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Calculation of Gourava topological indices in $HAC_5C_6C_7[p, q]$ nanotubes

Jaber Ramezani Tousi †
Massoud Ghods*
Faculty of Mathematics, Statistics and Computer Science
Department of Applied Mathematics
Semnan University
Semnan 35131-19111
Iran

Abstract

One of the best and most widely used carbon structures is carbon nanotubes. The most important features of carbon nanotubes are high durability, flexibility and good conductivity.

In this article, the graph of $HAC_5C_6C_7[p,q]$ carbon nanotube structure is investigated using a section of its surface. By presenting a method for obtaining the degree of vertices in the relevant area, the topological indices of Gourava and Hyper Gourava are calculated, and the relevant theorems are expressed. The Gourava indices and Hyper Gourava indices are then calculated for the line graph and subdivision graph of $HAC_5C_6C_7[p,q]$. Also, to compare the obtained values, the diagrams of Gourava and Hyper Gourava indices are drawn.

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1. Introduction

Today, graph theory is one of the most practical branches of mathematics due to its numerous applications in various fields such as nanotechnology, chemistry, computers, information networks, etc. Graph theory is used in chemistry for modeling.

† *E-mail:* jaber.ramezani@semnan.ac.ir
* *E-mail:* mghods@semnan.ac.ir (Corresponding Author)

The chemical graph of a molecule is obtained by assuming its atoms as vertices and its chemical bonds as edges. Graph theory provides a variety of valuable tools for chemists, including topological indices.

In a molecular graph, the topological index is expressed as a real number, and this number is attributed to the graphs, uniform with that molecule.

The topological index also indicates some of the properties of the molecule.

The Wiener Indices were presented by Wiener in 1947 [9]. One of the practical tools in studying the structure and properties of a molecule is the topological indices of its chemical graph [4].

Recently, topological indices for wheel graphs have been calculated and topological indices for its line graph and subdivision graph have been studied [1]. The calculation of topological indices using M-polynomials in molecular graphs has also been investigated[5, 8].

In nanoscience, the study of atomic, molecular, and macromolecular dimensions is discussed.

Study in nanoscale leads to drastic changes in material properties. Numerical calculations are of particular importance in nanoscale simulations.

In nanoscience, the study of atomic, molecular, and macromolecular dimensions was discussed, and research in these dimensions leads to a drastic change in the properties of materials. At the nanoscale, materials exhibit quantum properties that are often not measurable in practice. For this purpose, the desired systems should be mathematically modeled and the relevant equations should be solved for them.

Carbon nanotubes (CNTs) are types of nanostructures that are carbon allotropes and have a cylindrical shape. One of the best and most widely used carbon structures is carbon nanotubes, which in addition to high durability, also have good flexibility and conductivity.

2. Preliminaries

This section, provides some definitions needed. Suppose G = (V, E) is a simple and connected graph. We represent the set of edges with E(G) and the number of edges with $|E(G)|$ and the set of vertices with V (G) and the number of vertices with $|V(G)|$. We denote the degree of vertex u by d_u and if there is an edge between two vertices u, v, denote by $uv \in E(G)$.

The first and second Zagreb index were first introduced by Guttman et al. Zagreb indices have found many applications in QSPR and QSAR studies [6].

Motivated by the definitions of Zagreb indices and their wide applications, in 2017, Gourava indices were defined by V. R. Kulli [7].

Definition 2.1: The first Gourava index for graph G is defined as:

$$GO_1(G) = \sum_{uv \in E(G)} [(d_u + d_v) + (d_u . d_v)].$$

For each edge of $uv \in E(G)$, by defining $\psi_i = [(d_u + d_v) + (d_u . d_v)]$, the above formula can be defined as $GO_1(G) = \sum_{i=1}^{|E(G)|} \psi_i$.

Definition 2.2: The Second Gourava index for graph G is defined as:

$$GO_2(G) = \sum_{uv \in E(G)} [(d_u + d_v)(d_u . d_v)].$$

For each edge of $uv \in E(G)$, by defining $\psi_i' = [(d_u + d_v)(d_u . d_v)]$, the above formula can be defined as $GO_2(G) = \sum_{i=1}^{|E(G)|} \psi_i'$.

Definition 2.3: The first Hyper Gourava index for graph G is defined as:

$$HGO_1(G) = \sum_{uv \in E(G)} [(d_u + d_v) + (d_u . d_v)]^2.$$

For each edge of $uv \in E(G)$, by defining $\psi_i'' = [(d_u + d_v) + (d_u . d_v)]^2$, the above formula can be defined as $HGO_1(G) = \sum_{i=1}^{|E(G)|} \psi_i''$.

Definition 2.4: The Second Hyper Gourava index for graph G is defined as:

$$HGO_2(G) = \sum_{uv \in E(G)} [(d_u + d_v)(d_u . d_v)]^2.$$

For each edge of $uv \in E(G)$, by defining $\psi_i''' = [(d_u + d_v)(d_u . d_v)]^2$, the above formula can be defined as $HGO_2(G) = \sum_{i=1}^{|E(G)|} \psi_i'''$.

Definition 2.5: In a non-empty graph G, if each edge is considered as a vertex and the two vertices are connected, if the corresponding edges of the two vertices are adjacent to G, the resulting graph is denoted by L (G) and is called the line graph of G [2].

Definition 2.6: Subdivision graph of graph G is a graph that obtained by placing an extra vertex on each edge of G. In other words, each edge G is replaced by a path of length 2. The subdivision graph is denoted by S (G) [2].

3. The structure of the nanotube $HAC_5C_6C_7[p,q]$

In this section, to calculate the Gourava indices, the structure of the graph obtained from the $HAC_5C_6C_7[p,q]$ nanotube is investigated.

In this nanotube, p represents the number of pentagons in a row and q represents the number of periods, a period consisting of the first three rows with all its vertices and edges (Figure 1).

The number of nanotube vertices is obtained using the relation $\left|V(HAC_5C_6C_7[p,q])\right| = 16pq + 2p$.

We use $HAC_5C_6C_7[1,1]$ for ease of calculation (Figure 2) Because this structure is repeated throughout the nanotube.

The next section with reviews of edges in the nanotube $HAC_5C_6C_7[1,1]$, offered a formula for the number of indices are calculated Gourava and Hyper Gourava to help them.

4. Main results

In [3, 6], some topological indices for $HAC_5C_6C_7[p,q]$ nanotubes were calculated. In the following, Gourava and Hyper Gourava indices in the general state of nanotubes are obtained.

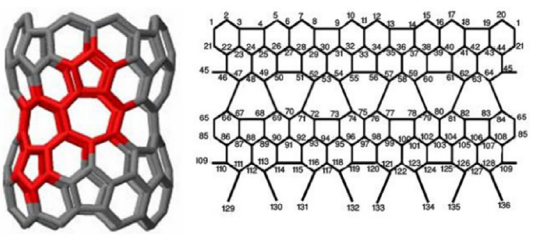

Figure 1
Nanotube $HAC_5C_6C_7$[4, 2].

Figure 2
Nanotube $HAC_5C_6C_7$[1, 1].

There are four types of edges in $HAC_5C_6C_7[p,q]$ as follows:

$e_1 = \{(d_u, d_v) \mid uv \in E(G), d_u = 1, d_v = 3\}$, $e_2 = \{(d_u, d_v) \mid uv \in E(G), d_u = 2, d_v = 2\}$,
$e_3 = \{(d_u, d_v) \mid uv \in E(G), d_u = 2, d_v = 3\}$ and $e_4 = \{(d_u, d_v) \mid uv \in E(G), d_u = 3, d_v = 3\}$.

We want to calculate the number of edges with the help of Figure (2) and the types of the above edges and obtain a general formula for it by generalizing it to the nanotube.

According to Figure (2), we have the Table (1) for molecular graph of $HAC_5C_6C_7[p, q]$

Table 1

Types and number of $HAC_5C_6C_7[p, q]$ edges.

Edge type	Number of edges	ψ_i	ψ_i'	ψ_i''	ψ_i'''
e_1	2p	7	12	49	144
e_2	2q+2	8	16	64	256
e_3	8q+4p-4	11	30	121	900
e_4	24pq-10q-6p+2	15	54	225	2916

As a result, the number of nanotube $HAC_5C_6C_7[p,q]$ edges is equal to:

$$\left|E(HAC_5C_6C_7[p,q])\right| = 24pq.$$

Nanotube line graph $HAC_5C_6C_7[p,q]$ In Figure (3) is shown.

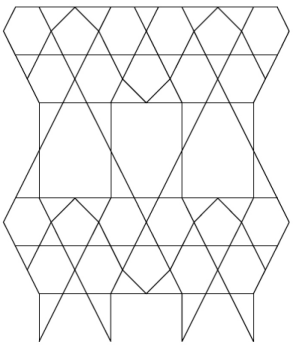

Figure 3
***L*(*HAC*$_5$*C*$_6$*C*$_7$[2, 2]).**

There are six types of edges in $L(HAC_5C_6C_7[p,q])$ as follows:

$e_1=\{(d_u,d_v)\,|\,uv\in E(\mathrm{L(G)}),\mathrm{d}_u=2,d_v=2\}$, $e_2=\{(d_u,d_v)\,|\,uv\in E(\mathrm{L(G)}),\mathrm{d}_u=2,d_v=3\}$,
$e_3=\{(d_u,d_v)\,|\,uv\in E(\mathrm{L(G)}),\mathrm{d}_u=2,d_v=4\}$, $e_4=\{(d_u,d_v)\,|\,uv\in E(\mathrm{L(G)}),\mathrm{d}_u=3,d_v=3\}$,
$e_5=\{(d_u,d_v)\,|\,uv\in E(\mathrm{L(G)}),\mathrm{d}_u=3,d_v=4\}$, $e_6=\{(d_u,d_v)\,|\,uv\in E(\mathrm{L(G)}),\mathrm{d}_u=4,d_v=4\}$.

Using Figure (3) and the types of edges above, the number of edges is calculated and by generalizing it to the nanotube line graph, a general formula is obtained for it.

According to Figure (3), we have the Table (2) for line graph of $L(HAC_5C_6C_7[p,q])$

Table 2

Types and number of $L(HAC_5C_6C_7[p,q])$ edges.

Edge type	Number of edges	ψ_i	ψ_i'	ψ_i''	ψ_i'''
e_1	2	8	16	64	256
e_2	4q+2	11	30	121	900
e_3	4p-2	14	48	196	2304
e_4	4q+3p-3	15	54	225	2916
e_5	12q+6p-8	19	84	361	130321
e_6	48pq-26q-16p+9	24	128	576	331776

As a result, the number of $L(HAC_5C_6C_7[p,q])$ edges is equal to:

$$\left|E(L(HAC_5C_6C_7[p,q]))\right|=48\,\mathrm{pq}-6\,\mathrm{q}-4\,\mathrm{p}.$$

Figure (4) shows the subdivision graph of nanotube $HAC_5C_6C_7[p,q]$.

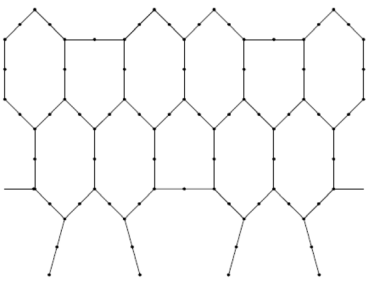

Figure 4

***S*($HAC_5C_6C_7$[2, 1]).**

There are three types of edges in $S(HAC_5C_6C_7[p,q])$ as follows:

$$e_1 = \{(d_u, d_v) \mid uv \in E(S(G)), d_u = 1, d_v = 2\},$$
$$e_2 = \{(d_u, d_v) \mid uv \in E(S(G)), d_u = 2, d_v = 2\} \text{ and}$$
$$e_3 = \{(d_u, d_v) \mid uv \in E(S(G)), d_u = 2, d_v = 3\}.$$

According to Figure (4), we have the Table (3) for subdivision graph of $HAC_5C_6C_7[p, q]$

Table 3

Types and number of $S(HAC_5C_6C_7[p, q])$ edges.

Edge type	Number of edges	ψ_i	ψ_i'	ψ_i''	ψ_i'''
e_1	2p	5	6	25	36
e_2	12q+4p	8	16	64	256
e_3	48pq-12q-6p	11	30	121	900

As a result, the number of $S(HAC_5C_6C_7[p,q])$ edges is equal to:

$$|S(HAC_5C_6C_7[p,q]))| = 48\,pq.$$

According to the above structure, the following theorems are expressed to calculate the Gourava indices.

Theorem 4.1: *Let G be the graph of* $HAC_5C_6C_7[p,q]$ *nanotube. Then we have,*

(i) $GO_1(G) = 360pq - 32p - 46q + 2$,

(ii) $GO_2(G) = 1296pq - 180p - 268q + 20$.

Proof: According to the values in Table (1) and definitions 2.1 and 2.2, the following relationships are obtained:

$$\begin{aligned} GO_1(G) &= \sum_{i=1}^{|E(G)|} \psi_i = 2p(7) + (2q+2)(8) + (8q+4p-4)(11) \\ &\quad + (24pq - 10q - 6p + 2)15 \\ &= 360pq - 32p - 46q + 2. \end{aligned}$$

Similarly we have,

$$\begin{aligned} GO_2(G) &= \sum_{i=1}^{|E(G)|} \psi_i' = 2p(12) + (2q+2)(16) + (8q+4p-4)(30) \\ &\quad + (24pq - 10q - 6p + 2)54 \\ &= 1296pq - 180p - 268q + 20. \end{aligned}$$

□

Theorem 4.2 : *Suppose G is graph of* $HAC_5C_6C_7[p,q]$ *nanotube. Then we have,*

(i) $\mathrm{H}GO_1(G) = 5400pq - 768p - 1154q + 94$,

(ii) $\mathrm{H}GO_2(G) = 69984pq - 13608p - 21448q + 2744$.

Proof: According to the values in Table (1) and definitions 2.3 and 2.4, the following relationships are obtained:

$$\begin{aligned} HGO_1(G) &= 2p(49) + (2q+2)(64) + (8q+4p-4)(121) \\ &\quad + (24pq - 10q - 6p + 2)225 \\ &= 5400pq - 768p - 1154q + 94. \end{aligned}$$

Similarly we have,

$$\begin{aligned} HGO_2(G) &= 2p(144) + (2q+2)(256) + (8q+4p-4)(900) \\ &\quad + (24pq - 10q - 6p + 2)2916 \\ &= 69984pq - 13608p - 21448q + 2744. \end{aligned}$$

□

Now, according to the above structure, the following theorems are used to calculate the Gourava indices for $L(HAC_5C_6C_7[p,q])$.

Theorem 4.3 : *Suppose* G' *is line graph of* $HAC_5C_6C_7[p,q]$ *nanotube. Then we have,*

(i) $GO_1(G') = 1152pq - 292q - 169p + 29$,

(ii) $GO_2(G') = 6144pq - 1984q - 1190p + 314$.

Proof: *According to the values in Table (2) and definitions 2.1 and 2.2, the following relationships are obtained:*

$$\begin{aligned} GO_1(G') &= 2(8) + 11(4q+2) + (4p-2)(14) + (4q+3p-3)(15) \\ &\quad + (12q+6p-8)(19) + (48pq - 26q - 16p + 9)(24) \\ &= 1152pq - 292q - 169p + 29. \end{aligned}$$

Similarly, we have,

$$\begin{aligned} GO_2(G') &= 2(16) + 30(4q+2) + (4p-2)(48) + (4q+3p-3)(54) \\ &\quad + (12q+6p-8)(84) + (48pq - 26q - 16p + 9)(128) \\ &= 6144pq - 1984q - 1190p + 314. \end{aligned}$$

Theorem 4.4 : *Suppose* G' *is line graph of* $HAC_5C_6C_7[p,q]$ *nanotube. Then we have,*

(i) $HGO_1(G') = 27648pq - 9260q - 5591p + 1599,$

(ii) $HGO_2(G') = 15925248pq - 7047060q - 4508526 + 1932372.$

Proof: According to the values in Table (2) and definitions 2.3 and 2.4, the following relationships are obtained:

$$\begin{aligned} HGO_1(G') &= 2(64) + 121(4q+2) + (4p-2)(196) + (4q+3p-3)(225) \\ &\quad + (12q+6p-8)(361) + (48pq-26q-16p+9)(576) \\ &= 27648pq - 9260q - 5591p + 1599. \end{aligned}$$

Similarly, we have,

$$\begin{aligned} HGO_2(G') &= 2(256) + 900(4q+2) + (4p-2)(2304) + (4q+3p-3)(2916) \\ &\quad + (12q+6p-8)(130321) + (48pq-26q-16p+9)(331776) \\ &= 15925248pq - 7047060q - 4508526 + 1932372. \end{aligned}$$

According to the above structure, the following theorems are used to calculate the Gourava indices for $S(HAC_5C_6C_7[p,q])$.

Theorem 4.5: *Suppose S is subdivision graph of* $HAC_5C_6C_7[p,q]$ *nanotube. Then we have,*

(i) $GO_1(S) = 528pq - 24p - 36q,$

(ii) $GO_2(S) = 1440pq - 104p - 168q.$

Proof: According to the values in Table (3) and definitions 2.1 and 2.2, the following relationships are obtained:

$$\begin{aligned} GO_1(S) &= \sum_{i=1}^{|E(G)|} \psi_i = 2p(5) + (12q+4p)(8) + (48pq-12q-6p)(11) \\ &= 528pq - 24p - 36q. \end{aligned}$$

Similarly, we have:

$$\begin{aligned} GO_2(S) &= \sum_{i=1}^{|E(G)|} \psi_i' = 2p(6) + (12q+4p)(16) + (48pq-12q-6p)(30) \\ &= 1440pq - 104p - 168q. \end{aligned}$$

□

Theorem 4.6: Suppose S is subdivision graph of $HAC_5C_6C_7[p,q]$ nanotube. Then we have,

(i) $HGO_1(S) = 5808pq - 420p - 684q,$

(ii) $HGO_2(S) = 43200pq - 4304p - 7728q.$

Proof: According to the values in Table (3) and definitions 2.3 and 2.4, the following relationships are obtained:

$$\begin{aligned} HGO_1(S) &= \sum_{i=1}^{|E(G)|} \psi_i'' = 2p(25) + (12q + 4p)(64) + (48pq - 12q - 6p)(121) \\ &= 5808pq - 420p - 684q. \end{aligned}$$

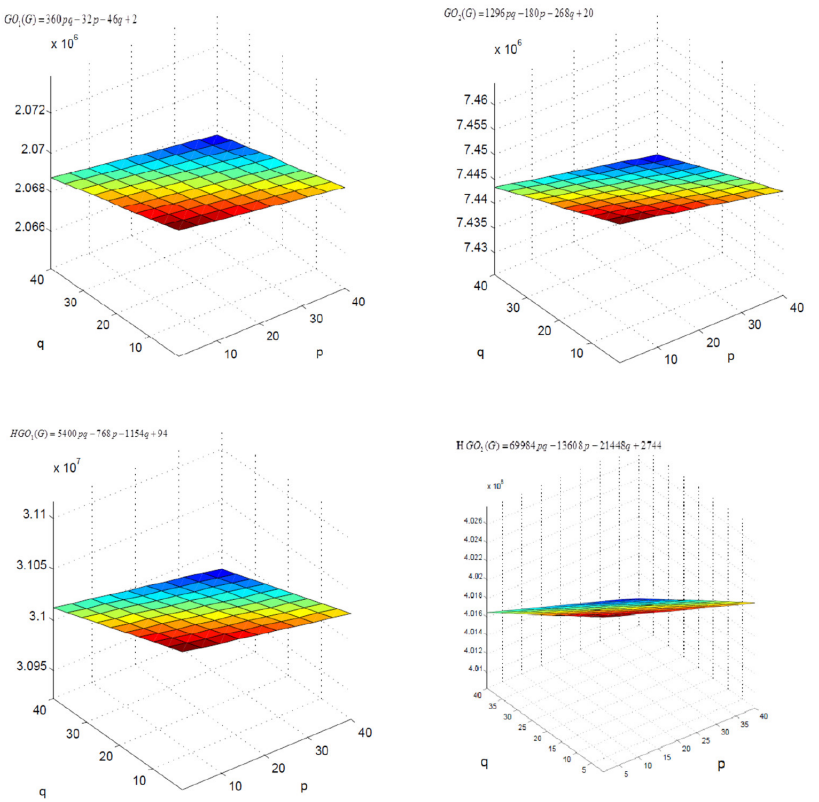

Figure 5

Diagrams of Gourava and Hyper Gourava indices for $HAC_5C_6C_7[p, q]$ nanotube.

Similarly we have,

$$HGO_2(S) = \sum_{i=1}^{|E(G)|} \psi_i''' = 2p(36) + (12q + 4p)(256) + (48pq - 12q - 6p)(900)$$
$$= 43200pq - 4304p - 7728q.$$

□

In the end, the diagrams obtained from drawing Gourava and Hyper Gourava indices are presented (Figure 5).

5. Conclusion

In this article, a method for calculating Gourava indices and Hyper Gourava indices for nanotubes is presented. The advantage of these methods is that it makes the calculation of Guarava indices much easier with the help of mathematical software. These indices were also expressed for $L(HAC_5C_6C_7[p,q])$ and $S(HAC_5C_6C_7[p,q])$. The above method can also be used for other nanotubes.

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