Chemistry: Bulgarian Journal of Science Education
Volume 27 Number 1, 2018
Природните науки в образованието

ZAGREB CONNECTION INDICES OF TiO_2 NANOTUBES

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Abstract. The Zagreb connection indices are molecular descriptors (topological indices) which have recently been introduced by Ali & Trinajstić (2018). A novel/old modification of the first Zagreb index, *Mol. Inform.*, to appear]. This paper is devoted to establishing general expressions for calculating the Zagreb connection indices of a well-known nanostructure, namely the Titania nanotube TiO_2.

Keywords: molecular structure descriptor; Zagreb connection indices; titania nanotube

Introduction

Chemical compounds are associated with physical and chemical properties, and some of these compounds have biological activities. Actually, in the search for new antibacterial and various other medicinal drugs, pharmaceutical companies synthesize and test annually millions of new chemical compounds, characterizing in detail those compounds that show some promise (Balaban, 2013). In 2017, the number of substances registered in the *Chemical Abstracts Service* databases reached 135 million. Testing for biological activity is expensive, therefore many theoretical methods have been devised for correlating structures with biological activities or physical-chemical properties. One of the simplest such methods involves molecular structure descriptors or topological indices (Balaban, 2013; Devillers & Balaban, 1999).

Mathematical chemistry deals with the study and development of mathematical models of chemical phenomena (Basak, 2013). Chemical graph theory is one of the branches of mathematical chemistry. In this branch, graphs are used to represent chemical compounds, in which vertices correspond to the atoms while edges represent the covalent bonds between atoms (Gutman & Polansky, 1986). A numerical quantity calculated from a molecular graph is said to be a molecular structure descriptor, or more precisely, a topological index if it is invariant under graph isomorphism (Devillers & Balaban, 1999). The Wiener index is the first topological index proposed by the chemist Wiener in 1947 to model the boiling point of hydrocarbons (Todeschini & Consonni, 2009). Later on, many other topological indices were devised to predict certain physicochemical properties of chemical compounds (Kier & Lowell, 1976).

Titanium is a chemical element discovered by a German Chemist Martin Heinrich Klaproth in 1791. Its symbol is Ti. Titanium dioxide has a chemical formula TiO_2, also known as titania, which is a naturally occurring oxide of titanium.

Radushkevich & Lukyanovich (1952) discovered the carbon nanotubes. The reference (Kasaga et al., 1999) is the first publication on Titania nanotube. After then titania became a highly studied compound and up till now thousands of publications have been appeared on this compound (Roy et al., 2011).

The distance between two vertices $u, v \in V(H)$ of a (connected) molecular graph H, is the length of the shortest path joining them. The number of vertices at distance 2 from a vertex $u \in V(H)$ of a (connected) molecular graph H, is known as the connection number of uu, and it will be denoted by $\sigma(u)$ throughout this paper. Certainly, the connection number of a vertex in H must be at least is 0 and at most $n-2$.

The first Zagreb connection index ZC_1, second Zagreb connection index ZC_2 and modified first Zagreb connection index ZC_1^* for a (connected) molecular graph H are defined (Ali & Trinajstić, 2017) as:

$$ZC_1(H) = \sum_{u \in V(G)} (\sigma(u))^2,$$

$$ZC_2(H) = \sum_{uv \in E(G)} \sigma(u)\sigma(v),$$

$$ZC_1^*(H) = \sum_{uv \in E(G)} (\sigma(u) + \sigma(v)).$$

In this paper, we find general expressions for calculating the first Zagreb connection index, second Zagreb connection index,, and modified first Zagreb connection index of the Titania nanotube TiO_2 (see Fig. 1 for its chemical structure and Fig. 2 for its molecular graph).

Main results

Denote by G the molecular graph of the TiO_2–nanotube (see Figs. 1 and 2). Clearly, the connection number of any vertex of the molecular graph G of the TiO_2–nanotube is among the numbers $3,4,5,6,7,9,10$. We partition the vertex set $V(G)$ of the graph G into some disjoint sets. Let $(G) = V_3 \cup V_4 \cup V_5 \cup V_6 \cup V_7 \cup V_9 \cup V_{10}$, where $V_3 = \{u \in V(G) \mid \sigma(u) = 3\}$, $V_4 = \{u \in V(G) \mid \sigma(u) = 4\}$, $V_5 = \{u \in V(G) \mid \sigma(u) = 5\}$, $V_6 = \{u \in V(G) \mid \sigma(u) = 6\}$, $V_7 = \{u \in V(G) \mid \sigma(u) = 7\}$, $V_9 = \{u \in V(G) \mid \sigma(u) = 9\}$, $V_{10} = \{u \in V(G) \mid \sigma(u) = 10\}$. Cardinalities of these sets are given in Table 1.

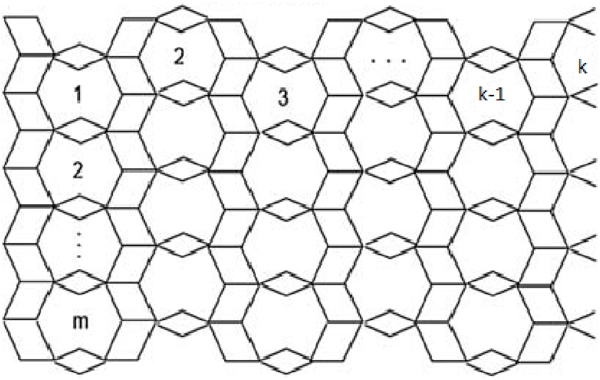

Figure 1. Chemical structure of TiO_2 $[m, k]$ –nanotube, where m denotes the number of octagons in a column and k denotes the number of octagons in a row of the Titania nanotube

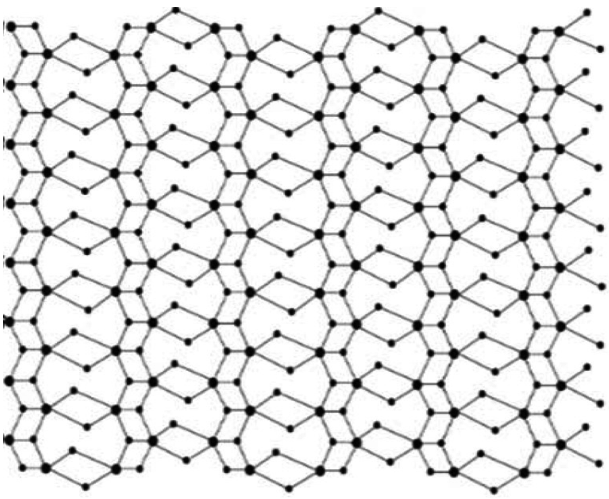

Figure 2. The molecular graph G of the TiO_2 $[m, k]$ – nanotube

Table 1. Cardinalities of the sets, which define a partition of $V(G)$

Set	Cardinality
V_3	$2k$
V_4	$2k$
V_5	$2mk$
V_6	$2k$
V_7	$2mk$
V_9	$2k$
V_{10}	$2mk - 2k$

Now, the first Zagreb connection index of G is defined as:

$$ZC_1(G) = \sum_{u \epsilon V(G)} [\sigma(u)]^2$$

This formula can be rewritten as:

$$ZC_1(G) = \sum_{u \epsilon V_3} [\sigma(u)]^2 + \sum_{u \epsilon V_4} [\sigma(u)]^2 + \sum_{u \epsilon V_5} [\sigma(u)]^2$$
$$+ \sum_{u \epsilon V_6} [\sigma(u)]^2 + \sum_{u \epsilon V_7} [\sigma(u)]^2$$
$$+ \sum_{u \epsilon V_9} [\sigma(u)]^2 + \sum_{u \epsilon V_{10}} [\sigma(u)]^2$$

$$ZC_1(G) = 9|V_3| + 16|V_4| + 25|V_5| + 36|V_6| + 49|V_7| + 81|V_9| + 100|V_{10}|$$

Substituting the values from Table 1, we get

$$ZC_1(G) = 348mk + 84k.$$

If we denote the number of vertices of a (connected) graph H having connection number i by $y_i(H)$, and φ_i is any non-negative real valued function depending on i, then we can define a more general atom's connection-number-based topological index:

$$ACN(H) = \sum_{0 \le i \le n-2} y_i(H) \cdot \varphi_i$$

where *n* is the total number of vertices in the graph *H*. For the molecular graph G of the TiO_2 $[m,k]$ – nanotube, we have

$$ACN(H) = 2k[\varphi_3 + \varphi_4 + \varphi_6 + \varphi_9 - \varphi_{10}] + 2mk[\varphi_5 + \varphi_7 + \varphi_{10}] \quad (1)$$

If we take $\varphi_i = i^2$, then Eq. (1) gives

$$ZC_1(G) = 2k[3^2 + 4^2 + 6^2 + 9^2 - 10^2] + 2mk[5^2 + 7^2 + 10^2]$$
$$+2mk[5^2 + 7^2 + 10^2] \; = 84k + 348mk = 84k + 348mk$$

Now, we calculate other two Zagreb connection indices of the molecular graph G of the TiO_2 $[m,k]$ – nanotube. For this, we partition the edge set $E(G)$ into some disjoint sets. Let us take

$$E_q = \{e = uv \in E(G)\, |\sigma(u) + \sigma(v) = q\}$$

and

$$E_s^* = \{e = uv \in E(G)\, |\sigma(u).\sigma(v) = s\}$$

Or more precisely,

$$E_8 = E_{15}^* = \{e = uv \in E(G) \mid \sigma(u) = 3, \sigma(u) = 5\}$$

$$E_9 = E_{18}^* = \{e = uv \in E(G) \mid \sigma(u) = 3, \sigma(u) = 6\}$$

$$E_{10} = E_{24}^* = \{e = uv \in E(G) \mid \sigma(u) = 4, \sigma(u) = 6\}$$

$$E_{11} = E_{28}^* = \{e = uv \in E(G) \mid \sigma(u) = 4, \sigma(u) = 7\}$$

$$E_{12} = E_{27}^* = \{e = uv \in E(G) \mid \sigma(u) = 3, \sigma(u) = 9\}$$

$$E_{12} = E_{35}^* = \{e = uv \in E(G) \mid \sigma(u) = 5, \sigma(u) = 7\}$$

$$E_{13} = E_{36}^* = \{e = uv \in E(G) \mid \sigma(u) = 4, \sigma(u) = 9\}$$

$$E_{14} = E_{40}^* = \{e = uv \in E(G) \mid \sigma(u) = 4, \sigma(u) = 10\}$$

$$E_{14} = E_{45}^* = \{e = uv \in E(G) \mid \sigma(u) = 5, \sigma(u) = 9\}$$

$$E_{15} = E_{50}^* = \{e = uv \in E(G) \mid \sigma(u) = 5, \sigma(u) = 10\}$$

Cardinalities of these sets are given in Table 2.

Table 2. The sets which define a partition of $E(G)$

Set		Cardinality
E_8	$E_{15}{}^*$	$4k$
E_9	$E_{18}{}^*$	$2k$
E_{10}	$E_{24}{}^*$	$2k$
E_{11}	$E_{28}{}^*$	$4k$
E_{12}	$E_{27}{}^*$	$2k$
	$E_{35}{}^*$	$4mk - 4k$
E_{13}	$E_{36}{}^*$	$2k$
E_{14}	$E_{40}{}^*$	$2k$
	$E_{45}{}^*$	$2k$
E_{15}	$E_{50}{}^*$	$6mk - 8k$

For the Table 2, we remark that

$$|E_{12}| = |E_{27}{}^* \cup E_{35}{}^*| = 4mk - 2k$$

and

$$|E_{14}| = |E_{40}{}^* \cup E_{45}{}^*| = 4k$$

It is clear that

$$E(G) = E_8 \cup E_9 \cup E_{10} \cup E_{11} \cup E_{12} \cup E_{13} \cup E_{14} \cup E_{15}.$$

By using the definition of the modified first Zagreb connection index and using Table 2, we have

$$ZC_1^*(G) = 138mk + 52k$$

Also, we have

$$E(G) = E_{15}{}^* \cup E_{18}{}^* \cup E_{24}{}^* \cup E_{27}{}^* \cup E_{28}{}^* \cup E_{35}{}^* \cup E_{36}{}^* \cup E_{40}{}^* \cup E_{45}{}^* \cup E_{50}{}^*$$

By using the definition of the second Zagreb connection index and using Table 2, we have

$$ZC_2(G) = 440mk + 12k.$$

Following (Ali & Trinajstić, 2018), denote by $y_{i,j}(H)$ the number of those edges of a (connected) graph H which connect the vertices having connection numbers i, j, and denote by $\varphi_{i,j}\varphi_{i,j}$ any non-negative real valued function depending on , then bond incident connection-number (BIC) indices are defined as

$$BIC(H) = \sum_{0 \le i,j \le n-2} y_{i,j}(G) \cdot \varphi_{i,j}$$

For the molecular graph G of the $TiO_2\ [m,k]$ – nanotube, we have

$$BIC(G) = 2k\left[2\varphi_{3,5} + \varphi_{3,6} + \varphi_{4,6} + \varphi_{3,9} + 2\varphi_{4,7} - 2\varphi_{5,7} + \varphi_{4,9} + \varphi_{4,10} + \varphi_{5,9} - 4\varphi_{5,10}\right] + 2mk\left[2\varphi_{5,7} + 3\varphi_{5,10}\right].$$

The above general expression can also be used to find the modified first Zagreb connection index and second Zagreb connection index of the molecular graph G of the TiO_2–nanotube.

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