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COMPUTING SOME TOPOLOGICAL INDICES OF CARBON NANOTUBES

Mohammad Javad Nikmehr[1], Najmeh Soleimani[2], Hamid Agha Tavallaee[3]

[1] Faculty of Mathematics, K. N. Toosi University of Technology, P.O. Box 16315-1618, Tehran, Iran
[2] Salehan Institute of Higher Education, Ghaemshahr, Iran
[3] Department of Mathematics, Tehran-North Branch, Islamic *Azad University*, Tehran, Iran
e-mail: nikmehr@kntu.ac.ir, soleimani.najmeh@gmail.com, tavallaee@iust.ac.ir

Abstract. In this paper, several topological indices are investigated for *H*-Phenylenic nanotube, *H*-Naphthylenic nanotube and *H*-Anthracenic nanotube. The calculated indices are product-connectivity index, sum-connectivity index, geometric-arithmetic index and atom-bond connectivity index.

Keywords: vertex-degree, topological indices, molecular graphs, carbon nanotubes.

AMS Subject Classification: 05C07, 05C40.

1. Introduction

The focus of many research activities in the last few decades have been the carbon nanotubes and nanostructures which is driven to a large extent by the quest for new materials with specific applications. A molecular graph is a simple graph such that its vertices correspond to the atoms and the edges to the bonds. A graph Gconsist of a set of vertices $V(G)$ and a set of edges $E(G)$. The vertices in $G$are connected by an edge if there exists an edge $uv \in E(G)$ connecting the vertices $u$and $v$in Gsuch that $u, v \in V(G)$. For any $u \in V(G)$, $d_u$represents the number of edges incident to u, called the degree of the vertex $u$in G. Here, a topological index is a real number that is derived from molecular graphs of chemical compounds. There are several topological indices already defined.

The product-connectivity index, also called *Randić index*$\chi(G)$ of a graph G and is defined such as:

$$\chi(G) = \sum_{uv \in E(G)} \frac{1}{\sqrt{d_u d_v}}.$$

This topological index was first proposed by Randić[4] in 1975.

In 2009, Zhou and Trinajstić [9] proposed another connectivity index, named the *sum-connectivity index*. This index is defined as follows:

$$X(G) = \sum_{uv \in E(G)} \frac{1}{\sqrt{d_u + d_v}}.$$

The *geometric-arithmetic* (GA) *index* is another topological index based on degrees of vertices defined by Vukičevićand Furtula [7]:

$$GA(G) = \sum_{uv\in E(G)} \frac{2\sqrt{d_u d_v}}{d_u + d_v}.$$

Estrada et al. [2] introduced *atom-bond connectivity* (*ABC*) *index*, which has been applied up to study the stability of alkanes and the strain energy of cycloalkanes. This index is defined as follows:

$$ABC(G) = \sum_{uv\in E(G)} \sqrt{\frac{d_u+d_v - 2}{d_u d_v}}.$$

In recent years, there has been considerable interest in the general problem of determining topological indices [1, 3, 5, 6, 8]. The aim of this paper is to compute some topological indices of lattice *H*-Phenylenic nanotube, *H*-Naphthylenic nanotube and *H*-Anthracenic nanotube, Figures 1, 2 and 3.

2. Results and discussion

In this section we calculate the Randić index, sum-connectivity index, geometric-arithmetic index and atom-bond connectivity index of *H*-Phenylenic nanotube, *H*-Naphthylenic nanotube and *H*-Anthracenic nanotube by use an algebraic method.

Remark 1. We denote a 2-dimensional lattice of *H*-Phenylenic nanotube by $G = GTUC[p,q]$(Figure 1). Now we consider the molecular graph G. It is easy to see that$|V(G)| = 6pq$and $|E(G)| = 9pq - 2q$. We partition the edges of Ginto three subsets $E_1(G), E_2(G)$ and $E_3(G)$. The following table gives the three types and gives the number of edges in each type.

Table 1. Computing the number of edges for molecular graph G.

$[d_u, d_v]$ where$uv \in E(G)$	Total Number of Edges
$E_1 = [2,2]$	2q
$E_2 = [2,3]$	$4q$
$E_3 = [3,3]$	$9pq - 8q$

Using Table 1, we give an explicit computing of some indices of G.

Theorem 1. Consider the graph G of lattice *H*-Phenylenic nanotube. Then

(i) $\chi(G) = \sum_{uv\in E(G)} \frac{1}{\sqrt{d_u d_v}} = \frac{|E_1|}{\sqrt{4}} + \frac{|E_2|}{\sqrt{6}} + \frac{|E_3|}{\sqrt{9}} = 3pq + \frac{2\sqrt{6}-5}{3} q.$

(ii) $X(G) = \sum_{uv\in E(G)} \frac{1}{\sqrt{d_u + d_v}} = \frac{|E_1|}{\sqrt{4}} + \frac{|E_2|}{\sqrt{5}} + \frac{|E_3|}{\sqrt{6}} = \frac{3\sqrt{6}}{2} pq + \left(1 + \frac{4\sqrt{5}}{5} - \frac{4\sqrt{6}}{3}\right) q.$

(iii) $GA(G) = \sum_{uv\in E(G)} \frac{2\sqrt{d_u d_v}}{d_u + d_v} = |E_1| \frac{2\sqrt{4}}{4} + |E_2| \frac{2\sqrt{6}}{5} + |E_3| \frac{2\sqrt{9}}{6} = 9pq + \left(\frac{8\sqrt{6}}{5} - 6\right) q.$

(iv) $ABC(G) = \sum_{uv \in E(G)} \sqrt{\frac{d_u+d_v-2}{d_u d_v}} = |E_1|\sqrt{\frac{2}{4}} + |E_2|\sqrt{\frac{3}{6}} + |E_3|\sqrt{\frac{4}{9}} = 6pq + \left(3\sqrt{2} - \frac{16}{3}\right)q.$

Remark 2. We denote a 2-dimensional lattice of *H*-Naphthylenic nanotube *by* $K = KTUC[p,q]$(Figure 2). Now we consider the molecular graph K. It is easy to see that $|V(K)| = 10pq$and $|E(K)| = 15pq - 2q$. We partition the edges of Kinto three subsets $E_1(K), E_2(K)$and $E_3(K)$. The following table gives the three types and gives the number of edges in each type.

Table 2.Computing the number of edges for molecular graph$K$.

$[d_u, d_v]$ where$uv \in E(K)$	Total Number of Edges
$E_1 = [2,2]$	2q
$E_2 = [2,3]$	$4q$
$E_3 = [3,3]$	$15pq - 8q$

Table 2 is used to compute, we give an explicit computing of some indices of K.

Theorem 2. Consider the graph K of lattice *H*-Naphthylenic nanotube. Then

(i) $\chi(K) = \sum_{uv \in E(K)} \frac{1}{\sqrt{d_u d_v}} = \frac{|E_1|}{\sqrt{4}} + \frac{|E_2|}{\sqrt{6}} + \frac{|E_3|}{\sqrt{9}} = 5pq + \frac{2\sqrt{6}-5}{3}q.$

(ii)$X(K) = \sum_{uv \in E(K)} \frac{1}{\sqrt{d_u + d_v}} = \frac{|E_1|}{\sqrt{4}} + \frac{|E_2|}{\sqrt{5}} + \frac{|E_3|}{\sqrt{6}} = \frac{5\sqrt{6}}{2}pq + \left(1 + \frac{4\sqrt{5}}{5} - \frac{4\sqrt{6}}{3}\right)q.$

(iii) $GA(K) = \sum_{uv \in E(K)} \frac{2\sqrt{d_u d_v}}{d_u + d_v} = |E_1|\frac{2\sqrt{4}}{4} + |E_2|\frac{2\sqrt{6}}{5} + |E_3|\frac{2\sqrt{9}}{6} = 15pq + \left(\frac{8\sqrt{6}}{5} - 6\right)q.$

(iv) $ABC(K) = \sum_{uv \in E(K)} \sqrt{\frac{d_u+d_v-2}{d_u d_v}} = |E_1|\sqrt{\frac{2}{4}} + |E_2|\sqrt{\frac{3}{6}} + |E_3|\sqrt{\frac{4}{9}} = 10pq + \left(3\sqrt{2} - \frac{16}{3}\right)q.$

Remark 3. We denote a 2-dimensional lattice of *H*-Anthracenic nanotube by $L = LTUC[p,q]$ (Figure 3). Now we consider the molecular graph L. It is easy to see that$|V(L)| = 14pq$and $|E(L)| = 21pq - 2q$. We partition the edges of Linto three subsets $E_1(L), E_2(L)$and $E_3(L)$. The following table gives the three types and gives the number of edges in each type.

Table 3.Computing the number of edges for molecular graph$L$.

$[d_u, d_v]$where$uv \in E(L)$	Total Number of Edges
$E_1 = [2,2]$	2q
$E_2 = [2,3]$	$4q$
$E_3 = [3,3]$	$21pq - 8q$

From this table, we give an explicit computing of some indices of L.

Theorem 3. Consider the graph L of lattice *H*-Anthracenic nanotube. Then

(i) $\chi(L)=\sum_{uv\in E(L)}\frac{1}{\sqrt{d_u d_v}}=\frac{|E_1|}{\sqrt{4}}+\frac{|E_2|}{\sqrt{6}}+\frac{|E_3|}{\sqrt{9}}=7pq+\frac{2\sqrt{6}-5}{3}q.$

(ii) $X(L)=\sum_{uv\in E(L)}\frac{1}{\sqrt{d_u+d_v}}=\frac{|E_1|}{\sqrt{4}}+\frac{|E_2|}{\sqrt{5}}+\frac{|E_3|}{\sqrt{6}}=\frac{7\sqrt{6}}{2}pq+\left(1+\frac{4\sqrt{5}}{5}-\frac{4\sqrt{6}}{3}\right)q.$

(iii) $GA(L)=\sum_{uv\in E(L)}\frac{2\sqrt{d_u d_v}}{d_u+d_v}=|E_1|\frac{2\sqrt{4}}{4}+|E_2|\frac{2\sqrt{6}}{5}+|E_3|\frac{2\sqrt{9}}{6}=21pq+\left(\frac{8\sqrt{6}}{5}-6\right)q.$

(iv) $ABC(L)=\sum_{uv\in E(L)}\sqrt{\frac{d_u+d_v-2}{d_u d_v}}=|E_1|\sqrt{\frac{2}{4}}+|E_2|\sqrt{\frac{3}{6}}+|E_3|\sqrt{\frac{4}{9}}=14pq+\left(3\sqrt{2}-\frac{16}{3}\right)q.$

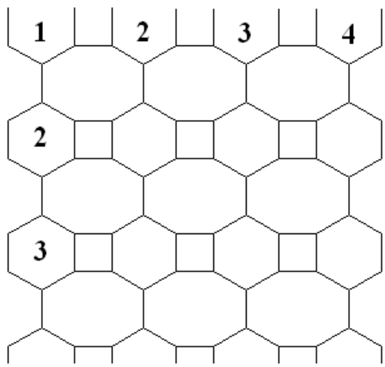

Figure 1. The 2-D graph lattice *H*-Phenylenic nanotube with $p=4$ and $q=3$.

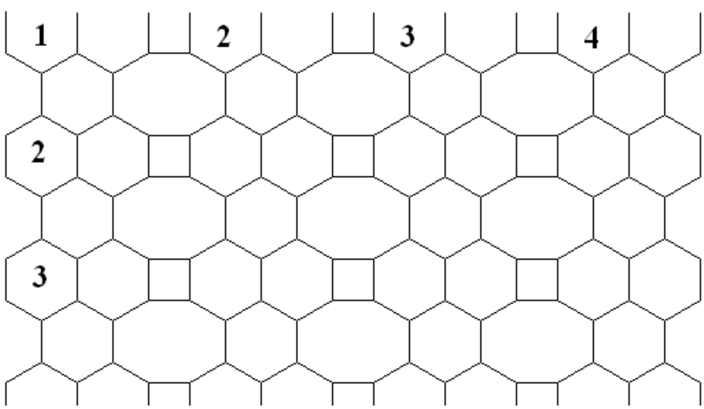

Figure 2. The 2-D graph lattice *H*-Naphthylenic nanotube with $p=4$ and $q=3$.

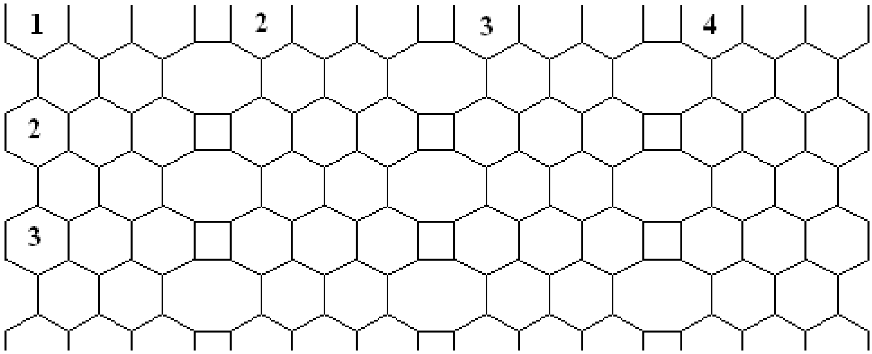

Figure 3. The 2-D graph lattice H-Anthracenic nanotube with $p = 4$ and $q = 3$.

3. Conclusion

This paper deals with the mathematical characterization of some families of nanotubes, that is, carbon nanotubes. Carbon nanotubes form an interesting class of carbon nanomaterials. Some chemical indices have been invented in theoretical chemistry, such as Randić index, sum-connectivity index, geometric-arithmetic index and atom-bond connectivity index, which, we compute theseindices for three types of carbon nanotubes.

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Karbon nanoboruların bəzi topoloji indekslərin hesablanması

Najmeh Süleymani, Məhəmməd Cavad Nikmehr,
Həmid Ağa Təvallei

XÜLASƏ

Bu məqalədə H-Phenylenic nanoborusu, H-Naphthylenic nanoborusu və H-Anthracenic nanoborusu üçün bir neçə topoloji indeks araşdırılmışdır. Hesablanan indekslər nəticə birləşməsi indeksi, cəm birləşməsi indeksi, həndəsi hesabi indeks və atom birləşməsi rabitəsi indeksidir.

Açar sözlər: dərəcənin təpələri, topoloji indekslər, molekulyar qraflar, karbon nanoboruları.

Вычисления некоторых топологических индексов углеродных нанотрубок

Нажмех Сулеймани, Мухаммад Джавад Никмехр,
Хамид Ага Таваллеи

РЕЗЮМЕ

В этой статье исследованы несколько топологические индексы для H-Phenylenic нанотрубки, H-Naphthylenic нанотрубки и H-Anthracenic нанотрубки. Рассчитанные индексы являются - индекс продукта соединения, индекс суммарной соединения, геометрической арифметическое индекс и индекс атом-облигаций связности.

Ключевые слова: вершина градусов, топологические индексы, молекулярные графы, углеродные нанотрубки.