

Edge and vertex PI index of nanotubes and nanotori covered by C_4

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In previous paper the authors computed the Wiener and Szeged indices of nanotubes and nanotori covered by C_4 . In this paper, we present the same for PI index.

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1. Introduction

Throughout this paper we consider only simple graphs, i.e. graphs without loops and multiple edges. It is possible to associate a graph to a molecule, named molecular graph. In this graph each vertex represented an atom of the molecule and covalent bonds between atoms are represented by edges between the corresponding vertices. Suppose $V(G)$ denotes the vertex set of a graph G . For two vertices $u, v \in V(G)$, $d(u, v)$ is defined as the number of edges in a minimal path connecting the vertices u and v .

Suppose R denotes the set of all real numbers, Y is a set and $d: Y \times Y \longrightarrow R$ is a function such that for every $x, y \in Y$:

- 1) $d(x, y) \geq 0$ (non-negativity)
- 2) $d(x, y) = 0$ if and only if $x = y$ (identity of indiscernibles)
- 3) $d(x, y) = d(y, x)$ (symmetry)
- 4) $d(x, z) \leq d(x, y) + d(y, z)$ (triangle inequality)

then (Y, d) is called a metric space. It is easy to see that the set $V(G)$ equipped with distance function $d_G(-, -)$ constitutes a metric space. A topological index for G is a real number $Top(G)$ such that for every graph H isomorphic to G , $Top(H) = Top(G)$.

The Wiener index W is the first topological index to be used in chemistry. It was introduced in 1947 by Harold Wiener [1], as the path number for characterization of alkanes. Wiener originally defined his index on trees and studied its use for correlation of physico chemical

properties of alkenes, alcohols, amines and their analogous compounds. This index is defined to be the count of all shortest distances in a graph. Padmakar Khadigar [2] introduced another topological index named PI index. It is defined as $PI(G) = \sum_{u,v \in V(G)} d(u, v)$, where

The authors computed the Wiener and Schultz indices of nanotubes and nanotori covered by C_4 . The aim of this paper is to present the same for PI index. Throughout this paper our notation is standard and taken mainly from [5,6].

2. Results and discussion

Suppose G and H are graphs. The Cartesian product $G \bullet H$ of graphs G and H has the vertex set $V(G \bullet H) = V(G) \times V(H)$ and $(a, x)(b, y)$ is an edge of $G \bullet H$ if $a = b$ and $xy \in E(H)$, or $ab \in E(G)$ and $x = y$. It is well known that the Cartesian product is commutative and associative, $|V(G \bullet H)| = |V(G)| \times |V(H)|$ and $|E(G \bullet H)| = |E(G)| \times |V(H)| + |V(G)| \times |E(H)|$. On the other hand, if (a, x) and (b, y) are vertices of $G \bullet H$ then $d_{G \bullet H}((a, x), (b, y)) = d_G(a, b) + d_H(x, y)$, see [5] for details.

We now assume that P_n and C_n denote the path and cycle with n vertices. Then $R = P_n \bullet C_m$ and $S = C_n \bullet C_m$ are nanotubes and nanotori with mn vertices. On the other hand, by above results $|E(R)| = 2mn - m$, $|E(S)| = 2mn$,

$$PI_e(P_n) = PI_v(P_n) = (n-1)(n-2)$$

and

$$PI_e(C_n) = \begin{cases} n(n-1) & \text{nisodd} \\ n(n-2) & \text{niseven} \end{cases} \quad \& \quad PI_v(C_n) = \begin{cases} n(n-3) & \text{nisodd} \\ n(n-2) & \text{niseven} \end{cases}$$

In [7,8], the authors proved that the vertex PI index and edge PI index of the Cartesian product of two graphs are given as $PI_v(G \bullet H) = PI_v(G)|V(H)|^2 + PI_v(H)|V(G)|^2$ and

$PI_e(G \bullet H) = |V(G)|^2|V(H)|E(H)PI_v(H) + |V(H)|^2|V(G)|E(G)PI_v(G)$. Then by these formulae, one can see that

$$\begin{aligned}
PI_e(R) &= \begin{cases} 2m^2n^2 - 4m^2n + 2m^2 - 3mn^2 + 2mn & m \text{ is even} \\ 2m^2n^2 - 4m^2n - 3mn^2 + 3mn + 2m^2 & m \text{ is odd} \end{cases} \\
PI_v(S) &= \begin{cases} 2m^2n^2 - 2m^2n - 2mn^2 & n \& m \text{ are even} \\ 2m^2n^2 - 3m^2n - 3mn^2 & n \& m \text{ are odd} \\ 2m^2n^2 - 2m^2n - 3mn^2 & n \text{ is even \& } m \text{ is odd} \\ 2m^2n^2 - 3m^2n - 2mn^2 & m \text{ is even \& } n \text{ is odd} \end{cases} \\
PI_v(R) &= \begin{cases} 2m^2n^2 - 3m^2n - 2mn^2 + 2m^2 & m \text{ is even} \\ 2m^2n^2 - 3m^2n - 3mn^2 + 2m^2 & m \text{ is odd} \end{cases} \\
PI_e(S) &= 4m^2n^2 - 4m^2n - 4mn^2
\end{aligned}$$

In [9-16] some exact formulae for the first and second Zagreb, PI and vertex PI, Schultz and Modified Schultz, edge Wiener, hyper-Wiener and edge Szeged indices of the Cartesian product of graphs are given. Using the main results of these papers, one can compute the corresponding topological indices of nanotubes and nanotori covered by C_4 . This shows that if Top is a given topological index for which $Top(G \square H)$ is computed then it is possible to compute the $Top(R)$ and $Top(S)$ immediately from the values of $Top(P_n)$ and $Top(C_n)$.

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