Research Article

On Molecular Topological Properties of TiO$_2$ Nanotubes

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Titania nanotube is a well-known semiconductor and has numerous technological applications. In chemical graph theory, topological indices provide an important tool to quantify the molecular structure and it is found that there is a strong correlation between the properties of chemical compounds and their molecular structure. Among different topological indices, degree-based topological indices are most studied and have some important applications. In this study, several old and new degree-based topological indices have been investigated for titania TiO$_2$ nanotubes.

1. Introduction

Chemical graph theory is an important branch of mathematical chemistry where we model the chemical phenomenon using graph theory. In chemical graph theory molecules are represented by a molecular graph, which is an unweighted, undirected graph without self-loop or multiple edges such that its vertices correspond to atoms and edges to the bonds between them. A topological index is a numeric quantity which is derived from a molecular graph and it does not depend on labeling or pictorial representation of a graph. It is found that there exist strong connections between the chemical characteristics of chemical compounds and drugs and their topological indices. Topological indices are used for studying quantitative structure-activity relationship (QSAR) and quantitative structure-property relationship (QSPR) for predicting different properties of chemical compounds and biological activities in chemistry, biochemistry, and nanotechnology.

Among different topological indices, degree-based topological indices are most studied and have some important applications in chemical graph theory. The first and second Zagreb indices were first introduced by Gutman and Trinajstić in 1972 [1] and it was reported that these indices are useful in anti-inflammatory activities study of certain chemicals.

Suppose $G$ is a simple connected graph. Let $V(G)$ and $E(G)$, respectively, denote the vertex set and edge set of $G$ and $n$ and $m$, respectively, denote the number of vertices and edges of $G$. Let, for any vertex $v \in V(G)$, $d_G(v)$ denote its degree, that is, the number of edges incident with that vertex. Thus, if $N(v)$ denotes the set of vertices which are the neighbors of the vertex $v$, then $|N(v)| = d_G(v)$. The first and second Zagreb indices of a graph are denoted by $M_1(G)$ and $M_2(G)$ and are, respectively, defined as

\[ M_1(G) = \sum_{v \in V(G)} d_G(v)^2 = \sum_{uv \in E(G)} [d_G(u) + d_G(v)], \]

\[ M_2(G) = \sum_{uv \in E(G)} d_G(u) d_G(v). \]  

(1)

These indices are one of the oldest and extensively studied topological indices in both mathematical and chemical literature; for details interested readers are referred to [2–7].

The $F$-index of a graph is defined as the sum of cubes of the vertex degrees of the graph which was introduced in 1972, in the same paper where the first and second Zagreb indices were introduced to study the structure-dependency of total $\pi$-electron energy. But this topological index was not further studied till then. Very recently, Furtula and Gutman [8] reinvestigated the index and named it “forgotten topological index” or “$F$-index.” Very recently the present authors studied this index for different graph operations [9] and also introduced its coindex version in [10]. In [11] Abdoa...
et al. investigate the trees extremal with respect to the $F$-index. Thus the $F$-index of a graph is defined as

$$F(G) = \sum_{u,v \in E(G)} [d_G(u)^2 + d_G(v)^2].$$  \hspace{1cm} (2)

Albertson in [12] defined another degree-based topological index called irregularity of $G$ as

$$iir(G) = \sum_{e=v \in E(G)} |d_G(u) - d_G(v)|.$$ \hspace{1cm} (3)

Tavakoli et al. in [13] found some new results on irregularity of graphs. In [14], De et al. derived irregularity of some composite graphs. Abdo and Dimitrov in [15] determined irregularity of graphs under different graph operations.

Miličević et al. [16] reformulated the Zagreb indices in terms of edge degrees instead of vertex degrees, where the degree of an edge $e = uv$ is defined as $d(e) = d(u) + d(v) - 2$, so the reformulated first and second Zagreb indices of a graph $G$ are defined as

$$EM_1(G) = \sum_{e \in E(G)} d(e)^2,$$ \hspace{1cm} (4)

$$EM_2(G) = \sum_{e \neq f} d(e)d(f).$$ \hspace{1cm} (5)

Here $e \sim f$ means that the edges $e$ and $f$ share a common vertex in $G$; that is, they are adjacent. These reformulated Zagreb indices are subject to large number of chemical and mathematical studies. Different properties of reformulated Zagreb indices have been studied in [17, 18]. In [19], bounds for the reformulated first Zagreb index of graphs with connectivity at most $k$ are obtained. De [20] found some upper and lower bounds of these indices in terms of some other graph invariants and also derived reformulated Zagreb indices of a class of dendrimers [21]. Ji et al. [22, 23] computed these indices for acyclic, unicyclic, bicyclic, and tricyclic graphs.

Recently, Shirdel et al. [24] investigate reformed first Zagreb index of some graph operations.

Recently, Shirdel et al. [25] introduced a new version of Zagreb index and named it as hyper-Zagreb index, which is defined as

$$HM(G) = \sum_{u,v \in E(G)} [d(u) + d(v)]^2.$$ \hspace{1cm} (6)

For different recent study of these indices, see [26–28].

During the last two decades, titania nanotubes were systematically synthesized using different methods. Since titania nanotubes are widely used in different applied fields, the study of titania nanotubes has received attention in both chemical and mathematical literature (see [29–31]). Though the study of molecular topological properties of titania nanotubes has been largely limited, we have been attracted to studying molecular topological properties of titania nanotubes. Recently, Malik and Imran [32] studied the Zagreb indices and Nadeem and Shaker [33] studied the eccentric connectivity index of an infinite class of titania nanotubes.

In this paper, we study some old and new degree-based topological indices such as $F$-index, reformulated first Zagreb index, third Zagreb index, and hyper-Zagreb index of this type of nanotubes.

### 2. Main Results

The molecular graph of $\text{TiO}_2[m,n]$ has total $2n + 2m$ rows and $m$ columns and is presented in Figure 1. For $\text{TiO}_2$ nanotubes $2 \leq d(v) \leq 5$, for all $v \in V(\text{TiO}_2)$. We denote the partitions of the vertex set of $\text{TiO}_2$ by $V_i(\text{TiO}_2)$, where $v \in V(\text{TiO}_2)$ if $d(v) = i$. Thus we have the following partitions of the vertex set:

$$V_2(\text{TiO}_2) = \{v \in V(\text{TiO}_2) : d(u) = 2\},$$

$$V_3(\text{TiO}_2) = \{v \in V(\text{TiO}_2) : d(u) = 3\},$$

$$V_4(\text{TiO}_2) = \{v \in V(\text{TiO}_2) : d(u) = 4\},$$

$$V_5(\text{TiO}_2) = \{v \in V(\text{TiO}_2) : d(u) = 5\}.$$ \hspace{1cm} (7)

From direct calculation we get $|V_2(\text{TiO}_2)| = 2mn + 4n$, $|V_3(\text{TiO}_2)| = 2mn$, $|V_4(\text{TiO}_2)| = 2n$, and $|V_5(\text{TiO}_2)| = 2mn$. 

Figure 1: The molecular graph of $\text{TiO}_2[m,n]$ for $m = 4$ and $n = 6$. 

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Top image

Cross section of image

1 2
2
n
n=1 n=2 n=3 n=4 n=5 ... }.

(7) From direct calculation we get $|V_2(\text{TiO}_2)| = 2mn + 4n$, $|V_3(\text{TiO}_2)| = 2mn$, $|V_4(\text{TiO}_2)| = 2n$, and $|V_5(\text{TiO}_2)| = 2mn$.
The vertex partition of TiO$_2$ nanotubes is given in Table 1.

| Vertex partition | $V_2$ | $V_3$ | $V_4$ | $V_5$ |
|------------------|-------|-------|-------|-------|
| Cardinality      | $2mn + 4n$ | $2mn$ | $2n$ | $2mn$ |

The edge partition of TiO$_2$ nanotubes is given in Table 2.

| Edge partition | $E_6$ | $E_7$ | $E_8$ | $E_{15}$ | $E_{10}$ | $E_{12}$ |
|----------------|-------|-------|-------|----------|----------|----------|
| Cardinality    | $6n$  | $4mn + 4n$ | $6mn - 2n$ | $4mn + 2n$ | $2n$ |

In the following we calculate the $F$-index, first reformulated Zagreb index, irregularity, and hyper-Zagreb index of the TiO$_2$[m,n] nanotube as defined in the previous section.

**Theorem 1.** The $F$-index of TiO$_2$[m,n] nanotube is given by

$$F(TiO_2) = 320mn + 160n.$$ (10)

**Proof.** From (2) and by cardinalities of the edge partitions of TiO$_2$ nanotube, we have

$$F(TiO_2) = \sum_{v \in V(TiO_2)} d(v)^3$$

$$= \sum_{v \in V_2} d(v)^3 + \sum_{v \in V_3} d(v)^3 + \sum_{v \in V_4} d(v)^3$$

$$+ \sum_{v \in V_5} d(v)^3$$

$$= 8 |V_2| + 27 |V_3| + 64 |V_4| + 125 |V_5|$$

$$= 8 (2mn + 4n) + 27 (2mn) + 64 (2n) + 125 (2n)$$

from where the desired result follows. \hfill \Box

**Theorem 2.** The third Zagreb index or irregularity of TiO$_2$[m,n] nanotube is given by

$$\text{irr}(TiO_2) = 316mn + 124n.$$ (12)

**Proof.** From (3) and by cardinalities of the edge partitions of TiO$_2$ nanotube, we have

$$\text{irr}(TiO_2) = \sum_{uv \in E(TiO_2)} |d(u) - d(v)|$$

$$= \sum_{uv \in E_2} |d(u) - d(v)| + \sum_{uv \in E_{10}} |d(u) - d(v)|$$

$$+ \sum_{uv \in E_{12}} |d(u) - d(v)|$$

$$= 2 |E_8^*| + 3 |E_{10}^*| + |E_{12}^*| + 2 |E_{15}^*|$$

$$= 2 (6n) + 3 (4mn + 2n) + 2n$$

$$+ 2 (6mn - 2n)$$

from where the desired result follows. \hfill \Box

**Theorem 3.** The reformulated first Zagreb index of TiO$_2$[m,n] nanotube is given by

$$EM_1(TiO_2) = 316mn + 124n.$$ (14)
Proof. From (4) and by cardinalities of the edge partitions of TiO$_2$ nanotube, we have

$$EM_1(TiO_2) = \sum_{uv \in E_1} [d(u) + d(v) - 2]^2$$

$$= \sum_{uv \in E_1} [d(u) + d(v) - 2]^2$$

$$+ \sum_{uv \in E_2} [d(u) + d(v) - 2]^2$$

$$+ \sum_{uv \in E_3} [d(u) + d(v) - 2]^2$$

$$= 16 |E_1| + 36 |E_3|$$

$$= 16(6n) + 36(4mn + 4n)$$

$$+ 36(6mn - 2n)$$

from where the desired result follows.

Theorem 4. The hyper-Zagreb index of TiO$_2$[$m,n$] nanotube is given by

$$HM(TiO_2) = 580mn + 284n.$$

Proof. From (6) and by cardinalities of the edge partitions of TiO$_2$ nanotube, we have

$$HM(TiO_2) = \sum_{uv \in E} [d(u) + d(v)]^2$$

$$= \sum_{uv \in E_1} [d(u) + d(v)]^2$$

$$+ \sum_{uv \in E_2} [d(u) + d(v)]^2$$

$$+ \sum_{uv \in E_3} [d(u) + d(v)]^2$$

$$= 36|E_1| + 64|E_2|$$

$$= 36(6n) + 64(4mn + 4n)$$

$$+ 64(6mn - 2n)$$

from where the desired result follows.

3. Conclusion

In this paper, the expressions for some old and new degree-based topological indices such as F-index, reformulated first Zagreb index, third Zagreb index, and hyper-Zagreb index of titania TiO$_2$ nanotubes have been derived. These explicit formulae can correlate the chemical structure of titania nanotubes to information about their physical structure.

Competing Interests

The author declares no conflict of interests.

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