The Hosoya polynomial of one-quadrilateral carbon nanocone

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Let G be a chemical graph with vertex set $V(G)$ and $d_G(u,v)$ the distance between vertices u and v in G. The Hosoya polynomial in variable x of graph G is $\sum_{\{u,v\}\subseteq V(G)} x^{d_G(u,v)}$. In this paper, we give an analytical expression for calculating the Hosoya polynomial of one-quadrilateral carbon nanocone. Furthermore, a series of distance-based molecular structure descriptors, such as the well-known Wiener index, the hyper-Wiener index etc., can be easily obtained.

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1. Introduction

The occurrence of hollow carbon structures is a fascinating phenomenon. Except Fullerenes and nanotubes, carbon nanocones have been observed as caps on the ends of the nanotubes [1,2], or also as freestanding structures on a flat graphite surface by Ge and Sattler [3]. Mathematical calculations are necessary to explore important concepts in chemistry; chemical graph theory is an important tool for studying molecular structures [4]. In a sense, this research plays a positive promotive role in chemistry. A topological index is a real number related to a structural graph of a molecule, it does not depend on the labeling or pictorial representation of a graph.

So far, there are many topological indices that have been proposed, especially distance-based indices, such as the Wiener index, hyper-Wiener index, Tratch-Stankevitch-Zefirov index, and so on. They all play important roles in Quantitative Structure-Activity Relationship (QSAR) and Quantitative Structure-Property Relationship (QSPR) studies. The QSAR and QSPR studies are the areas of chemical research that focus structure-dependent chemical behavior of molecules [5,6].

The Wiener index is the oldest one of the distance-based topological indices of a chemical graph that correlate with some of the physicochemical properties of the compound, it was introduced by the chemist HAROLD WIENER [7] about 60 years ago as a descriptor for explaining the boiling points of paraffins. The effect of approximation was surprisingly good. The Wiener index of a chemical graph G with 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 vertices u and v in G (i.e., the number of edges on a shortest path connecting u and v), the subscript is omitted when it is clear from the context.

H. Hosoya introduced a distance-based counting polynomial named *Wiener polynomial* [8], but we call it *Hosoya polynomial* in honor of H. Hosoya. The *Hosoya polynomial* in variable x of a chemical graph G with vertex set $V(G)$, is defined as:

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

where the summation is over all (unordered) pairs $\{u;v\}$ of distinct vertices in $V(G)$. Note that there is no constant term, while it contains the number of vertices as constant term in some literature.

The Hosoya polynomial not only contains more information concerning distance in the chemical graph than any of the hitherto proposed distance-based molecular structure descriptors [9,10], but also deduces some of them. For example, the Wiener index $W(G)$ of a molecular graph G is equal to the first derivative of the Hosoya polynomial in $x=1$:

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

The chemical applications and mathematical properties of the Wiener index are well documented [11-14]. Moreover, the hyper-Wiener index $WW(G)$ [15], Tratch-Stankevitch-Zefirov index $TSZ(G)$ [16] can also be deduced from $H(G,x)$ as follows:

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

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

It seems that the formulas (2) and (3) were first reported in [17, 18], 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 in Refs. [18, 19]. On the other hand, recently Brückler etc. [18] 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) decrease 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 [20-25], and computation [17,26-34].

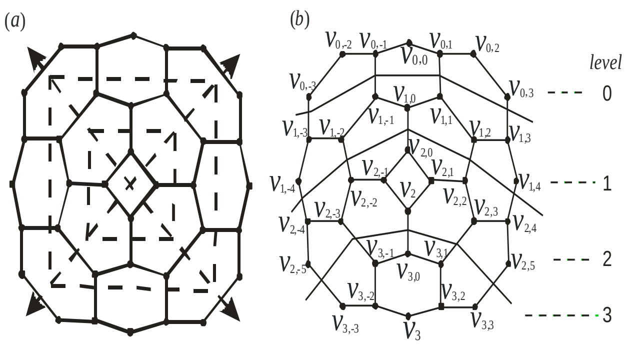

Fig. 1. (a) The one-quadrilateral nanocone $CNC_4[3]$ is represented by solid lines, dotted quadrilaterals indicate $CNC_4[3]$'s recursive construction, dotted rays indicate $CNC_4[3]$'s symmetric structure; (b) Labeling of vertices in $CNC_4[3]$.

In this paper we consider about a nanocone with a quadrilateral in the center, denote by $CNC_4[n]$, n is parameter (see the next section for the details). In 2010 ALI RETA ASHRAFI and FARZANEH GHOLAMI-NEZHAAD finished the computation of PI and edge Szeged indices of $CNC_4[n]$ [35]. We shall discuss about the Hosoya polynomial of $CNC_4[n]$, and give an explicit analytical expression for it. Furthermore, a series of topological indices, such as the Wiener index, the hyper-Wiener index, etc., can be easily obtained from the expression.

2. Preliminaries

First, we define a one-quadrilateral carbon nanocone $CNC_4[n]$ from a geometrical view of point. It is a plane graph and its bounded face boundaries consist of one quadrilateral and remained hexagons. When $n=1$ $CNC_4[n]$ is exactly a single quadrangle. When $n\geq 2$ $CNC_4[n]$ is obtained from $CNC_4[n-1]$ by identifying the inner boundary of an additional appropriate circular hexagonal chain with the outer boundary of $CNC_4[n-1]$, the construction is indicated by dotted regular quadrangle in Fig. 1(a) for $n=3$. In a word, $CNC_4[n]$ consists of one quadrangle and $n-1$ layers of circular hexagonal chains around it. Evidently (and in the sequel), for $1\leq i<j\leq n$, $CNC_4[i]$ can be considered as a substructure (or a subgraph) of $CNC_4[j]$.

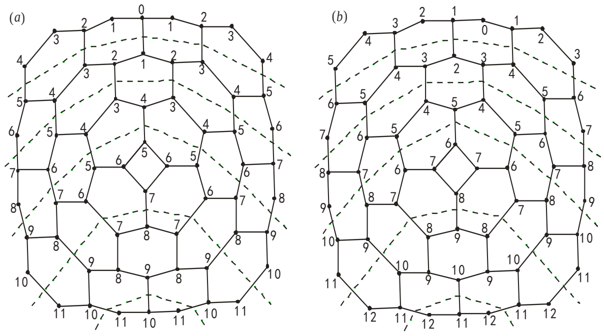

Fig. 2. (a) and (b) show distances from vertices in $CNC_4[4]$ to $v_{0,0}$ and $v_{0,1}$, respectively.

In order to facilitate discussion, we label vertices in $CNC_4[n]$. First, we partition vertices into *levels* $0,1,2,\cdots,\left\lfloor\frac{3n-2}{2}\right\rfloor$ from top to bottom, which are indicated by dotted curves in Fig. 1(b). From the structure, when $0\leq i\leq n-2$, there are $2n+2i+1$ vertices in level i, say $v_{i,-(n+i)},\cdots,v_{i,-1}$, $v_{i,0}$, $v_{i,1}$, $\cdots$, $v_{i,n+i}$ from left to right; when $i=n-1$ (i.e., the level containing the whole unique quadrilateral), there are $4n$ vertices in level

$n-1$, say $v_{i,-(n+i)},\cdots,v_{i,-1},v_{i,0},v_{i,1},\cdots,v_{i,n+i}$ from left to right and the special middle lower vertex v_i; when $n \le i \le \left\lfloor \frac{3n-4}{2} \right\rfloor$, there are $12n-8i-4$ vertices in level i, say, $v_{i,-(6n-4i-3)}$, $\cdots,v_{i,-1},v_{i,0},v_{i,1},\cdots$, $v_{i,6n-4i-3}$ from left to right and the special middle lower vertex v_i; when $i = \left\lfloor \frac{3n-2}{2} \right\rfloor$, we divide two cases according to the parity of n. When n is even, there are $12n-8i-5$ vertices in level i, say $v_{i,-(6n-4i-3)}$ $\cdots,v_{i,-1},v_{i,0},v_{i,1},\cdots$, $v_{i,6n-4i-3}$, when n is odd, there are $12n-8i-4$ vertices, say $v_{i,-(6n-4i-3)}$, $\cdots,v_{i,-1},v_{i,0}$, $v_{i,1}$ $\cdots$, $v_{i,6n-4i-3}$ and the special middle lower vertex v_i. (See Fig. 1(b)).

By the symmetry of $CNC_4[n]$, we just need to consider n vertices among the vertices on the outer boundary of $CNC_4[n]$. For example, in Fig. 1(b), we need to consider $v_{0,0}, v_{0,1}, v_{0,2}$. So we define a distance sequence, denoted by $\bar{S}(k,i)$, between a special vertex $v_{0,k}$ $(0 \le k \le n-1)$ and vertices in level i (expect the special vertex v_i ($i \ge n-1$) if it exists) as:

when $0 \le i \le n-1$,

$$(d(v_{0,k},v_{i,-(n+i)}), d(v_{0,k},v_{i,-(n+i)+1}),\cdots,d(v_{0,k},v_{i,n+i}));$$

when $n \le i \le \left\lfloor \frac{3n-2}{2} \right\rfloor$,

$$(d(v_{0,k},v_{i,-(6n-4i-3)}),\ d(v_{0,k},v_{i,-(6n-4i-3)+1}),\cdots,\ d(v_{0,k},v_{i,6n-4i-3}));$$

Distances between $v_{0,0}$ (resp., $v_{0,1}$) and all vertices in $CNC_4[4]$ are shown in Fig. 2(a) (resp., Fig. 2(b)), which also indicate $\bar{S}(0,i)$ (resp., $\bar{S}(1,i)$) for $0 \le i \le 5$.

For the sake of convenience, in $CNC_4[n]$, for $0 \le k \le n-1$ and $0 \le i \le \left\lfloor \frac{3n-2}{2} \right\rfloor$, we define the distance sequence $S(k,i)$ as the sequence obtained from $\bar{S}(k,i)$ by (if necessary) inserting the distance between $v_{0,k}$ and the special vertex v_i to some appropriate position of $\bar{S}(k,i)$, because the order in the distance sequence is irrelevant to the discussion of the Hosoya polynomial of $CNC_4[n]$. Hence $S(k,i)$ is some distance sequence of distances between $v_{0,k}$ and all vertices in level i.

To express $S(k,i)$ in a short manner, we define the following notations. Given nonnegative integers m, n and s, we define

$$m,\uparrow,n := m,m+1,m+2,\cdots,n \qquad (m \le n);$$

$$m,\downarrow,n := m,m-1,m-2,\cdots,n \qquad (m \ge n);$$

$$m,\leftrightarrow s,n := \overbrace{m,n,m,n,\cdots,m,n}^{2s\ terms} \qquad (m \ne n).$$

Combined Lemma 2.3 in [29] with the structure of $CNC_4[n]$, we obtain $S(k,i)$ in $CNC_4[n]$ for $0 \le k \le n-1$ and $0 \le i \le \left\lfloor \frac{3n-2}{2} \right\rfloor$ as follows.

Lemma 1. If $n+k$ is even, $0 \le k \le 1$, then $S(k,i) =$

$$\begin{cases} (n+2i+k,\downarrow,2i,2i-1 \leftrightarrow i,2i,2i+1,\uparrow,n+2i-k), & 0 \le i \le n-2; \\ (n+2i+k,\downarrow,2i+1,2i+1,2i \leftrightarrow i,2i-1,2i,\uparrow,\ n+2i-k), & i = n-1; \\ (3n+k-1,\downarrow,2i+1,2i+1,2i \leftrightarrow 3n-2i-2,2i-1,2i,\uparrow,3n-k-1), & n \le i \le \left\lfloor \frac{3n-4}{2} \right\rfloor; \\ (3n+k-1,\downarrow,2i+1,2i+1,2i \leftrightarrow 3n-2i-2,2i-1,2i,\uparrow,3n-k-1), & i = \left\lfloor \frac{3n-2}{2} \right\rfloor, n = odd; \\ (3n+k-1,\downarrow,2i+1,2i \leftrightarrow 3n-2i-2,2i-1,2i,\uparrow,3n-k-1), & i = \left\lfloor \frac{3n-2}{2} \right\rfloor, n = even. \end{cases}$$

If $n+k$ is even, $k \ge 2$, then $S(k,i) =$

$$\begin{cases} (n+2i+k,\downarrow,2i,2i-1 \leftrightarrow i,2i,2i+1,\uparrow,n+2i-k), & 0 \le i \le n-2; \\ (n+2i+k,\downarrow,2i+1,2i+1,2i \leftrightarrow i,2i-1,2i,\uparrow,\ n+2i-k), & i = n-1; \\ (3n+k-1,\downarrow,2i+1,2i+1,2i \leftrightarrow 3n-2i-2,2i-1,2i,\uparrow,3n-k-1), & n \le i \le \left\lfloor \frac{3n-k-2}{2} \right\rfloor; \\ (6n-2i-3,\downarrow,2i+1,2i+1,2i \leftrightarrow 3n-2i-1,2i-1), & \left\lfloor \frac{3n-k}{2} \right\rfloor \le i \le \left\lfloor \frac{3n-4}{2} \right\rfloor; \\ (6n-2i-3,\downarrow,2i+1,2i \leftrightarrow 3n-2i-1,2i-1), & i = \left\lfloor \frac{3n-2}{2} \right\rfloor, n = even; \\ (6n-2i-3,\downarrow,2i+1,2i+1,2i \leftrightarrow 3n-2i-1,2i-1), & i = \left\lfloor \frac{3n-2}{2} \right\rfloor, n = odd. \end{cases}$$

If $n+k$ is odd, $0 \le k \le 2$, then $S(k,i) =$

$$\begin{cases}(n+2i+k,\downarrow,2i+1,2i \leftrightarrow i+1,2i+1,2i+2\uparrow,n+2i-k), & 0\le i\le n-2;\\ (n+2i+k,\downarrow,2i+2,2i+2,2i+1\leftrightarrow i+1,2i,2i+1,\uparrow,n+2i-k), & i=n-1;\\ (3n+k-1,\downarrow,2i+2,2i+2,2i+1\leftrightarrow 3n-2i-1,2i,2i+1,\uparrow,3n-k-1), & n\le i\le \left\lfloor\frac{3n-4}{2}\right\rfloor;\\ (3n+k-1,\downarrow,2i+2,2i+2,2i+1\leftrightarrow 3n-2i-1,2i,2i+1,\uparrow,3n-k-1), & i=\left\lfloor\frac{3n-2}{2}\right\rfloor, n=odd;\\ (3n+k-1,\downarrow,2i+2,2i+1\leftrightarrow 3n-2i-1,2i,2i+1,\uparrow,3n-k-1), & i=\left\lfloor\frac{3n-2}{2}\right\rfloor, n=even.\end{cases}$$

If $n+k$ is odd, $k\ge 3$, then $S(k,i)=$

$$\begin{cases}(n+2i+k,\downarrow,2i+1,2i \leftrightarrow i+1,2i+1,2i+2\uparrow,n+2i-k), & 0\le i\le n-2;\\ (n+2i+k,\downarrow,2i+2,2i+2,2i+1\leftrightarrow i+1,2i,2i+1,\uparrow,n+2i-k), & i=n-1;\\ (3n+k-1,\downarrow,2i+2,2i+2,2i+1\leftrightarrow 3n-2i-1,2i,2i+1,\uparrow,3n-k-1), & n\le i\le \left\lfloor\frac{3n-k-1}{2}\right\rfloor;\\ (6n-2i-2,\downarrow,2i+2,2i+2,2i+1\leftrightarrow 3n-2i-1,2i), & \left\lfloor\frac{3n-k+1}{2}\right\rfloor\le i\le \left\lfloor\frac{3n-4}{2}\right\rfloor;\\ (6n-2i-2,\downarrow,2i+2,2i+1\leftrightarrow 3n-2i-1,2i), & i=\left\lfloor\frac{3n-2}{2}\right\rfloor, n=even;\\ (6n-2i-2,\downarrow,2i+2,2i+2,2i+1\leftrightarrow 3n-2i-1,2i), & i=\left\lfloor\frac{3n-2}{2}\right\rfloor, n=odd.\end{cases}$$

Note that the value which appears twice consecutively in $S(k,i)$ represents the distance the distance between $v_{0,k}$ and the special vertex v_i.

3. Calculating $H(CNC_4[n],x)$

First, we give some notations. In $CNC_4[n]$, for $0\le k\le n-1$, we denote by $H_k(n,x)$ the contribution of the vertex $v_{0,k}$ to $H(CNC_4[n],x)$, by $Hb_k(n,x)$ the contribution of distances between $v_{0,k}$ and the boundary vertices in $CNC_4[n]$ (i.e., vertices in $CNC_4[n]$ but not in $CNC_4[n-1]$) to $H(CNC_4[n],x)$, and by $Hb(n,x)$ the contribution of the boundary vertices to $H(CNC_4[n],x)$.

From the structure of $CNC_4[n]$, there are n orbits of the automorphism group *Aut*($CNC_4[n]$) on the boundary vertices of $CNC_4[n]$. We take $\{v_{0,0},v_{0,1},v_{0,2},\cdots,v_{0,n-1}\}$ as a set of the orbital representatives. Among all 8 automorphisms of $CNC_4[n]$, each vertex in $\{v_{0,1},v_{0,2},\cdots,v_{0,n-1}\}$ has 8 isomorphic images, the vertex $v_{0,0}$ has 4 isomorphic images. Then we can give the expression of $Hb(n,x)$ in terms of $H_k(n,x)$ and $Hb_k(n,x)$ as follows.

Lemma 2.

$$Hb(n,x)=(8\sum_{k=1}^{n-1}H_k(n,x)+4H_0(n,x))-(4\sum_{k=1}^{n-1}Hb_k(n,x)+2Hb_0(n,x)).$$

Note that the last term of the right-hand side of the above expression is the contribution of distances between two vertices of boundary vertices to $H(CNC_4[n],x)$, which arises because they are counted twice in the first term of the right-hand side of the above expression.

According to Lemmas 1 and 2, Using the software MATHEMATICA 7.0, we obtain

Lemma 3. When n is even,

$$Hb(n,x)=\frac{4x^{4n-2}(x^3+1)}{(x-1)^3}+\frac{2}{(x+1)(x-1)^3}(2x^2+2nx^{2n-1}+(6n-2)x^3-2x^{3n-3}+2(n-4)x^{2n+2}+(4-6n)x+2(n-1)x^{2n}-4x^{2n+1}-5x^{3n+2}-2(n+1)x^{2n+3}+3x^{3n-2}-14x^{3n}+2x^{3n+1}+4x^{4n}).$$

When n is odd,

$$Hb(n,x)=\frac{-4x^2}{(x-1)^2(x+1)}-\frac{4nx^{2n}(x^3-1)}{x(x-1)^3}-\frac{4(x^{3n}-x^{4n})}{x^2(x-1)^3(x+1)}-\frac{x^{3n}-x^{4n}}{(x-1)^3(x+1)x}-\frac{2}{(x+1)}\frac{1}{(x-1)^3}((6n-4)x-6nx^3+2x^{2n}+4x^{2n+1}-4x^{4n}-8x^{2n+2}+2x^{2n+3}-14x^{3n+1}+x^{3n+3}-2x^{3n+2}-2x^{4n+1}-2x^{4n+2}).$$

Since $CNC_4[n]$ can be considered as a graph obtained from its isometric subgraph $CNC_4[n-1]$ (i.e., $d_{CNC_4[n-1]}(x,y)=d_{CNC_4[n]}(x,y)$ for vertices x,y in $CNC_4[n-1]$) by adding the boundary vertices of

$CNC_4[n]$, we have

Lemma 4.

$$H(CNC_4[n],x)=\sum_{j=1}^{n}Hb(j,x).$$

Note that the initial condition $H(CNC_4[1],x)=2x^2+4x.$

So we can get the main theorem: the Hosoya polynomial of $CNC_4[n]$.

Theorem 1. Let $CNC_4[n]$ be the one-quadrilateral carbon nanocone. Then when n is even,

$$H(CNC_4[n],x)=\frac{2(x^{4n+2}+x^{4n+7}-nx^{2n}+x^6-1)}{(x-1)^3(x+1)^2(x^4+x^2+1)}+\frac{3n^2x(x^6-1)}{(x+1)(x-1)^3(x^4+x^2+1)}+\frac{2x-2}{x^4+x^3+x+1}(x^2-3x-2)x^{3n}+\frac{nx(x^6-1)}{(x-1)^4(x^4+x^2+1)}-\frac{2x^2}{(x-1)^4(x+1)^2(x^4+x^2+1)}(x^2-1+2x^3-3x^4+5x^6-2x^7+2x^8+x^9-2x^{2n}(x^5-4x^4-4x^6+4x^8-x^9-3x^7)-x^{3n}(3x+14x^3+6x^5+14x^7)+2x^{4n}(2x^4+x^5+2x^6+x^7+x^8));$$

when n is odd,

$$H(CNC_4[n],x)=\frac{2(x^{4n+2}+x^{4n+7}-nx^{2n}+x^6-1)}{(x-1)^3(x+1)^2(x^4+x^2+1)}+\frac{3n^2x(x^6-1)}{(x+1)(x-1)^3(x^4+x^2+1)}+\frac{nx(x^6-1)}{(x-1)^4}\frac{1}{x^4+x^2+1}-\frac{2x^{2n}(x^5-x-4x^4-4x^6)}{(x-1)^4(x+1)^2(x^4+x^2+1)}(2-2x^8+x^9+2x^2(1+x^2+2x^3-3x^4+5x^6-2x^7)+x^{3n}(3x+14x^3+6x^5+14x^7)-2x^{4n}(2x^4+x^5+2x^6+x^7+x^8)).$$

In what follows, we give some corollaries of Theorem 1. First, we define a notation z associated with an integer n as follows. When n is odd, $z=15$; when n is even, $z=0$. From Theorem 1, we immediately obtain the Wiener index $W(CNC_4[n])$ of $CNC_4[n]$.

Corollary 1. Let $CNC_4[n]$ be the one-quadrilateral carbon nanocone. Then

$$W(CNC_4[n])=\frac{2}{15}(87n^5-20n^3+15n^2-37n+z).$$

Similarly, we can deduce the Hyper-Wiener index, Tratch-Stankevitch-Zefirov index of one-quadrilateral carbon nanocone $CNC_4[n]$ as follows.

Corollary 2. Let $CNC_4[n]$ be the one-quadrilateral carbon nanocone. Then

$$WW(CNC_4[n])=\frac{1}{15}(87n^5+60n^4-20n^3-37n+z).$$

$$TSZ(CNC_4[n])=\frac{1}{45}(87n^5+60n^4-20n^3-37n+z).$$

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