

Among all 12 automorphisms of C_r, each vertex in $\{v_{1,0}, v_{2,0}, \cdots, v_{r-1,0}\}$ has 12 isomorphic images (including itself), vertex $v_{r,0}$ has 6 isomorphic images. Denote by $Hb(C_r, x)$ the contribution of the boundary vertices to the Hosoya polynomial of C_r. By Lemma 3.1, we have

Lemma 3.2.

$$\begin{aligned}
&Hb(C_r,x)\\
=&12\sum_{i=1}^{r-1}H_{v_{i,0}}(C_r,x)+6H_{v_{r,0}}(C_r,x)-\left(6\sum_{i=1}^{r-1}Hb_{v_{i,0}}(C_r,x)+3Hb_{v_{r,0}}(C_r,x)-6r+3\right) \qquad (7)\\
=&-3+6r+6H_{v_{r,0}}(C_r,x)-3Hb_{v_{r,0}}(C_r,x)+6\sum_{i=1}^{r-1}\big(2H_{v_{i,0}}(C_r,x)-Hb_{v_{i,0}}(C_r,x)\big).
\end{aligned}$$

Note that the last term of right-hand side of Eq. (7) is the contribution of the distances between the vertices on the boundary of C_r to the Hosoya polynomial of C_r.

Substituting Lemma 3.1 into Lemma 3.2, we obtain

Lemma 3.3.

$$\begin{aligned}
&Hb(C_r,x)\\
=&\frac{6r(2x^2-x+2)}{(x-1)^2}+\frac{6(-x^3+2x^2-x+1)}{(x-1)^3}+\frac{3r^2(x^5-x^4-x+1)x^{4r-3}}{(x-1)^3}+\frac{6r(x-1)x^{4r-3}}{(x-1)^3}\\
&-\frac{3(x^3+x^2+x-1)x^{4r-3}}{(x-1)^3}-\frac{6(x^2+1)(x^{4r}-x^{2r+2})}{(x-1)^3(x+1)}+\frac{6(x^2+1)(rx^{4r-2}-x^{2r})}{(x-1)^2}. \qquad (8)
\end{aligned}$$

Since C_r can be obtained from C_{r-1} by adding the boundary vertices of C_r, and C_{r-1} can be considered as an isometric subgraph of C_r by the constitution, the Hosoya polynomial $H(C_r, q)$ of C_r is equal to

$$H(C_r, q) = \sum_{i=1}^{r} Hb(C_i, q). \tag{9}$$

Substituting Eq. (8) into Eq. (9), we get the main theorem: the Hosoya polynomial of circumcoronene C_r.

Theorem 3.4.

$$\begin{aligned}&H(C_r, x)\\ =&\frac{3r(2rx^3 - 3rx^2 + x^2 + 3rx + x - 2r)}{(x-1)^3} + \frac{3x\big(r^2x^{4r}(x-1)(x^4-1) - x^2(x+1)(x^{4r}-1)\big)}{(x-1)^4(x+1)(x^2+1)}\\ -&\frac{6x^2(-rx^{4r+4} + rx^{4r} + x^{4r+4} + x^{4r+2} + x^{4r} - x^{2r+4} - 2x^{2r+2} - x^{2r} + x^2)}{(x-1)^4(x+1)^2(x^2+1)}.\end{aligned}$$

From Theorem 3.4, we immediately obtain the Wiener index $W(C_r)$ and the hyper-Wiener index $WW(C_r)$ of circumcoronene C_r.

Corollary 3.5. *[8, 20, 26, 30]*

$$\begin{aligned}W(C_r) &= \frac{1}{5}(164r^5 - 30r^3 + r);\\ WW(C_r) &= \frac{1}{30}r(1096r^5 + 492r^4 - 275r^3 - 90r^2 + 34r + 3).\end{aligned}$$

4 Acknowledgements

We wish to thank the anonymous referees for their careful reading and valuable comments on the paper. The work is partially supported by NSFC (grant Nos. 10826075, 11001113). The work of X. Lin is partially supported by Science Foundation of Jimei University, China (grant No. ZQ2009011), FJCEF (grant No. JA11163). The work of S.-J. Xu is partially supported by the National Science Foundation for Post-doctoral Scientists of China(grant No. 20080440071), the Fundamental Research Funds for the Central Universities (grant No. lzujbky-2009-51).

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