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Use of Structure Codes (Counts) for Computing Topological Indices of Carbon Nanotubes: Sadhana (Sd) Index of Phenylenes and its Hexagonal Squeezes

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ABSTRACT

Structural codes vis-a-vis structural counts, like polynomials of a molecular graph, are important in computing graph-theoretical descriptors which are commonly known as topological indices. These indices are most important for characterizing carbon nanotubes (CNTs). In this paper we have computed Sadhana index (Sd) for phenylenes and their hexagonal squeezes using structural codes (counts). Sadhana index is a very simple W-Sz-PI-type topological index obtained by summing the number of edges on both sides of the elementary cuts of benzenoid graphs. It has the similar discriminating power as that of the Weiner (W)-, Szeged (Sz)-, and PI-indices.

Keywords: Sadhana index, graph-theoretical descriptor, structural codes, structural counts phenylene, hexagonal squeeze, benzenoids.

1. INTRODUCTION

Carbon nanotubes (CNTs) are *peri*-condensed benzenoids that are ordered in graphite-like hexagonal pattern. They can be derived from graphite by rolling up the rectangular sheets along certain vectors. All benzenoids, including graphite and CNTs are aromatic structure.

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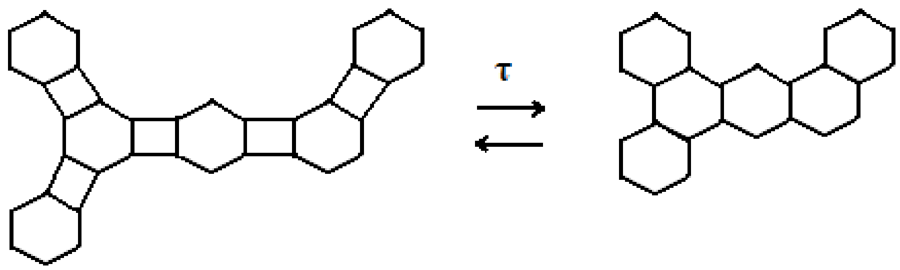
The unique properties of CNTs have made this new form of solid carbon the most studied nano-material for the last few years. They are among the stiffest and strongest fibers known, and have remarkable electronic properties and many other unique characteristics. Consequently, CNTs have attracted tremendous academic and industrial interest. It is, thus, of interest to study the mathematical properties of CNTs. The important among the mathematical properties of nanotubes is to compute their topological indices [1, 2].

In the present paper, therefore, an attempt has been made for computing Sd index of phenylenes and its hexagonal squeezes using structural codes [3]. The structure code can be used to represent graph and likewise the structure codes can be used for computing topological index.

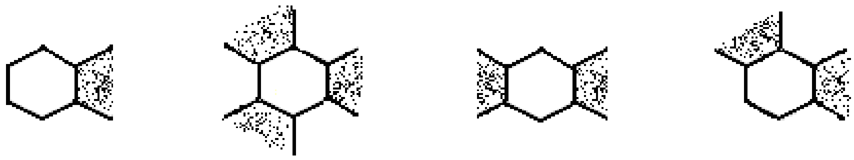
2. COMPUTATION OF SADHANA INDEX (SD) OF PHENYLENE (PH) AND ITS HEXAGONAL SQUEEZES (HS) USING STRUCTURE CODES

Phenylenes are polycyclic conjugated molecules, composed of four-and six-membered rings such that every four membered ring is adjacent to two six-membered rings, and no two six membered rings are mutually adjacent. Each four-membered ring lies between two six membered rings, and each six-membered ring is adjacent only to four-membered rings. Because of such structural features phenylenes are very interesting conjugated species [4 – 8]. The rapid development of the experimental study of phenylenes motivated a number of recent theoretical studies of thee conjugated π-electron systems. Consequently, in the present paper we report computation of Sadhana index (Sd) of PH and its HS using structural codes (counts) for computing. The transformation of PH into its HS is demonstrated below:



PH HS

The hexagons of HS and also of PH are denoted by end-, branching-, linear-, and kink hexagons respectively:



end - **branching -** **linear -** **kink -**

Let e = e(HS) = e(PH); b = b(HS) = b(PH); l = l(HS) = l(PH); and k = k(HS) = k(PH); denote the number of end-, branching-, linear-, and kink- hexagons respectively. Clearly, e + b + l + k = h = number of hexagons, h = h (HS) = h (PH) and e = b + 2.

Let c = number of orthogonal cuts, S_i = i^{th} orthogonal cuts, $m_i = |S_i|$ = number of edges of S_i, m = Σ mi = number of edges of graph, where i = 1, 2, …, c.

Theorem 1: Let PH be a phenylene and HS be its hexagonal squeeze with h hexagons. Then Sd(PH) = Sd(HS) = m(c – 1), where m is the number of edges and c is the number of orthogonal cuts in a PH and HS, respectively.

Proof: The definition of Sadhana index of a bipartite SCO-graph G is

$$Sd(G) = \sum_{i=1}^{c}[m(G) - m_i(G)] \quad (1)$$

For a PH, let s = s (PH) denote the number of squares of a PH, where s = h – 1, m = 5h + 1 + 3s, c_2 = 2e + 2l + k + s (m_i = 2), $m_i = l_i + 3 + s_i$, where s_i is the number of squares in segment S_i and c – c_2 = 2b + k + 1. Thus, by equation (1) we get

$$
\begin{aligned}
Sd(PH) &= \sum_{i=1}^{c}[m - m_i] \\
&= mc - \sum_{i=1}^{c} m_i \\
&= mc - \sum_{m_i=2} m_i - \sum_{m_i>2} m_i \\
&= mc - \sum_{i=1}^{c_2} m_i - \sum_{i=1+c_2}^{c} m_i \\
&= mc - (2(2e + 2l + k + s) + \sum_{i=1+c_2}^{c}[l_i + 3 + s_i] \\
&= mc - (4e + 4l + 2k + 2s + l + s + 3(c - c_2)) \\
&= mc - (4e + 5l + 2k + 3s + 3(2b + k + 1)) \\
&= mc - (4e + 5(l + k) + 6b + 3s + 3) \\
&= mc - (5h - e + b + 3s + 3) \\
&= mc - (5h + 1 + 3s) \\
&= mc - m \\
&= m(c - 1)
\end{aligned}
$$

Similarly, in an HS, m = 5h + 1, the number of cuts with m_i = 2 is c_2 = 2e + 2l + k and for all other cuts of HS, $m_i = l_i + 3$, where l_i denote the number of hexagons of l-type (in segment S_i).

$$\begin{aligned}
\mathrm{Sd(HS)} &= \textstyle\sum_{i=1}^{c}[m - m_i] \\
&= \mathrm{mc} - \textstyle\sum_{i=1}^{c} m_i \\
&= \mathrm{mc} - \textstyle\sum_{m_i=2} m_i - \sum_{m_i>2} m_i \\
&= \mathrm{mc} - \textstyle\sum_{i=1}^{c_2} m_i - \sum_{i=1+c_2}^{c} m_i \\
&= \mathrm{mc} - (2(2e + 2l + k) + \textstyle\sum_{i=1+c_2}^{c}[l_i + 3] \\
&= \mathrm{mc} - (4e + 4l + 2k + 3(c - c_2) + \textstyle\sum_{i=1+c_2}^{c} l_i) \\
&= \mathrm{mc} - (4e + 5l + 2k + 3(2b + k + 1)) \\
&= \mathrm{mc} - (4e + 5(l + k) + 6b + 3) \\
&= \mathrm{mc} - (5h - e + b + 3) \\
&= \mathrm{mc} - (5h + 1) \\
&= \mathrm{mc} - m \\
&= m\,(c - 1).
\end{aligned}$$
□

Corollary 2: For a PH with h hexagons, Sd(PH) = $24h^2 - 14h + 2$.

Proof: The result is trivial. □

Corollary 3: For an HS with h hexagons, Sd(HS) = $10h^2 + 2h$.

Proof: The result is trivial. □

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