Fullerene, Nanotubes and Carbon Nanostructures

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The Omega Index of Polyomino Chain, Phenylene Graphs and Carbon Nanocones

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The Omega index of a graph G is defined as \( \Omega(G) = \sum_{s} m(G, s) \), where \( m(G, s) \) is the number of strips of length \( s \). In this paper, we compute this index for \( k \)-polyomino chain, phenylenes and carbon nanocones.

Keywords Omega index, polyomino chain, carbon nanocones, phenylene

Introduction

The structure of a molecule could be represented in a variety of ways. The information on the chemical constitution of molecule is conventionally represented by a molecular graph. Graph theory has successfully provided the chemist with a variety of useful tools, namely, topological index. The first reported use of a topological index in chemistry was by Wiener (11) in the study of paraffin boiling points. Since then, in order to model various molecular properties, many topological indices have been designed (10). Such a proliferation is still ongoing and is becoming counter productive.

Let \( G = (E, V) \) be a connected graph, with the vertex set \( V(G) \) and edge set \( E(G) \). Two edges \( e = uv \) and \( f = xy \) of \( G \) are called codistant if they obey the following relation (7,8):

\[
d(v, x) = d(v, y) + 1 = d(u, x) + 1 = d(u, y)
\]

Relation \( co \) is reflexive; that is, \( e \ co \ e \) holds for any edge \( e \) of \( G \). It is also symmetric, if \( e \ co \ f \) then \( f \ co \ e \). In general, relation \( co \) is not transitive, an example showing this fact is the complete bipartite graph \( K_{2,n} \). If “\( co \)” is also transitive, thus an equivalence relation, then \( G \) is called a co-graph and the set of edges \( C(e) = \{ f \in E(G) | f \ co \ e \} \) is called an orthogonal cut of \( G \), \( E(G) \) being the union of disjoint orthogonal cuts: \( E(G) = C_1 \cup C_2 \cup \cdots \cup C_k \), \( C_i \cap C_j = \phi, i \neq j \). Klavžar in (6) has shown that relation \( co \) is a theta Djoković-Winkler relation; see (4,12).

Let \( e = uv \) and \( f = xy \) be two edges of \( G \) which are opposite or topologically parallel and denote this relation by \( e \ op \ f \). A set of opposite edges, within the same face/ring, eventually forming a strip of adjacent faces/rings, is called an opposite edge strip ops, which is a quasi-orthogonal cut qoc (i.e., the transitivity relation is not necessarily obeyed). Note that \( co \) relation is defined in the whole graph while \( op \) is defined only in a face/ring.

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The length of $ops$ is maximal irrespective of the starting edge. Let $m(G,s)$ be the number of $ops$ strips of length $s$. The Omega index is defined as $\Omega(G) = \sum_s m(G,s)$.

In this paper we compute this index for $k$-polyomino chain, phenylenes and carbon nanocones.

The Omega Index of Polyomino Chains of 4k– Cycles

A $k$-polyomino system is a finite 2-connected plane graph such that each interior face (also called cell) is surrounded by a regular $4k$-cycle of length one. In other words, it is an edge-connected union of cells. For the origin of polyominoes, see, for example, Klarner (5) and Golomb (7,8).

For calculating the omega index of a $k$-polyomino chain, we introduce some concepts for a $k$-polyomino chain. A kink of a $k$-polyomino chain is any branched or angularly connected $4k$-cycle. A segment of a $k$-polyomino chain is a maximal linear chain in the polyomino chain, including the kinks and/or terminal $4k$-cycles at its end. The number of $4k$-cycles in a segment $S$ is called its length and is denoted by $\ell(S)$. For any segment $S$ of a polyomino chain with $n \geq 2$ $4k$-cycles, one has $2 \leq \ell(S) \leq n$. In particular, a $k$-polyomino chain is a linear chain if and only if it contains exactly one segment (see Figure 1).

A $k$-polyomino chain is a zig-zag chain if and only if the length of each segment is 2 (see Figure 2).

A $k$-polyomino chain consists of a sequence of segments $S_1, S_2, \ldots, S_s$, $s \geq 1$, with lengths $\ell(S_i) \equiv \ell_i, i = 1, 2, \ldots, s$, where $\sum_{i=1}^s \ell_i = n + s - 1$

Figure 1. The linear chain of 8-cycles.

Figure 2. The zig-zag chain of 8-cycles.
Figure 3. The graph $B_{5,2|3}$. 

$(n$ denotes the number of $4k$-cycles of the polyomino chain) since two neighboring segments have always one $4k$-cycle in common. In the following we will abbreviate the vector of lengths by $\ell$, that is, $\ell = (\ell_1, \ldots, \ell_s)$.

**Theorem 1.** Let $B_{n,k|\ell}$ be a $k$-polyomino chain with $n$ $4k$-cycles consisting of $s \geq 1$ segments $S_1, S_2, \ldots, S_s$ with lengths $\ell_1, \ell_2, \ldots, \ell_s$. Then $\Omega(B_{n,k|\ell}) = (2k - 1)n + 1$.

**Proof.** Let us first observe that the edges of $B_{n,k|\ell}$ fall into two distinct classes, namely the ones which are cut across by the straight line passing through the centers of the $4k$-cycles of $S_i$ and those which are not. We denote the edges of the first type contained in $S_i$ by $E_c(S_i)$.

The edges $E_c(S_i)$ $(1 \leq i \leq s)$ in each $S_i$ form a strip $C_i$ of length $\ell_i + 1$ $(1 \leq i \leq s)$. On other hand, two opposite edges in each $4k$-cycle (except the edges, which belong to $E_c(S_i)$) form a strip $C_0$ of length 2 (see Figure 3). Thus the number of strips of length 2 is equal to $m(G, |C_0|) = \frac{1}{2}(|E(G)| - \sum_{i=1}^{s} |E_c(S_i)|)$. But

$|E(G)| = (4k - 1)n + 1$ and $|E_c(S_i)| = \ell_i + 1$ for every $i$.

So

$$m(G, |C_0|) = (2k - 1)n - s + 1$$

Therefore

$$\Omega(G) = (2k - 1)n - s + 1 + \sum_{i=1}^{s} 1 = (2k - 1)n + 1$$

The result follows.

The above theorem implies that omega index of $B_{n,k|\ell}$ only depends on the number of $4k$-cycle and dose not depend on the length and number of segments. Thus we have the following result.

**Corollary 1.** Let $L_{n,k}$ and $Z_{n,k}$ be the linear chain and zig-zag chain, respectively. Then

$$\Omega(B_{n,k|\ell}) = \Omega(L_{n,k}) = \Omega(Z_{n,k})$$
Omega Index of Phenylennes and Their Hexagonal Squeezes

Phenylennes are a class of chemical compounds in which the carbon atoms form 6- and 4-membered cycles. Each 4-membered cycle (=square) is adjacent to two disjoint 6-membered cycles (=hexagons), and no two hexagons are adjacent. Their respective molecular graphs are also referred to as phenylennes. By eliminating, or “squeezing out,” the squares from a phenylene, a catacondensed hexagonal system (which may be jammed) is obtained, called the hexagonal squeeze of the respective phenylene (10). Clearly, there is a one-to-one correspondence between a phenylene (PH) and its hexagonal squeeze (HS). Both possess the same number \( n \) of hexagons. In addition, a PH with \( n \) hexagons possesses \( n - 1 \) squares. The number of vertices of PH and HS are \( 6n \) and \( 4n + 2 \), respectively. The number of edges of PH and HS are \( 8n - 2 \) and \( 5n + 1 \), respectively. An example of PH and its HS is shown in Figure 3.

For PHs and their HS, some results related to the mathematical properties of Wiener index, Randić index and the second-order Randić index have been reported in the literature (3,9,13). In this section, we will give a formula for calculating the omega index of PHs and establish a simple relation between the Omega index of a PH and of the corresponding HS.

For calculating the omega index of a PH, we introduce some conceptions in a PH analogously in a hexagonal system. The linear chain PH is a PH without kinks, where the kinks are the branched or angularly connected hexagons. A segment of a PH is a maximal linear chain in the PH, including the kinks and/or terminal hexagons at its end. The number of hexagons in a segment \( S \) is called its length and is denoted by \( \ell(S) \). For any segment \( S \) of a PH, \( 2 \leq \ell(S) \leq n \). Particularly, a PH is a full kink one if and only if the lengths of its segment are all equal to 2.

A PH consists of a sequence of segments \( S_1, S_2, \ldots, S_s, s \geq 1 \), with lengths \( \ell(S_i) = \ell_i \), \( i = 1, 2, \ldots, s \), where \( \sum_{i=1}^{s} \ell_i = n + s - 1 \), since two neighboring segments have always one hexagon in common.

**Theorem 2.** The Omega index of PH is equal to \( \Omega(PH) = 3n \).

*Proof.* The proof is similar to the proof in Theorem 1. Thus this graph has \( s \) strips \( C_i \) of length \( 2\ell_i \), and \( 3n-s \) strips of length 2 (see Figure 4). Therefore, \( \Omega(G) = 3n - s + s = 3n \), as desired.

In comparing with PH, graph HS has \( n-1 \) squares less than PH. Since two opposite edges in every square form a strip of length 2, so HS has \( n-1 \) strips less than PH. Thus we have the following result which is relation between the Omega index of a phenylene and the corresponding hexagonal squeeze.

**Corollary 2.** \( \Omega(HS) = \Omega(PH) - (n - 1) \).

Omega Index of the Carbon Nanocones

In recent years, nanostructures involving carbon have been the focus of an intense research activity driven to a large extent by the quest for new materials with specific applications. One pentagonal carbon nanocone originally discovered by Ge and Sattler in 1994 (2). These are constructed from a graphene sheet by removing a 60° wedge and joining the edges produces a cone with a single pentagonal defect at the apex. If a 120° wedge is considered
then a cone with a single square defect at the apex is obtained. The case of 240° wedge yields a single triangle defect at the apex. Two types of carbon nanocones are evident in Figure 5, one-triangle and one-square (1,2).
Theorem 3. The Omega index of \( \text{CNC}_m[n] \) is equal to

\[
\Omega(\text{CNC}_m[n]) = \begin{cases}
  k(2n + 1) & m = 2k \\
  (2k + 1)(n + 1) & m = 2k + 1
\end{cases}
\]

Proof. The edges that are opposite every edge of central apex form a strip \( C_0 \). Also the edges that are parallel in every layer form a strip \( C_i \) \((1 \leq i \leq n)\) (see Figure 5). The number of strips of length \(|C_0|\) is equal to \( m \) or \( m/2 \) in respective cases \( m \) is odd or even. The number of strips of length \(|C_i|\) is equal to \( m \). Thus,

\[
\Omega(G) = m + \sum_{i=1}^{n} m = m(n + 1)
\]

if \( m \) is odd and

\[
\Omega(G) = \frac{m}{2} + \sum_{i=1}^{n} m = \frac{m}{2}(2n + 1)
\]

if \( m \) is even. Therefore the proof is completed.

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