American Journal of Chemical Engineering
2017; 5(6): 163-168
http://www.sciencepublishinggroup.com/j/ajche
doi: 10.11648/j.ajche.20170506.18
ISSN: 2330-8605 (Print); ISSN: 2330-8613 (Online)

On *ve*-Degree and *ev*-Degree Zagreb Indices of Titania Nanotubes

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To cite this article:
Murat Cancan, Mehmet Şerif Aldemir. On *ve*-Degree and *ev*-Degree Zagreb Indices of Titania Nanotubes. *American Journal of Chemical Engineering*. Vol. 5, No. 6, 2017, pp. 163-168. doi: 10.11648/j.ajche.20170506.18

Received: July 18, 2017; **Accepted**: October 13, 2017; **Published**: November 30, 2017

Abstract: Titania nanotubes are among the most investigated nanomaterials relating to their common applications in the manufacturing of corrosion-resistant, gas sensing and catalytic molecules. Topological indices which are graph invariants derived from molecular graphs of molecules are used in QSPR researches for modelling physicochemical properties of molecules. Topological indices are important tools for determining the underlying topology of a molecule in view of theoretical chemistry. Most of the topological indices are defined by using classical degree concept of graph theory. Recently two novel degree concepts have been defined in graph theory: *ve*-degrees and *ev*-degrees. By using both novel graph invariants, as parallel to their classical degree versions, the *ev*-degree Zagreb index, the *ve*-degree Zagreb indices and the *ve*-degree Randić index have been defined very recently. In this study the *ev*-degree Zagreb index, the *ve*-degree Zagreb indices and the *ve*-degree Randić index of titania nanotubes were computed.

Keywords: *ev*-Degree Zagreb Index, *ve*-Degree Randić Index, *ve*-Degree Zagreb Indices, QSPR Researches, Titania Nanotubes

1. Introduction

Graph theory which is one of the most important branch of applied mathematics and chemistry has many applications from the basic sciences to the engineering sciences especially for solving and modelling of real-world problems. Chemical graph theory is the common place for graph theory and chemistry. Topological indices are indispensable tools for QSPR researches in view of theoretical chemistry and chemical graph theory. Topological indices have been used more than seventy years predicting and modelling physicochemical properties of chemical substances.

A graph $G=(V,E)$ consists of two nonempty sets V and 2-element subsets of V namely E. The elements of V are called vertices and the elements of E are called edges. For a vertex v, $\deg(v)$ show the number of edges that incident to v. The set of all vertices which adjacent to v is called the open neighborhood of v and denoted by $N(v)$. If the vertex v is added to $N(v)$, then the closed neighborhood of v, $N[v]$ is got. For the vertices u and v, $d(u,v)$ denotes the distance between u and v which means that minimum number of edges between u and v.

The first distance based topological index is the Wiener index which was defined by H. Wiener to modelling the boiling points of paraffin molecules [1]. Wiener, computed all distances between all atoms (vertices) in the molecular graph of paraffin molecules and named this graph invariant as "path number". The Wiener index of a simple connected graph G defined as follows;

$$W = W(G) = \sum_{\{u,v\}\subseteq V(G)} d(u,v) \quad (1)$$

Many years later the path number renamed as "Wiener index" to honor Professor Harold Wiener for valuable contribution to mathematical chemistry. In the same year, the first degree based topological index was proposed by Platt for modeling physical properties of alcanes [2]. The Platt index of a simple connected graph G defined as follows;

$$I_{Pl} = I_{Pl}(G) = \sum_{uv\in E(G)} [\deg(u) + \deg(v) - 2] \quad (2)$$

After these both studies, approximately twenty five years later the well-known degree based Zagreb indices were defined by Gutman and Trinijastić to modelling π-electron energy of alternant carbons [3]. The first Zagreb index of a simple connected graph defined as;

$$M_1 = M_1(G) = \sum_{v \in V(G)} \deg(v)^2 \quad (3)$$

And the second Zagreb index of a simple connected graph defined as;

$$M_2 = M_2(G) = \sum_{uv \in E(G)} \deg(u) \deg(v) \quad (4)$$

An alternative definition of the second Zagreb index of a simple connected graph is given the following formula;

$$M_2 = M_2(G) = \sum_{uv \in E(G)} (\deg(u) + \deg(v)) \quad (5)$$

In 1975, Randić defined the "Randić index" [4] to modelling molecular branching of carbon skeleton atoms as follows;

$$R = R(G) = \sum_{uv \in E(G)} (\deg(u) . \deg(v))^{-1/2} \quad (6)$$

Among the all topological indices, the above mentioned topological indices have been used for QSPR researches more considerably than any other topological indices in chemical and mathematical literature. The interested reader are referred to the following citations for up to date information about these well-known and the most used topological indices [5], [6], [7], [8], [9], [10], [11], [12], [13], [14], [15].

Titania nanotubes which have been produced fifteen years ago have many applications on the very broad of science from medicine to electronics [16], [17], [18], [19], [20]. Computing certain topological indices of titania nanotubes have been started recently. Since 2015, there are many studies to compute the exact value of some topological indices of titania nanotubes [21], [22], [23], [24], [25], [26], [27], [28], [29].

Recently two new degree definitions in graph theory have been given by Chellali *et al* [30]. The authors of [30] found the close relationship between the first Zagreb index and the total *ev*-degrees (*ve*-degrees). It was suggested in [30] that these novel degree concepts may be used to define novel degree based topological indices. Following this suggestion, *ev*-degree and *ve*-degree topological indices have been defined in [31], [32], [33], [34]. These novel *ev*-degree and *ve*-degree topological indices have been showed that give considerably good correlations to predict some physicochemical properties of octane molecules than well-known and above mentioned topological indices; Wiener, Zagreb and Randić indices.

The aim of this paper is to compute the exact values of *ev*-degree and *ve*-degree topological indices of titania nanotubes.

2. Results and Discussions

In this section, the definitions of *ev*-degree and *ve*-degree concepts which were given by Chellali *et al.* in [30] and the definitions and properties of ev-degree and ve-degree topological indices which were given in [31] are introduced. After that, ev-degree and ve-degree topological indices of titania nanotubes are computed.

Definition 1. [30] Let G be a connected graph and $v \in V(G)$. The ve-degree of the vertex v, $deg_{ve}(v)$, equals the number of different edges that incident to any vertex from the closed neighborhood of v. For convenience, the ve-degree of the vertex v are showed, by c_v.

Definition 2. [30] Let G be a connected graph and $e = uv \in E(G)$. The ev-degree of the edge e, $deg_{ev}(e)$, equals the number of vertices of the union of the closed neighborhoods of u and v. For convenience the ev-degree of the edge $e = uv$ by are showed by c_e or c_{uv}.

Observation 3. [30] For any connected graph G,

$$c_e = c_{uv} = \deg(u) + \deg(v) - n_e. \quad (7)$$

Where n_e denotes the number of triangles contain the edge *e*.

Lemma 4. [31] Let G be a connected graph and $v \in V(G)$, then;

$$c_v = \sum_{u \in N(v)} \deg(u) - n_v. \quad (8)$$

Where n_v denotes the number of triangles contain the vertex *v*.

Definition 5. [30] Let G be a connected graph and $v \in V(G)$. The total *ev*-degree of the graph G is defined as;

$$T_e = T_e(G) = \sum_{e \in E(G)} c_e. \quad (9)$$

And the total *ve*-degree of the graph G is defined as;

$$T_v = T_v(G) = \sum_{v \in V(G)} c_v. \quad (10)$$

Observation 6. [30] For any connected graph G,

$$T_e(G) = T_v(G). \quad (11)$$

The following theorem states the relationship between the first Zagreb index and the total *ve*-degree of a connected graph G.

Theorem 7. [30] For any connected graph G,

$$T_e(G) = T_v(G) = M_1(G) - 3n(G). \quad (12)$$

where $n(G)$ denotes the total number of triangles in G.

Definition 8. [31] Let G be a connected graph and $e \in E(G)$. The *ev*-degree Zagreb index of the graph G is defined as;

$$S = S(G) = \sum_{e \in E(G)} c_e^2. \quad (13)$$

Definition 9. [31] Let G be a connected graph and $v \in V(G)$. The first *ve*-degree Zagreb alpha index of the graph G is defined as;

$$S^\alpha = S^\alpha(G) = \sum_{v \in V(G)} c_v^2. \quad (14)$$

Definition 10. [31] Let G be a connected graph and

$uv \in E(G)$. The first *ve*-degree Zagreb beta index of the graph G is defined as;

$$S^{\beta} = S^{\beta}(G) = \sum_{uv \in E(G)} (c_u + c_v). \quad (15)$$

Definition 11. [31] Let G be a connected graph and $uv \in E(G)$. The second *ve*-degree Zagreb index of the graph G is defined as;

$$S^{\mu} = S^{\mu}(G) = \sum_{uv \in E(G)} c_u c_v. \quad (16)$$

Definition 12. [31] Let G be a connected graph and $uv \in E(G)$. The *ve*-degree Randić index of the graph G is defined as;

$$R^{\alpha}(G) = \sum_{uv \in E(G)} (c_u c_v)^{-1/2}. \quad (17)$$

And now, to compute the *ev*-degree and *ve*-degree Zagreb indices of titania nanotubes are given. The following Figure 1, the molecular graph of titania nanotubes are given.

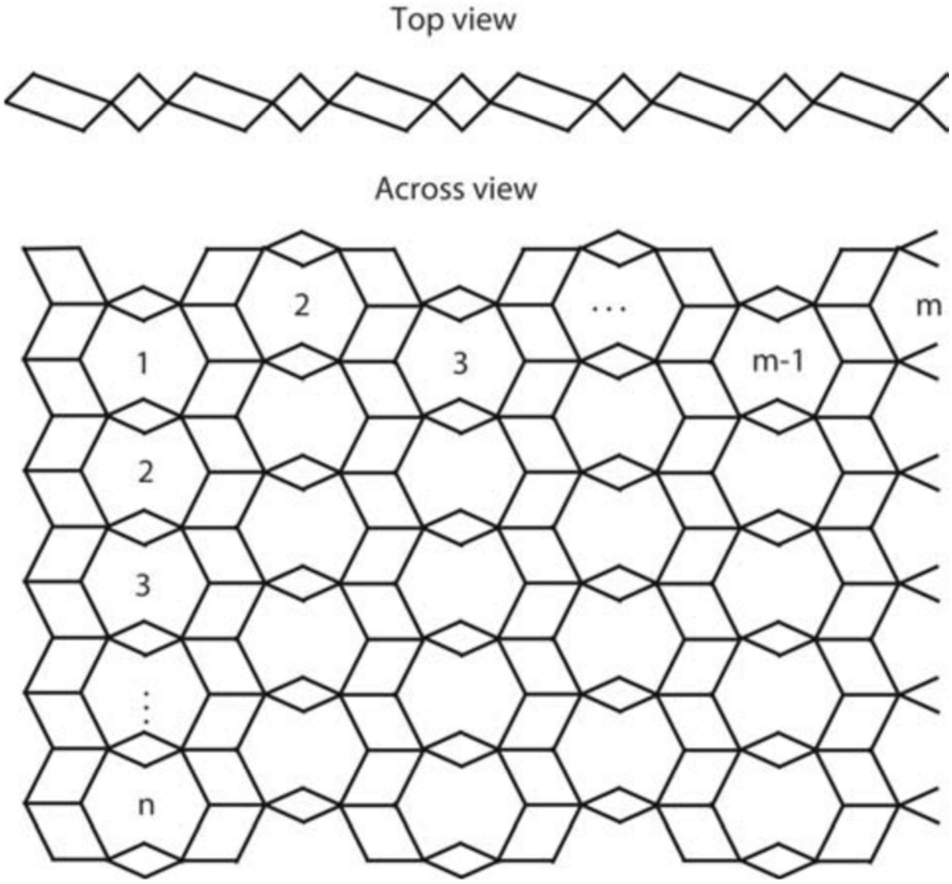

Figure 1. *The Molecular Graph of Titania Nanotubes.*

It is preferred to show titania nanotubes as TiO_2 $[m, n]$ where *m, n* denote the number of octagons in a row and in a column, respectively. Note that any vertex and edge of titania does not lie in any triangle. From this fact it is got that;

$$c_v = \sum_{u \in N(v)} \deg(u) \quad (18)$$

$$c_e = c_{uv} = \deg(u) + \deg(v) \quad (19)$$

for any vertex and any edge of titania respectively.

From the Figure 1, it is got the following Table 1 which give the classification of edges in relation to their *ev*-degrees.

Table 1. *ev-Degree Classification of the Edges of Titania Nanotubes.*

Edges *e=uv*	Number of edges	*ev*-degrees $c_e = c_{uv}$
deg(u)=2 and deg(v)=4	6n	6
deg(u)=2 and deg(v)=5	4mn+2n	7
deg(u)=3 and deg(v)=4	2n	7
deg(u)=3 and deg(v)=5	6mn-2n	8

From the Figure 1, it is got the following Table 2 which give the classification of vertices (atoms) in relation to their *ve*-degrees.

Table 2. *ve-Degree Classification of the Vertices of Titania Nanotubes.*

Degrees deg(v)	Number of vertex	*ve*-degrees c_v
deg(v)=2	2mn+4n-8m	10
deg(v)=2	4m	9
deg(v)=2	4m	8
deg(v)=3	2mn-2m	15
deg(v)=3	2m	14
deg(v)=4	2n	9
deg(v)=5	2m	12
deg(v)=5	2mn-2m	13

From the Figure 1, it is got the following Table 3 which gives the classification of edges in relation to their *ve*-degrees of end vertices.

Table 3. *The Classification of Edges in Relation to Their ve-Degrees of End Vertices.*

(c_u, c_v) for e=uv	The number of edges	(c_u, c_v) for e=uv	The number of edges
(8, 9)	$4n$	(10, 13)	$4mn-4n$
(9, 9)	$2n$	(12, 14)	$2n$
(9, 12)	$2n$	(12, 15)	$2n$
(9, 14)	$2n$	(13, 14)	$2n$
(10, 12)	$4n$	(13, 15)	$6mn-8n$

Theorem 7. Let G be a molecular graph of titania nanotubes TiO_2 [m, n]. Then the *ev*-degree Zagreb index of G equals;

$$S(G) = 580mn + 284n.$$

Proof. From Equation 13 and Table 1, it can be directly wrote that;

$$S = S(G) = \sum_{e \in E(G)} c_e^2 = 36.6n + 49(4mn + 2n) + 49.2n + 64.(6mn - 2n) = 580mn + 284.$$

Theorem 8. Let G be a molecular graph of titania nanotubes TiO_2 [m, n]. Then the first *ve*-degree Zagreb alpha index of G equals;

$$S^{\alpha}(G) = 1018mn - 398m + 562n.$$

Proof. From Equation 14 and Table 2 it can be directly wrote that;

$$S^{\alpha} = S^{\alpha}(G) = \sum_{v \in V(G)} c_v^2 = 100.(2mn + 4n - 8m) + 81.4\mathrm{m} + 64.4\mathrm{m} + 225.(2\mathrm{mn} - 2\mathrm{m})$$

$$+196.2m + 81.2n + 144.2m + 169.(2mn - 2m)$$

$$= 200mn + 400n - 800m + 324m + 256m + 450mn - 450m + 392m + 162n + 288m + 368mn - 368m$$

$$= 1018mn - 398m + 562n.$$

Theorem 9. Let G be a molecular graph of titania nanotubes TiO_2 [m, n]. Then the first *ve*-degree Zagreb beta index of G equals;

$$S^{\beta}(G) = 1018mn - 398m + 562n.$$

Proof. From Equation 15 and Table 3, it can be directly wrote that;

$$S^{\beta} = S^{\beta}(G) = \sum_{uv \in E(G)} (c_u + c_v) = 17.4n + 18.2n + 21.2n + 23.2n + 22.4n + 23.(4mn - 4n) + 26.2n + 27.2n + 27.2n + 28.(6mn - 8n)$$

$$= 68n + 36n + 42n + 46n + 88n + 92mn - 92n + 52n + 54n + 54n + 168mn - 224n$$

$$= 260mn + 124n.$$

Theorem 10. Let G be a molecular graph of titania nanotubes TiO_2 [m, n]. Then the second *ve*-degree Zagreb index of G equals;

$$S^{\beta}(G) = 1018mn - 398m + 562n.$$

Proof. From Equation 16 and Table 3, it can be directly wrote that;

$$S^{\mu} = S^{\mu}(G) = \sum_{uv \in E(G)} c_u c_v = 72.4n + 81.2n + 108.2n + 126.2n + 120.4n + 130.(4mn - 4n)$$

$$+168.2n + 180.2n + 182.2n + 195.(6mn - 8n)$$

$$= 288n + 162n + 216n + 252n + 480n + 520mn - 520n + 336n + 360n + 364n + 1170mn - 1560n$$

$$= 1690mn + 378n.$$

Theorem 11. Let G be a molecular graph of titania nanotubes TiO_2 [m, n]. Then the *ve*-degree Randić index of the graph G equals;

$$R^{\alpha}(G) = \frac{6mn}{\sqrt{195}} + \frac{4mn}{\sqrt{130}} + \frac{2n}{9} + \frac{2n}{3\sqrt{2}} + \frac{n}{3\sqrt{3}} + \frac{2n}{3\sqrt{14}} + \frac{2n}{\sqrt{30}} + \frac{n}{\sqrt{42}} + \frac{2n}{6\sqrt{5}} + \frac{2n}{\sqrt{182}} - \frac{4n}{\sqrt{130}} - \frac{8n}{\sqrt{195}}$$

Proof. From Equation 17 and Table 3 it can be directly wrote that;

$$R^{\alpha}=R^{\alpha}(G)=\sum_{uv\in E(G)}(c_u c_v)^{-1/2}=\frac{4n}{\sqrt{72}}+\frac{2n}{\sqrt{81}}+\frac{2n}{\sqrt{108}}+\frac{2n}{\sqrt{126}}+\frac{4n}{\sqrt{120}}+\frac{4mn-4n}{\sqrt{130}}+\frac{2n}{\sqrt{168}}+\frac{2n}{\sqrt{180}}+\frac{2n}{\sqrt{182}}+\frac{6mn-8n}{\sqrt{195}}$$

$$=\frac{4n}{6\sqrt{2}}+\frac{2n}{9}+\frac{2n}{6\sqrt{3}}+\frac{2n}{3\sqrt{14}}+\frac{4n}{2\sqrt{30}}+\frac{4mn-4n}{\sqrt{130}}+\frac{2n}{2\sqrt{42}}+\frac{2n}{6\sqrt{5}}+\frac{2n}{\sqrt{182}}+\frac{6mn-8n}{\sqrt{195}}$$

$$=\frac{6mn}{\sqrt{195}}+\frac{4mn}{\sqrt{130}}+\frac{2n}{9}+\frac{2n}{3\sqrt{2}}+\frac{n}{3\sqrt{3}}+\frac{2n}{3\sqrt{14}}+\frac{2n}{\sqrt{30}}+\frac{n}{\sqrt{42}}+\frac{2n}{6\sqrt{5}}+\frac{2n}{\sqrt{182}}-\frac{4n}{\sqrt{130}}-\frac{8n}{\sqrt{195}}$$

3. Conclusions

In this study, the exact values of newly defined *ev*-degree and *ve*-degree topological indices of titania nanotubes were computed. This calculation will help to predict and model some physicochemical, optical and biological properties of titania nanotubes. It can be interesting to compute the *ev*-degree and *ve*-degree topological indices of some other nanotubes and networks for further studies.

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