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Gourava Indices and Hyper-Gourava Indices of Line Graph of $HAC_5C_6C_7$ Carbon Nanotube

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Abstract: ***The first Gourava index $GO_1(G)$ is defined as sum$(d_u + d_v) + d_u d_v$ for all edges uv in the graph, while the first hyper-Gourava index $HGO_1(G)$ squares this sum. In this paper first, second Gourava indices, first and second hyper-Gourava indices of L($HAC_5C_6C_7$), T(G), some transformation graphsG^{xy}, G^{xyz} and their complements of L($HAC_5C_6C_7$) are studied.***

Keywords: Gourava index, hyper-Gourava index, line graph, line vertex degree, point vertex degree, transformation graph

1. Introduction

Let $G = (V,E)$ be a graph with order $|V(G)| = n$ and size $|E(G)| = m$. The degree of a vertex is denoted by d_u and is defined as the number of vertices adjacent to $u \in V(G)$. The edge connecting the vertices u and v is denoted by uv [1].Let G=(V,E) be a graph and x,y,z be three variables taking values [+ or -].The total graph T(G) of a graph G is the graph whose vertex set is V(G)UE(G),such that two vertices are adjacent if and only if they are either adjacent or incident in G [2].In a non-empty graph G,if each edge is considered as a vertex and the vertices are connected if the corresponding edges of the two vertices are adjacent in G, the resulting graph is denoted by L(G) and is called the line graph of G [3-4].Complement of the graph G is a simple graph $(\overline{G})$ with same vertex set and there is an edge between the vertex u and v in G. The point vertex represents the same vertex v of the original graph but its edges now reflect more complex relationships. A topological index is a numeric value associated with a chemical compound graph, that describes its topology while being invariant under graph automorphism [5]. Gourava indices find applications in chemical graph theory for predicting the physico-chemical properties of molecules and nanostructures by QSPR. Zagreb indices, Randic indices, Gourava indices when computed from point vertex degree of transformation graphs, measure how reactivity, branching and stability vary across the molecules. Higher values of such indices often correlate with increased polarizability, greater chemical reactivity, lower stability. Chemical reactivity depends on local atomic environments (number of bonds, types of neighbours), bond adjacencies, all these are encoded in the topology of the molecular graph.

The second Gourava index and hyper-Gourava index of line graph of subdivision graph of a triangular benzenoid were computed in [6]. The $ReZG_3(G)$ redefined third Zagreb index which was introduced in [7] is actually second Gourava index [8]. Leap Zagreb polynomials of generalized transformation graphs of triangle with pendant graph and path graph P_4 were studied in [9]. The F-index and F-coindex of the line graphs of the subdivision graphs were studied in [10]. The Gourava coindices are expressed in terms of first and second Zagreb coindices in [11] and first and second Gourava indices for trees with acyclic structures were studied in [12]. In $HAC_5C_6C_7$ nanotube 2-D structure, which is hexagonal-alternate (HA) lattice made of carbon rings with size 5,6 and 7. $HAC_5C_6C_7$ means the unit cell contains pentagons(C_5), hexagons(C_6) and heptagons(C_7) arranged in alternating pattern. The 2-D lattice of $HAC_5C_6C_7$[p,q] consists of p rows and q periods. The more C_5/C_7 defects are present, the higher the curvature stress. In nanotubes, this stress influences stability, electronic properties and mechanical strength. There are three partitions of edge set corresponding to their degrees of end vertices, as E_{23}=4p, E_{13}=2p and E_{33}=24pq-6p [13-15]. Different types of Gourava indices of graphs were studied in [16-18]. Gourava indices and hyper-Gourava indices are degree-based topological indices defined [19-24] as

1) First Gourava index $= GO_1(G) = \sum_{uv \in E(G)}[(d_u + d_v) + d_u d_v]$.
2) Second Gourava index $= GO_2(G) = \sum_{uv \in E(G)}[(d_u + d_v)d_u d_v]$.
3) First hyper-Gourava index $= HGO_1(G) = \sum_{uv \in E(G)}[(d_u + d_v) + d_u d_v]^2$.
4) Second hyper-Gourava index $= HGO_2(G) = \sum_{uv \in E(G)}[(d_u + d_v)d_u d_v]^2$.

All the symbols and notations used in this paper are standard and mainly taken from books of graph theory [25-27]. The different transformation graphs of line graph of $HAC_5C_6C_7$[p,q] carbon nanotubes are considered. In this paper first, second Gourava indices, first and second hyper-Gourava indices of L($HAC_5C_6C_7$) =L(G),complement of L($HAC_5C_6C_7$)=$\overline{\mathbf{L(G)}}$, total graph T(L(G)), complement of total graph = $\overline{\mathbf{T(L(G))}}$, G^{++}(L(G)), $\overline{\mathbf{G^{++}(L(G))}}$, G^{--}(L(G)) , $\overline{\mathbf{G^{--}(L(G))}}$,T^{++1}(L(G)) , $\overline{\mathbf{T^{++1}(L(G))}}$,T^{001}(L(G)) and$\overline{\mathbf{T^{001}(L(G))}}$transformation graphs are studied.

2. Materials and Methods

Let G = (V, E) be a graph then the point vertex degree is denoted by $d_G(u)$ and line vertex degree by $d_G(e)$ respectively. Let the line graph L(G) = L(HA $C_5C_6C_7$).By applying graph operation, a new graph is obtained. The transformation graphs in G^{xy}, $\overline{G^{xy}}$, G^{xyz} and $\overline{G^{xyz}}$are used to get the point, line vertex degrees and edge partition of line graph of $HAC_5C_6C_7$[p,q] carbon nanotube. The edge partition for these graphs is defined in terms of: E_1-point-

point pair, E_2-point-line pair and E_3-line-line pair. 2-D graph of $HAC_5C_6C_7$[p,q] carbon nanotube, line graph and some transformation graphs of line graph of $HAC_5C_6C_7$ are shown in figure (1). To compute Gourava indices and hyper-Gourava indices of line graph of $HAC_5C_6C_7$, some transformation graphs and their complements their point, line vertex degrees and edge partition-E_1, E_2 and E_3 are observed from corresponding graphs.

3. Results and Discussion

The vertex of G^{xy} corresponding to a vertex v of G is referred as a point vertex and the vertex of G^{xy} corresponding to an edge e of G is referred as a line vertex. The degrees of point $d_G(u)$and line vertices $d_G(e)$and partition of the edge set as E_1, E_2 and E_3 where E_1: edge joining point-point, E_2: edge joining point-line and E_3: edge joining line-line vertices are represented in table (1). Graphs between Gourava indices and hyper-Gourava indices with $L(HAC_5C_6C_7)$ and some transformation graphs of it is represented in figure (2). Some Gourava and hyper-Gourava indices of these graphs are computed as follows.

Theorem 1.1: The first Gourava index of L(G) is 470.

Proof. By using table (1), point, line vertex degrees and E_1, E_2 and E_3 values for L(G), we have

$GO_1L(G)=\sum_{uv\in E(G)}[(d_u+d_v)+d_u\times d_v]$
$=\sum_{uv\in E_1}[(4+4)+4\times 4]+\sum_{uv\in E_2}[(4+2)+4\times 2]+\sum_{uv\in E_3}[(2+2)+2\times 2]$
$=10[(4+4)+4\times 4]+5[(4+2)+4\times 2]+20[(2+2)+2\times 2]=470.$

Theorem 1.2: The second Gourava index of L(G) is 1840.

Proof. By using table (1), $d_G(u)$, $d_G(e)$ and E_1, E_2 and E_3 values for L(G) graph, we have

$GO_2L(G)=\sum_{uv\in E(G)}[(d_u+d_v)d_u\times d_v]$
$=\sum_{uv\in E_1}[(4+4)4\times 4]+\sum_{uv\in E_2}[(4+2)4\times 2]+\sum_{uv\in E_3}[(2+2)2\times 2]$
$=10[(4+4)4\times 4]+5[(4+2)4\times 2]+20[(2+2)2\times 2]=1840.$

Theorem 1.3: The first hyper-Gourava index of L(G) is 8020.

Proof. By using table (1), $d_G(u)$,$d_G(e)$ and E_1, E_2 and E_3 values for L(G) graph, we have

$HGO_1L(G)=\sum_{uv\in E(G)}[(d_u+d_v)+d_u\times d_v]^2$
$=\sum_{uv\in E_1}[(4+4)+4\times 4]^2+\sum_{uv\in E_2}[(4+2)+4\times 2]^2+\sum_{uv\in E_3}[(2+2)+2\times 2]^2$
$=10[(4+4)+4\times 4]^2+5[(4+2)+4\times 2]^2+20[(2+2)+2\times 2]^2=8020.$

Theorem 1.4: The second hyper-Gourava index of L(G) is 180480.

Proof. By using table (1), $d_G(u)$, $d_G(e)$ and E_1, E_2 and E_3 values for L(G), we have

$HGO_2L(G)=\sum_{uv\in E(G)}[(d_u+d_v)d_u\times d_v]^2$
$=\sum_{uv\in E_1}[(4+4)4\times 4]^2+\sum_{uv\in E_2}[(4+2)4\times 2]^2+\sum_{uv\in E_3}[(2+2)2\times 2]^2$
$=10[(4+4)4\times 4]^2+5[(4+2)4\times 2]^2+20[(2+2)2\times 2]^2=180480.$

Theorem 2.1: The first Gourava index of complement of total graph of L(G) is 827.

Proof. By using table (1), point, line vertex degrees and E_1, E_2 and E_3 values for complement of total graph of L(G) graph, we have

$GO_1\overline{T(L(G))}=\sum_{uv\in E(G)}[(d_u+d_v)+d_u\times d_v]$
$=\sum_{uv\in E_1}[(2+2)+2\times 2]+\sum_{uv\in E_2}[(2+3)+2\times 3]+\sum_{uv\in E_3}[(3+3)+3\times 3]$
$=14[(2+2)+2\times 2]+50[(2+3)+2\times 3]+11[(3+3)+3\times 3]=827.$

Theorem 2.2: The second Gourava index of complement of total graph of L(G) is 2318.

Proof. By using table (1), $d_G(u)$, $d_G(e)$and E_1, E_2 andE_3 values for complement of total graph of L(G), we have

$GO_2\overline{T(L(G))}=\sum_{uv\in E(G)}[(d_u+d_v)d_u\times d_v]$
$=\sum_{uv\in E_1}[(2+2)2\times 2]+\sum_{uv\in E_2}[(2+3)2\times 3]+\sum_{uv\in E_3}[(3+3)3\times 3]$
$=14[(2+2)2\times 2]+50[(2+3)2\times 3]+11[(3+3)3\times 3]=2318.$

Theorem 2.3: The first hyper-Gourava index of complement of total graphof L(G) is 9421.

Proof. By using table (1), $d_G(u)$, $d_G(e)$ and E_1, E_2 and E_3 values for complement of total graph of L(G) graph, we have

$HGO_1\overline{T(L(G))}=\sum_{uv\in E(G)}[(d_u+d_v)+d_u\times d_v]^2$
$=\sum_{uv\in E_1}[(2+2)+2\times 2]^2+\sum_{uv\in E_2}[(2+3)+2\times 3]^2+\sum_{uv\in E_3}[(3+3)+3\times 3]^2$
$=14[(2+2)+2\times 2]^2+50[(2+3)+2\times 3]^2+11[(3+3)+3\times 3]^2=9421.$

Theorem 2.4: The second hyper-Gourava index of complement of total graph of L(G) is 80660.

Proof. By using table (1),$d_G(u)$, $d_G(e)$and E_1, E_2 andE_3 values for complement of total graph of L(G) graph, we have

$HGO_2\overline{T(L(G))}=\sum_{uv\in E(G)}[(d_u+d_v)d_u\times d_v]^2$
$=\sum_{uv\in E_1}[(2+2)2\times 2]^2+\sum_{uv\in E_2}[(2+3)2\times 3]^2+\sum_{uv\in E_3}[(3+3)3\times 3]^2$
$=14[(2+2)2\times 2]^2+50[(2+3)2\times 3]^2+11[(3+3)3\times 3]^2=80660.$

Theorem 3.1: The first Gourava index of graph $G^{++}(L(G))$ is 334.

Proof. By using table (1), point, line vertex degrees and E_1, E_2 and E_3 values for $G^{++}(L(G))$, we have

$GO_1G^{++}(L(G))=\sum_{uv\in E(G)}[(d_u+d_v)+d_u\times d_v]$
$=\sum_{uv\in E_2}[(2+3)+2\times 3]+\sum_{uv\in E_3}[(3+3)+3\times 3]$
$=14[(2+3)+2\times 3]+12[(3+3)+3\times 3]=334.$

Theorem 3.2: The second Gourava index of $G^{++}(L(G))$ is 1068.

Proof. By using table (1), $d_G(u)$, $d_G(e)$and E_1, E_2 andE_3 values for $G^{++}(L(G)$, we have
$GO_2G^{++}(L(G)) = \sum_{uv\in E(G)}[(d_u + d_v)d_u \times d_v]$
$= \sum_{uv\in E_2}[(2 + 3)2 \times 3] + \sum_{uv\in E_3}[(3 + 3)3 \times 3]$
$= 14[(2 + 3)2 \times 3] + 12[(3 + 3)3 \times 3] = 1068.$

Theorem 3.3: The first hyper-Gourava index of $G^{++}(L(G))$ is 4394.

Proof. By using table (1), $d_G(u)$, $d_G(e)$ and E_1, E_2 and E_3 values for $G^{++}(L(G))$, we have
$HGO_1G^{++}(L(G)) = \sum_{uv\in E(G)}[(d_u + d_v) + d_u \times d_v]^2$
$= \sum_{uv\in E_2}[(2 + 3) + 2 \times 3]^2 + \sum_{uv\in E_3}[(3 + 3) + 3 \times 3]^2$
$= 14[(2 + 3) + 2 \times 3]^2 + 12[(3 + 3) + 3 \times 3]^2 = 4394.$

Theorem 3.4: The second hyper-Gourava index of $G^{++}(L(G))$ is 47592.

Proof. By using table (1), $d_G(u)$, $d_G(e)$and E_1, E_2 and E_3 values for $G^{++}(L(G))$, we have
$HGO_2G^{++}(L(G)) = \sum_{uv\in E(G)}[(d_u + d_v)d_u \times d_v]^2$
$= \sum_{uv\in E_2}[(2 + 3)2 \times 3]^2 + \sum_{uv\in E_3}[(3 + 3)3 \times 3]^2$
$= 14[(2 + 3)2 \times 3]^2 + 12[(3 + 3)3 \times 3]^2 = 47592.$

Theorem 4.1: The first Gourava index of $T^{++1}(L(G))$ is 732.

Proof. By using table (1), point, line vertex degrees and E_1, E_2 andE_3 values for $T^{++1}(L(G))$, we have
$GO_1T^{++1}(L(G)) = \sum_{uv\in E(G)}[(d_u + d_v) + d_u \times d_v]$
$= \sum_{uv\in E_1}[(4 + 4) + 4 \times 4] + \sum_{uv\in E_2}[(4 + 2) + 4 \times 2] + \sum_{uv\in E_3}[(2 + 2) + 2 \times 2]$
$= 16(4 + 4) + 4 \times 4] + 18[(4 + 2) + 4 \times 2] + 12[(2 + 2) + 2 \times 2] = 732.$

Theorem 4.2: The second Gourava index of $T^{++1}(L(G))$is 3104.

Proof. By using table (1), $d_G(u)$, $d_G(e)$and E_1, E_2 andE_3 values for $T^{++1}(L(G))$, we have
$GO_2T^{++1}(L(G)) = \sum_{uv\in E(G)}[(d_u + d_v)d_u \times d_v]$
$= \sum_{uv\in E_1}[(4 + 4)4 \times 4] + \sum_{uv\in E_2}[(4 + 2)4 \times 2] + \sum_{uv\in E_3}[(2 + 2)2 \times 2]$
$= 16[(4 + 4)4 \times 4] + 18[(4 + 2)4 \times 2] + 12[(2 + 2)2 \times 2] = 3104.$

Theorem 4.3: The first hyper-Gourava index of $T^{++1}(L(G))$ is 13512.

Proof. By using table (1), $d_G(u)$, $d_G(e)$ and E_1, E_2 and E_3 values for$T^{++1}(L(G))$, we have
$HGO_1T^{++1}(L(G)) = \sum_{uv\in E(G)}[(d_u + d_v) + d_u \times d_v]^2$
$= \sum_{uv\in E_1}[(4 + 4) + 4 \times 4]^2 + \sum_{uv\in E_2}[(4 + 2) + 4 \times 2]^2 + \sum_{uv\in E_3}[(2 + 2) + 2 \times 2]^2$
$= 16[(4 + 4) + 4 \times 4]^2 + 18[(4 + 2) + 4 \times 2]^2 + 12[(2 + 2) + 2 \times 2]^2 = 13512.$

Theorem 4.4: The second hyper-Gourava index of $T^{++1}(L(G))$ is 306688.

Proof. By using table (1), $d_G(u)$, $d_G(e)$ and E_1, E_2 andE_3 values for$T^{++1}(L(G))$, we have
$HGO_2T^{++1}(L(G)) = \sum_{uv\in E(G)}[(d_u + d_v)d_u \times d_v]^2$
$= \sum_{uv\in E_1}[(4 + 4)4 \times 4]^2 + \sum_{uv\in E_2}[(4 + 2)4 \times 2]^2 + \sum_{uv\in E_3}[(2 + 2)2 \times 2]^2$
$= 16[(4 + 4)4 \times 4]^2 + 18[(4 + 2)4 \times 2]^2 + 12[(2 + 2)2 \times 2]^2 = 306688.$

Table 1: Point, line vertex degrees and edge partition for $L(HAC_5C_6C_7)$, transformation graphs of $L(HAC_5C_6C_7)$ and their complements

Graph	$d_G(u)$	$d_G(e)$	E_1	E_2	E_3
$L(G)$	4	2,3	10	5	20
$\overline{L(G)}$	3	4	12	18	20
$T(L(G))$	3,4	2,3	00	00	36
$\overline{T(L(G))}$	2,3	2,3,4	14	50	11
$G^{++}L(G)$	2	3	00	14	12
$\overline{G^{++}L(G)}$	2	3	12	16	18
$G^{--}L(G)$	2,3	4	10	16	3
$\overline{G^{--}L(G)}$	2	3,4	4	6	8
$T^{++1}L(G)$	4,6	2,3,4	16	18	12
$\overline{T^{++1}L(G)}$	2	3,6	00	24	12
$T^{001}L(G)$	2,3	2,3	00	42	18
$\overline{T^{001}L(G)}$	3,4,6	2	8	24	12

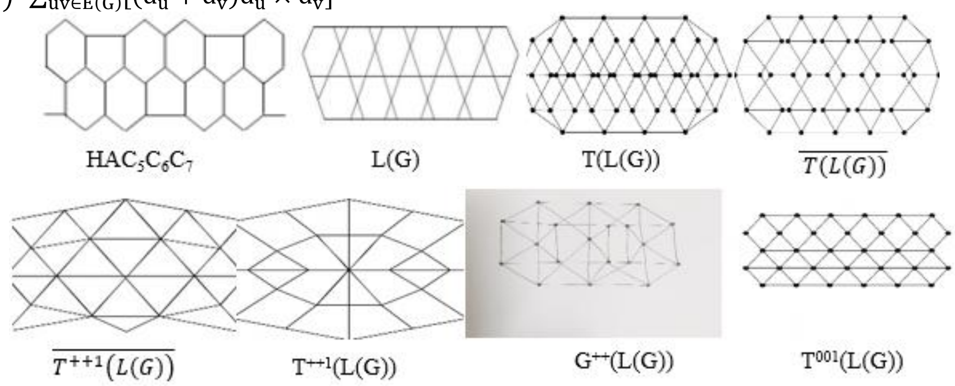

Figure 1.2: D graph of $HAC_5C_6C_7$[p,q]carbon nanotube, $L(HAC_5C_6C_7)$, total graph of $L(HAC_5C_6C_7)$, complement graph of total graph of $L(HAC_5C_6C_7)$, $\overline{T^{++1}(L(G))}$, $T^{++1}L((G))$, $G^{++}(L(G))$ and $T^{001}(L(G))$ graphs.

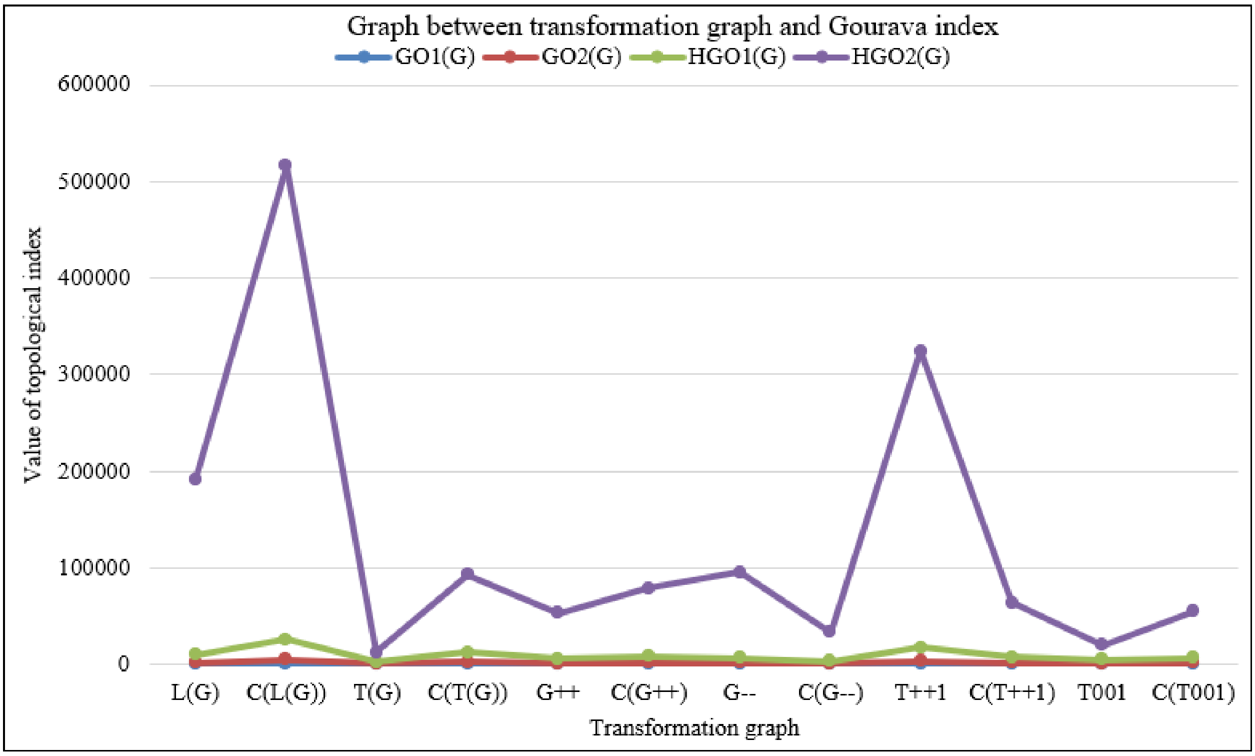

Figure 2: Graphical representation $L(HAC_5C_6C_7)$ and transformation graphs of $L(HAC_5C_6C_7)$ and their complements with $GO_1(G)$, $GO_2(G)$, $HGO_1(G)$ and $HGO_2(G)$ indices.

4. Conclusion

In this paper first, second Gourava indices, first and second hyper-Gourava indices of $L(HAC_5C_6C_7)$, complement of $L(HAC_5C_6C_7)$, total graph $T(L(G))$, $\overline{\mathbf{T(L(G))}}$, $G^{++}(L(G))$, $\overline{\mathbf{G^{++}(L(G))}}$, $G^{--}(L(G))$, $\overline{\mathbf{G^{--}(L(G))}}$, $T^{++1}(L(G))$, $\overline{\mathbf{T^{++1}(L(G))}}$, $T^{001}(L(G))$ and $\overline{\mathbf{T^{001}(L(G))}}$ are obtained. Gourava indices and hyper-Gourava indices studied graphically for these graphs. Second hyper-Gourava indices has larger values among these transformation graphs.

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