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Dedicated to Professor Mircea Diudea on the Occasion of His 65th Anniversary

THE INVERSE SUM INDEG INDEX OF SOME NANOTUBES

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ABSTRACT. Discrete Adriatic indices have been defined by Vukičević and Gašperov (2010), as a way of generalizing well-known molecular descriptors defined as the sum of individual bond contributions. One of these indices is the inverse sum indeg index which is a significant predictor of total surface area of octane isomers. In this paper, exact formulas for computing the inverse sum indeg index of some nanotubes are presented.

Keywords: *ISI index, Nanotube.*

INTRODUCTION

A *molecular descriptor* (also known as *topological index*, *measure* or *graph invariant*) is any function on a graph that does not depend on a labeling of its vertices. In organic chemistry, topological indices have been found use in chemical documentation, isomer discrimination, structure-property relationships (SPR), structure-activity relationships (SAR), and pharmaceutical drug design [1,2]. Some of the most famous molecular descriptors are *bond-additive*, *i.e.*, they can be presented as the sum of edge contributions. *Discrete Adriatic indices* were defined by Vukičević and Gašperov [3] as a way of generalizing well-known bond-additive molecular descriptors. One hundred forty eight discrete Adriatic indices have been defined [3] and QSAR and QSPR studies of them have been performed [3] on the benchmark sets [4] proposed by the International Academy of Mathematical Chemistry [5]. Twenty

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of these indices have shown good predictive properties. One of these twenty indices is the *inverse sum indeg index* that was selected in [3] as a significant predictor of total surface area for octane isomers. The inverse sum indeg index $ISI(G)$ of a simple graph *G* is defined as

$$ISI(G) = \sum_{uv \in E(G)} \frac{1}{\frac{1}{d_u} + \frac{1}{d_v}} = \sum_{uv \in E(G)} \frac{d_u d_v}{d_u + d_v},$$

where $E(G)$ is the edge set of *G*; and d_u and d_v are the degrees of the vertices *u* and *v* in *G*, respectively. For more information on ISI index see [6].

A nanostructure is an object of intermediate size between molecular and microscopic structures. It is a product derived through engineering at molecular scale. The most important class of these new materials is that of carbon nanotubes. Carbon nanotubes (CNTs) are allotropes of carbon with molecular structure and tubular shape, having diameters ranging from a few nanometers and lengths up to several millimeters. Nanotubes are categorized as single-walled (SWNTs) and multi-walled (MWNTs) nanotubes. In 1991, Iijima [7] discovered carbon nanotubes as multi-walled structures. In this paper, we present exact formulas for computing the inverse sum indeg index of some well-known nanotubes such as $TUAC_6$, $TUZC_6$, $TUC_4C_8(R)$, $TUC_4C_8(S)$, $TUHC_5C_7$, $TUSC_5C_7$, $TUHAC_5C_7$, and $TUHAC_5C_6C_7$. For more information on computing topological indices of nanostructures see [8-19]. The symbols, nomenclature and some of the following figures were taken from refs. [9,10] by permission of Professor Diudea.

RESULTS AND DISCUSSION

In this section, we compute ISI index of $TUAC_6$, $TUZC_6$, $TUC_4C_8(R)$, $TUC_4C_8(S)$, $TUHC_5C_7$, $TUSC_5C_7$, $TUHAC_5C_7$, and $TUHAC_5C_6C_7$ nanotubes.

Let *G* be one of the above-mentioned nanotubes. It is easy to see that, the degree of each vertex in *G* is either 2 or 3. So, we can partition the edge set of *G* into the three sets as follows:

$$E_1(G) = \{uv \in E(G) : d_u = d_v = 2\};$$
$$E_2(G) = \{uv \in E(G) : d_u = 2, d_v = 3\};$$
$$E_3(G) = \{uv \in E(G) : d_u = d_v = 3\}.$$

Now, the ISI index of the nanotube *G* can be computed from the following formula:

$$ISI(G) = \frac{2\times 2}{2+2}|E_1(G)| + \frac{2\times 3}{2+3}|E_2(G)| + \frac{3\times 3}{3+3}|E_3(G)|$$
$$= |E_1(G)| + \frac{6}{5}|E_2(G)| + \frac{3}{2}|E_3(G)|. \quad (1)$$

Consequently, for computing the ISI index of the nanotube G, it is enough to find the cardinality of the sets $E_1(G)$, $E_2(G)$, and $E_3(G)$.

Polyhex nanotubes

A polyhex net is a trivalent covering made entirely by hexagons C_6. Two classes of polyhex nanotubes are armchair and zig-zag polyhex nanotubes.

$TUAC_6$ nanotubes

Let $G=TUAC_6(p,q)$ be an armchair polyhex nanotube, where p is the number of hexagons in each row and q is the number of rows in the molecular graph of G (see Fig. 1).

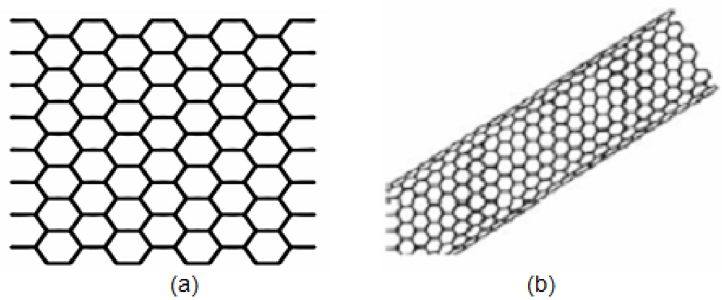

Figure 1. (a) The 2-dimensional lattice of $TUAC_6(4,8)$ nanotube, (b) $TUAC_6$ nanotube.

It is easy to see that, $|E_1(G)| = 2p$, $|E_2(G)| = 4p$, and $|E_3(G)| = 6pq - 8p$. Now using Eq. (1), we easily arrive at:

Theorem 1. The ISI index of $G=TUAC_6(p,q)$ nanotube is given by:

$$ISI(G) = 9pq - \frac{26}{5}.$$

$TUZC_6$ nanotubes

Let $G=TUZC_6(p,q)$ be a zigzag polyhex nanotube, where p is the number of hexagons in each row and q is the number of zigzag lines in the molecular graph of G (see Fig. 2).

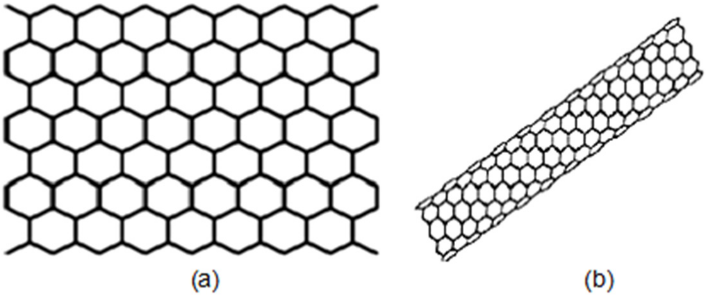

Figure 2. (a) The 2-dimensional lattice of *$TUZC_6(8,8)$* nanotube, (b) *$TUZC_6$* nanotube.

It is easy to see that, $|E_1(G)| = 0$, $|E_2(G)| = 4p$, and $|E_3(G)| = 3pq - 5p$. Now using Eq. (1), we easily arrive at:

Theorem 2. The ISI index of *$G=TUZC_6(p,q)$* nanotube is given by:

$$ISI(G) = \frac{9}{2}pq - \frac{27}{10}p\,.$$

TUC_4C_8 nanotubes

A *C_4C_8* net is a trivalent decoration constructed from alternating squares *C_4* and octagons *C_8*. Two classes of these nanotubes are *$TUC_4C_8(R)$* nanotubes and *$TUC_4C_8(S)$* nanotubes.

$TUC_4C_8(R)$ nanotubes

Let *$G=TUC_4C_8(R)$* (see Fig. 3). We denote the number of squares in each row of by *p* and the number of squares in each column by *q*.

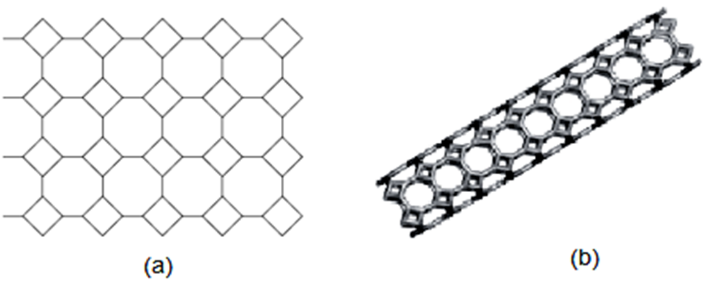

Figure 3. (a) The 2-dimensional lattice of *$TUC_4C_8(R)$* nanotube with *p*=5 and *q*=4, (b) *$TUC_4C_8(R)$* nanotube.

It is easy to see that, $|E_1(G)| = 0$, $|E_2(G)| = 4p$, and $|E_3(G)| = 6pq - 5p$. Now using Eq. (1), we easily arrive at:

Theorem 3. The ISI index of $G=TUC_4C_8(R)$ nanotube is given by:

$$ISI(G) = 9pq - \frac{27}{10}p\,.$$

$TUC_4C_8(S)$ nanotubes

Let $G=TUC_4C_8(S)$ (see Fig. 4). We denote the number of squares in each row of by p and the number of rows by q.

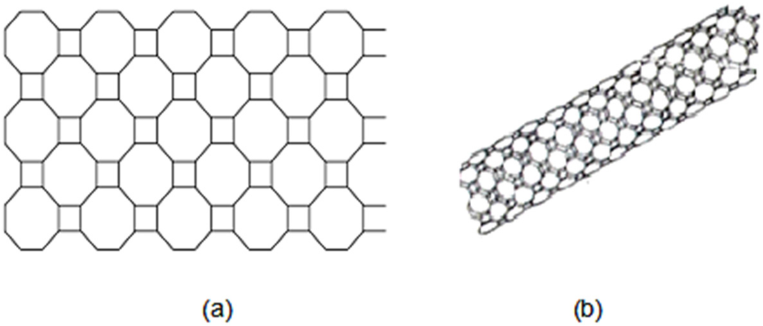

Figure 4. (a) The 2-dimensional lattice of $TUC_4C_8(S)$ nanotube with p=5 and q=6, (b) $TUC_4C_8(S)$ nanotube.

It is easy to see that, $|E_1(G)| = 2p$, $|E_2(G)| = 4p$, and $|E_3(G)| = 6pq - 8p$. Now using Eq. (1), we easily arrive at:

Theorem 4. The ISI index of $G=TUC_4C_8(S)$ nanotube is given by:

$$ISI(G) = 9pq - \frac{26}{5}p\,.$$

TUC_5C_7 nanotubes

A C_5C_7 net is a trivalent decoration constructed from alternating pentagons C_5 and heptagons C_7. Three members of these nanotubes are $TUHC_5C_7$ nanotubes, $TUSC_5C_7$ nanotubes, and $TUHAC_5C_7$ nanotubes.

$TUHC_5C_7$ nanotubes

Let $G=TUHC_5C_7(p,q)$ (see Fig. 5). We denote the number of pentagons in each row by p. In this nanotube, the four first rows of vertices and edges are repeated, alternatively. We denote the number of this repetition by q.

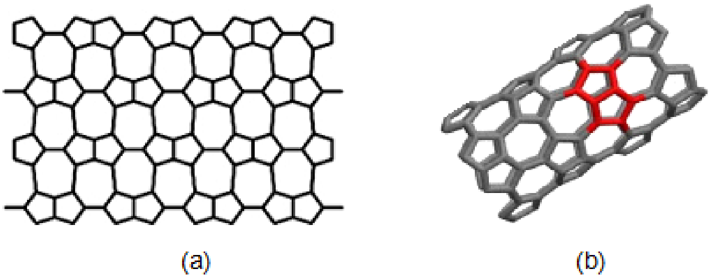

Figure 5. (a) The 2-dimensional lattice of *TUHC₅C₇(8,2)* nanotube, (b) *TUHC₅C₇* nanotube.

It is easy to see that, $|E_1(G)| = 0$, $|E_2(G)| = 4p$, and $|E_3(G)| = 12pq - 5p$. Now using Eq. (1), we easily arrive at:

Theorem 5. The ISI index of $G = TUHC_5C_7(p,q)$ nanotube is given by:

$$ISI(G) = 18pq - \frac{27}{10}p.$$

$TUSC_5C_7$ nanotubes

Let $G = TUSC_5C_7(p,q)$ (see Fig. 6). We denote the number of pentagons in each row by *p*. In this nanotube, the two first rows of vertices and edges are repeated, alternatively. We denote the number of this repetition by *q*.

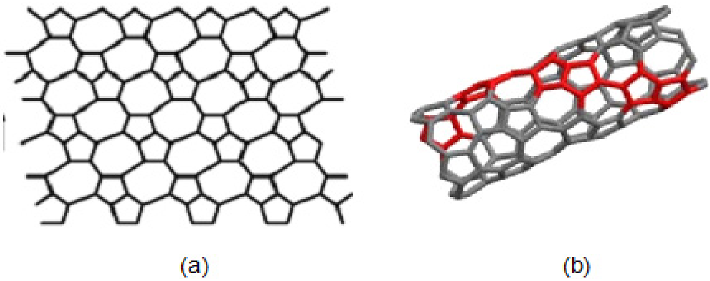

Figure 6. (a) The 2-dimensional lattice of $TUSC_5C_7(4,4)$ nanotube, (b) $TUSC_5C_7$ nanotube.

It is easy to see that, $|E_1(G)| = p$, $|E_2(G)| = 6p$, and $|E_3(G)| = 12pq - 12p$. Now using Eq. (1), we easily arrive at:

Theorem 6. The ISI index of $G = TUSC_5C_7(p,q)$ nanotube is given by:

$$ISI(G) = 18pq - \frac{49}{5}p.$$

$TUHAC_5C_7$ nanotubes

Let $G=TUHAC_5C_7(p,q)$ (see Fig. 7). We denote the number of heptagons in each row by p. In this nanotube, the three first rows of vertices and edges are repeated, alternatively. We denote the number of this repetition by q.

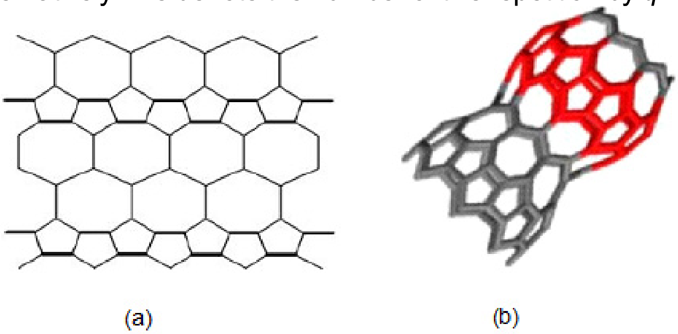

Figure 7. (a) The 2-dimensional lattice of $TUHAC_5C_7(4,2)$ nanotube, (b) $TUHAC_5C_7$ nanotube.

It is easy to see that, $|E_1(G)| = 0$, $|E_2(G)| = 4p$, and $|E_3(G)| = 12pq - 5p$. Now using Eq. (1), we easily arrive at:

Theorem 7. The ISI index of $G=TUHAC_5C_7(p,q)$ nanotube is given by:

$$ISI(G) = 18pq - \frac{27}{10}p.$$

$TUHAC_5C_6C_7$ nanotube

A $C_5C_6C_7$ net is a trivalent decoration constructed from alternating pentagons C_5, hexagons C_6, and heptagons C_7. Let $G=TUHAC_5C_6C_7(p,q)$ (see Fig. 8). We denote the number of pentagons in each row by p. In this nanotube, the three first rows of vertices and edges are repeated, alternatively. We denote the number of this repetition by q.

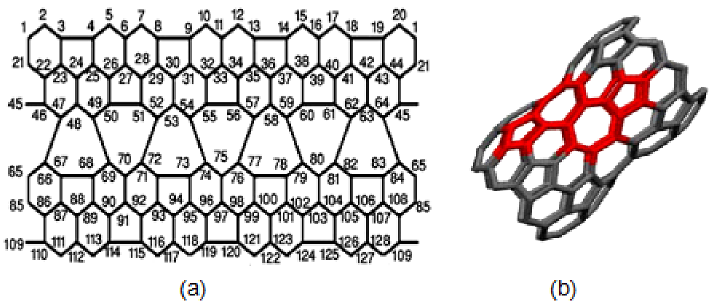

Figure 8. (a) The 2-dimensional lattice of $TUHAC_5C_6C_7(4,2)$ nanotube, (b) $TUHAC_5C_6C_7$ nanotube.

It is easy to see that, $|E_1(G)| = 0$, $|E_2(G)| = 8p$, and $|E_3(G)| = 24pq - 10p$. Now using Eq. (1), we easily arrive at:

Theorem 8. The ISI index of *G=TUHAC₅C₆C₇(p,q)* nanotube is given by:

$$ISI(G) = 36pq - \frac{27}{5}p .$$

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