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Computation of some Gourava Indices of Titania Nanotubes

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Abstract. A titania nanotube is studied in materials science. Recently, Kulli introduced the first and second Gourava indices of the molecular graph. In this paper, we define a generalized version of these indices and compute exact formulae for titania nanotubes.

Keywords: Gourava indices, hyper-Gourava indices, sum connectivity Gourava index, product connectivity index, titania nanotubes.

AMS Mathematics Subject Classification (2010): 05C05, 05C07, 05C90

1. Introduction

Let G be a finite, simple and connected graph with a vertex set $V(G)$ and an edge set $E(G)$. The degree $d_G(v)$ of a vertex v is the number of vertices adjacent to v. For all further notation and terminology, we refer the reader to [1].

A molecular graph is a graph such that its vertices correspond to the atoms and the edges to the bonds. Chemical graph theory is a branch of Mathematical Chemistry which has an important effect on the development of the Chemical Sciences. A single number that can be computed from the molecular graph, and used to characterize some property of the underlying molecule is said to be a topological index or molecular structure descriptor. Numerous such descriptors have been considered in theoretical chemistry, and have found some applications, especially in *QSPR/QSAR* research see [2, 3].

The first and second Gourava indices of a molecular graph G are defined as

$$GO_1(G)=\sum_{uv\in E(G)}\left[\left(d_G(u)+d_G(v)\right)+d_G(u)d_G(v)\right]. \tag{1}$$

$$GO_2(G)=\sum_{uv\in E(G)}\left(d_G(u)+d_G(v)\right)\left(d_G(v)d_G(u)\right) \tag{2}$$

These indices were introduced by Kulli in [4].

The first and second hyper-Gourava indices [5] of a molecular graph G are defined as

$$HGO_1(G)=\sum_{uv\in E(G)}\left[\left(d_G(u)+d_G(v)\right)+d_G(u)d_G(v)\right]^2. \tag{3}$$

$$HGO_2(G)=\sum_{uv\in E(G)}\left[\left(d_G(u)+d_G(v)\right)d_G(u)d_G(v)\right]^2. \tag{4}$$

Motivated by the definition of the product connectivity index or Randic index [6], Kulli introduced the sum connectivity Gourava index [7] and product connectivity Gourava index [8] of a graph as follows:

The sum connectivity Gourava index of a graph G is defined as

$$SGO(G)=\sum_{uv\in E(G)}\frac{1}{\sqrt{\left(d_G(u)+d_G(v)\right)+d_G(u)d_G(v)}}. \tag{5}$$

The product connectivity Gourava index of a graph G is defined as

$$PGO(G)=\sum_{uv\in E(G)}\frac{1}{\sqrt{\left(d_G(u)+d_G(v)\right)d_G(u)d_G(v)}}. \tag{6}$$

In this paper, we continue this generalization and define the general first and second Gourava indices of a graph G as

$$GO_1^a(G)=\sum_{uv\in E(G)}\left[\left(d_G(u)+d_G(v)\right)+d_G(u)d_G(v)\right]^a \tag{7}$$

$$GO_2^a(G)=\sum_{uv\in E(G)}\left[\left(d_G(u)+d_G(v)\right)d_G(u)d_G(v)\right]^a \tag{8}$$

Recently, some topological indices were studied, for example, in [9, 14-29].
The study of titania nanotubes has received much attention in the mathematical and chemical literature (see [10, 11, 12, 13]).
In this paper, we compute Gourava indices, hyper-Gourava indices, sum connectivity Gourava index, product connectivity Gourava index and general Gourava indices for titania nanotubes.

2. Results for TiO_2 nanotubes

Titania is studied in materials science. The titania nanotubes usually symbolized as $TiO_2[m, n]$ for any $m, n \in N$, in which m is the number of octagons C_8 in a row and n is the number of octagons C_8 in a column. The graph of $TiO_2[m, n]$ is shown in Figure 1.

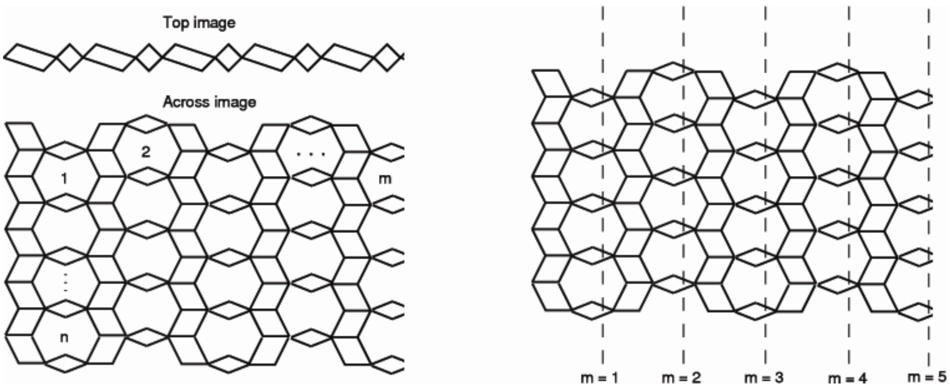

Figure 1: The graph of TiO_2 $[m, n]$ nanotubes

Let G be the graph of titania nanotube $TiO_2[m, n]$ with $|V(TiO_2 [m, n])|=6n (m+1)|$ and $|E(TiO_2 [m, n])| = 10mn+8n$. In $TiO_2[m,n]$, by algebraic method, there are four types of edges based on the degrees of end vertices of each edge, as follows:

$E_8 = \{uv \in E(G) \mid d_G(u) = 2, d_G(v) = 4\}$, $|E_8| = 6n$.
$E_{10} = \{uv \in E(G) \mid d_G(u) = 2, d_G(v) = 5\}$, $|E_{10}| = 4mn+2n$.
$E_{12} = \{uv \in E(G) \mid d_G(u) = 3, d_G(v) = 4\}$, $|E_{12}| = 2n$.
$E_{15} = \{uv \in E(G) \mid d_G(u) = 3, d_G(v) = 5\}$, $|E_{15}| = 6mn - 2n$.

In the following theorem, we compute the first Gourava index of titania nanotubes $TiO_2\,[m,n]$.

Theorem 1. The first Gourava index of $TiO_2\,[m, n]$ nanotubes is $GO_1(TiO_2) = 206mn + 92n$.

Proof: Let $G = TiO_2[m, n]$ be the molecular graph of titania nanotubes. From equation (1) and by cardinalities of the edge partitions of $TiO_2[m, n]$ nanotubes, we have

$$GO_1(TiO_2) = \sum_{uv\in E(G)} \left[\left(d_G(u)+d_G(v)\right)+d_G(u)d_G(v)\right]$$

$$= \sum_{uv\in E_8} \left[\left(d_G(u)+d_G(v)\right)+d_G(u)d_G(v)\right] + \sum_{uv\in E_{10}} \left[\left(d_G(u)+d_G(v)\right)+d_G(u)d_G(v)\right]$$

$$+ \sum_{uv\in E_{12}} \left[\left(d_G(u)+d_G(v)\right)+d_G(u)d_G(v)\right] + \sum_{uv\in E_{15}} \left[\left(d_G(u)+d_G(v)\right)+d_G(u)d_G(v)\right]$$

$= (6+8)|E_8| + (7+10)|E_{10}| + (7+12)|E_{12}| + (8+15)|E_{15}|$
$= 14(6n) + 17(4mn+2n) + 19(2n) + 23(6mn - 2n)$
$= 206mn + 92n$.

In the following theorem, we compute the second Gourava index of titania nanotubes $TiO_2\,[m, n]$.

Theorem 2. The second Gourava index of $TiO_2[m, n]$ nanotubes is $GO_2(TiO_2) = 1000\,mn + 356n$.

Proof: Let $G = TiO_2[m, n]$ be the molecular graph of titania nanotubes. From equation (2) and by cardinalities of the edge partitions of $TiO_2[m, n]$ nanotubes, we have

$$GO_2(TiO_2) = \sum_{uv\in E(G)} \left(d_G(u)+d_G(v)\right)\left(d_G(u)d_G(v)\right)$$

$$= \sum_{uv\in E_8} \left(d_G(u)+d_G(v)\right)\left(d_G(u)d_G(v)\right) + \sum_{uv\in E_{10}} \left(d_G(u)+d_G(v)\right)\left(d_G(u)d_G(v)\right)$$

$$+ \sum_{uv\in E_{12}} \left(d_G(u)+d_G(v)\right)\left(d_G(u)d_G(v)\right) + \sum_{uv\in E_{15}} \left(d_G(u)+d_G(v)\right)\left(d_G(u)d_G(v)\right)$$

$= (6 \times 8)\,|E_8| + (7\times10)\,|E_{10}| + (7 \times 12)\,|E_{12}| + (8 \times 15)\,|E_{15}|$
$= 48(6n) + 70\,(4mn + 2n) + 84(2n) + 120(6mn - 2n)$
$= 1000\,mn + 356n$.

In the following theorem, we compute the first hyper-Gourava index of titania nanotubes $TiO_2[m, n]$.

Theorem 3. The first hyper-Gourava index of $TiO_2[m, n]$ nanotubes is

$HGO_1(TiO_2) = 4330mn + 1418n$.

Proof: Let $G = TiO_2\,[m, n]$ be the molecular graph of titania nanotubes. From equation (3) and by cardinalities of the edge partitions of $TiO_2\,[m, n]$ nanotubes, we have

$$HGO_1(TiO_2)=\sum_{uv\in E(G)}\left[\left(d_G(u)+d_G(v)\right)+d_G(u)d_G(v)\right]^2$$

$$=\sum_{uv\in E_8}\left[\left(d_G(u)+d_G(v)\right)+d_G(u)d_G(v)\right]^2+\sum_{uv\in E_{10}}\left[\left(d_G(u)+d_G(v)\right)+d_G(u)d_G(v)\right]^2$$

$$+\sum_{uv\in E_{12}}\left[\left(d_G(u)+d_G(v)\right)+\left(d_G(u)d_G(v)\right)\right]^2+\sum_{uv\in E_{15}}\left[\left(d_G(u)+d_G(v)\right)+\left(d_G(u)d_G(v)\right)\right]^2$$

$= (6 + 8)^2 |E_8|+ (7+10)^2|E_{10}|+ (7+12)^2|E_{12}|+(8+15)^2 |E_{15}|$
$= 14^2(6n) + 17^2(4mn +2n) + 19^2(2n) + 23^2 (6mn – 2n)$
$= 4330mn + 1418n.$

In the following theorem, we compute the second hyper-Gourava index of titania nanotubes TiO_2 [*m*, *n*].

Theorem 4. The second hyper-Gourava index of $TiO_2[m, n]$ nanotubes is

$$HGO_2(TiO_2) = 106000mn + 8936n.$$

Proof: Let $G = TiO_2[m, n]$ be the molecular graph of titania nanotubes. From equation (4) and by cardinalities of the edge partitions of $TiO_2[m, n]$ nanotube, we have

$$HGO_2(TiO_2)=\sum_{uv\in E(G)}\left[\left(d_G(u)+d_G(v)\right)\left(d_G(u)d_G(v)\right)\right]^2$$

$$=\sum_{uv\in E_8}\left[\left(d_G(u)+d_G(v)\right)\left(d_G(u)d_G(v)\right)\right]^2+\sum_{uv\in E_{10}}\left[\left(d_G(u)+d_G(v)\right)\left(d_G(u)d_G(v)\right)\right]^2$$

$$+\sum_{uv\in E_{12}}\left[\left(d_G(u)+d_G(v)\right)\left(d_G(u)d_G(v)\right)\right]^2+\sum_{uv\in E_{15}}\left[\left(d_G(u)+d_G(v)\right)\left(d_G(u)d_G(v)\right)\right]^2$$

$= (6 \times 8)^2 |E_8| + (7\times10)^2 |E_{10}| + (7 \times 12)^2 |E_{12}|+ (8 \times 15)^2 |E_{15}|$
$= 48^2(6n) + 70^2(4mn + 2n) + 84^2(2n) + 120^2 (6mn – 2n)$
$= 106000\, mn + 8936n.$

In the following theorem, we compute the sum connectivity Gourava index of titania nanotubes TiO_2 [*m*, *n*].

Theorem 5. The sum connectivity Gourava index of TiO_2 [*m*, *n*] nanotubes is

$$SGO(TiO_2)=\left(\frac{4}{\sqrt{17}}+\frac{6}{\sqrt{23}}\right)mn+\left(\frac{6}{\sqrt{14}}+\frac{2}{\sqrt{17}}+\frac{2}{\sqrt{19}}-\frac{2}{\sqrt{23}}\right)n.$$

Proof: Let $G = TiO_2[m, n]$ be the molecular graph of titania nanotubes. From equation (5) and by cardinalities of the edge partitions of $TiO_2[m, n]$ nanotubes, we have

$$SGO(TiO_2)=\sum_{uv\in E(G)}\frac{1}{\sqrt{\left(d_G(u)+d_G(v)\right)+d_G(u)d_G(v)}}.$$

$$=\sum_{uv\in E_8}\frac{1}{\sqrt{\left(d_G(u)+d_G(v)\right)+d_G(u)d_G(v)}}+\sum_{uv\in E_{10}}\frac{1}{\sqrt{\left(d_G(u)+d_G(v)\right)+d_G(u)d_G(v)}}$$

$$+\sum_{uv\in E_{12}}\frac{1}{\sqrt{\left(d_G(u)+d_G(v)\right)+d_G(u)d_G(v)}}+\sum_{uv\in E_{15}}\frac{1}{\sqrt{\left(d_G(u)+d_G(v)\right)+d_G(u)d_G(v)}}$$

$$=\frac{1}{\sqrt{6+8}}|E_8|+\frac{1}{\sqrt{7+10}}|E_{10}|+\frac{1}{\sqrt{7+12}}|E_{12}|+\frac{1}{\sqrt{8+15}}|E_{15}|$$

$$=\frac{1}{\sqrt{14}}(6n)+\frac{1}{\sqrt{17}}(4mn+2n)+\frac{1}{\sqrt{19}}(2n)+\frac{1}{\sqrt{23}}(6mn-2n)$$

$$=\left(\frac{4}{\sqrt{17}}+\frac{6}{\sqrt{23}}\right)mn+\left(\frac{6}{\sqrt{14}}+\frac{2}{\sqrt{17}}+\frac{2}{\sqrt{19}}-\frac{2}{\sqrt{23}}\right)n.$$

In the following theorem, we compute the product connectivity Gourava index of titania nanotubes TiO_2 [m, n].

Theorem 6. The product connectivity Gourava index of $TiO_2[m, n]$ nanotubes is

$$PGO(TiO_2)=\left(\frac{4}{\sqrt{70}}+\frac{3}{\sqrt{30}}\right)mn+\left(\frac{3}{2\sqrt{3}}+\frac{2}{\sqrt{70}}+\frac{1}{\sqrt{21}}-\frac{1}{\sqrt{30}}\right)n.$$

Proof: Let $G = TiO_2$ [m, n] be the molecular graph of titania nanotubes. From equation (6) and by cardinalities of the edge partitions of TiO_2 [m, n] nanotubes, we have

$$PGO(TiO_2)=\sum_{uv\in E(G)}\frac{1}{\sqrt{\left(d_G(u)+d_G(v)\right)d_G(u)d_G(v)}}.$$

$$=\sum_{uv\in E_8}\frac{1}{\sqrt{\left(d_G(u)+d_G(v)\right)d_G(u)d_G(v)}}+\sum_{uv\in E_{10}}\frac{1}{\sqrt{\left(d_G(u)+d_G(v)\right)d_G(u)d_G(v)}}$$

$$+\sum_{uv\in E_{12}}\frac{1}{\sqrt{\left(d_G(u)+d_G(v)\right)d_G(u)d_G(v)}}+\sum_{uv\in E_{15}}\frac{1}{\sqrt{\left(d_G(u)+d_G(v)\right)d_G(u)d_G(v)}}$$

$$=\frac{1}{\sqrt{6\times 8}}|E_8|+\frac{1}{\sqrt{7\times 10}}|E_{10}|+\frac{1}{\sqrt{7\times 12}}|E_{12}|+\frac{1}{\sqrt{8\times 15}}|E_{15}|$$

$$=\frac{1}{4\sqrt{3}}(6n)+\frac{1}{\sqrt{70}}(4mn+2n)+\frac{1}{2\sqrt{21}}(2n)+\frac{1}{2\sqrt{30}}(6mn-2n)$$

$$=\left(\frac{4}{\sqrt{70}}+\frac{3}{\sqrt{30}}\right)mn+\left(\frac{3}{2\sqrt{3}}+\frac{2}{\sqrt{70}}+\frac{1}{\sqrt{21}}-\frac{1}{\sqrt{30}}\right)n.$$

In the following theorem, we compute the general first Gourava index of titania nanotubes TiO_2 [m, n].

Theorem 7. The general first Gourava index of TiO_2 [m, n] nanotubes is

$$GO_1^a(TiO_2)=\left(4\times 17^a+6\times 23^a\right)mn+\left(6\times 14^a+2\times 17^a+2\times 19^a-2\times 23^a\right)n.$$

Proof: Let $G = TiO_2[m, n]$ be the molecular graph of titania nanotubes. From equation (7) and by cardinalities of the edge partitions of $TiO_2[m, n]$ nanotubes, we have

$$GO_1^a(TiO_2)=\sum_{uv\in E(G)}\left[\left(d_G(u)+d_G(v)\right)+d_G(u)d_G(v)\right]^a$$

$$= \sum_{uv\in E_8}\left[\left(d_G(u)+d_G(v)\right)+d_G(u)d_G(v)\right]^a + \sum_{uv\in E_{10}}\left[\left(d_G(u)+d_G(v)\right)+d_G(u)d_G(v)\right]^a$$

$$+ \sum_{uv\in E_{12}}\left[\left(d_G(u)+d_G(v)\right)+d_G(u)d_G(v)\right]^a + \sum_{uv\in E_{15}}\left[\left(d_G(u)+d_G(v)\right)+d_G(u)d_G(v)\right]^a$$

$= (6 + 8)^a |E_8| + (7 + 10)^a|E_{10}| + (7 + 12)^a|E_{12}| + (8+15)^a|E_{15}|$

$= 14^a(6n) + 17^a(4mn+2n) + 19^a(2n) + 23^a(6mn - 2n)$

$= \left(4\times17^a + 6\times23^a\right)mn + \left(6\times14^a + 2\times17^a + 2\times19^a - 2\times23^a\right)n.$

In the next theorem, we compute the general second Gourava index of titania nanotubes $TiO_2[m, n]$.

Theorem 8. The general second Gourava index of $TiO_2[m, n]$ nanotubes is

$$GO_2^a\left(TiO_2\right) = \left(4\times70^a + 6\times120^a\right)mn + \left(6\times48^a + 2\times70^a + 2\times84^a - 2\times120^a\right)n.$$

Proof: Let $G = TiO_2[m, n]$ be the molecular graph of titania nanotubes. From equation (8) and by cardinalities of the edge partitions of TiO_2 $[m, n]$ nanotubes, we have

$$GO_2^a\left(TiO_2\right) = \sum_{uv\in E(G)}\left[\left(d_G(u)+d_G(v)\right)d_G(u)d_G(v)\right]^a$$

$$= \sum_{uv\in E_8}\left[\left(d_G(u)d_G(v)\right)d_G(u)d_G(v)\right]^a + \sum_{uv\in E_{10}}\left[\left(d_G(u)+d_G(v)\right)d_G(u)d_G(v)\right]^a$$

$$+ \sum_{uv\in E_{12}}\left[\left(d_G(u)+d_G(v)\right)d_G(u)d_G(v)\right]^a + \sum_{uv\in E_{15}}\left[\left(d_G(u)+d_G(v)\right)d_G(u)d_G(v)\right]^a$$

$= (6 \times 8)^a |E_8| + (7 \times 10)^a|E_{10}| + (7 \times 12)^a|E_{12}| + (8\times15)^a|E_{15}|$

$= 48^a(6n) + 70^a(4mn + 2n) + 84^a(2n) + 120^a(6mn - 2n)$

$= (4 \times 70^a + 6 \times 120^a)mn + (6 \times 48^a + 2 \times 70^a + 2 \times 84^a - 2 \times 120^a)n.$

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