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HARMONIC POLYNOMIAL AND HARMONIC INDEX OF MOLECULAR GRAPH

Raut Nagsen Khanderao

Abstract

Let G be a graph with vertex set V (G) and edge set E (G). The Harmonic polynomial is defined as H(G,x) = 2 $\sum_{u\,v \in E\,(G)} x^{\,d(u)+\,d(\,v)-1}$, where d(v) is the degree of vertex v in G. In this paper degree, inverse degree and Revan vertex degree based Harmonic polynomials for 2, 2, 3-trimethyl pentane, carbon nanocone $C_5[2]$ and carbon nanotube $TUAC_6$ are investigated.

Keywords: Topological indices; molecular graph; inverse degree; Revan vertex degree; Harmonic polynomial.

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1. Introduction

Let G = (V, E) be a graph with set V (G) and edge set E (G). The degree of vertex v in a graph G is the number of edges incident to v, except that each loop at v counts twice [1].The Harmonic index and relation of it with different topological indices are studied in [2-4]. The degree based topological indices are dealt in [5-6].The different topological polynomials are investigated by [7-19]. Hosaya polynomial is the key polynomial in the area of distance-based topological indices .The edge version of Harmonic polynomial is studied by R. Nasir et al. [20].Let G be a graph with u, v ∈ V (G) and e = uv ∈ E (G) then $d_e = d_u + d_v$ -2.The multiplicative version of reverse index and Revan index are studied for ABC, product connectivity, sum connectivity, GA for dendrimer nanostars in many papers. Let G be a simple connected graph of order n with m edges and let P, Δ and δ denote the number of pendent vertices, maximum vertex degree and minimum degree of G respectively. The reverse vertices and Revan vertices of uv edge are defined in [22].The reverse degree of a vertex u is $c_u = \Delta G - d_G - 1$ and the Revan vertex degree of a vertex u in G is $rG(u) = \Delta(G) - \delta_{(G)} - d_G(u)$. In this paper Harmonic Revan vertex degree polynomial and Harmonic reverse vertex degree polynomial and their corresponding Harmonic indices are studied for molecular graphs of 2, 2 ,3-trimethyl pentane, carbon nanocone C_5[2] and carbon nanotube $TUAC_6$.

2. Research Method

The Harmonic polynomial is defined in [21] as, $H(G, x) = 2 \sum_{uv \in E(G)} x^{d(u)+d(v)-1}$.

And the corresponding Harmonic index as $H(G) = \frac{\partial H(G,x)}{\partial x} /_{x=1}$

The Harmonic Revan vertex degree polynomial and Harmonic reverse vertex polynomial [23] can be defined as, Harmonic Revan vertex degree polynomial:

$H(G,x) = 2 \sum_{uv \in E(G)} x^{r(u)+r(v)-1}$.

Harmonic vertex degree polynomial,

$H(G,x) = 2 \sum_{uv \in E(G)} x^{d(u)+d(v)-1}$.

$H(G) = \frac{\partial H(G,x)}{\partial x} /_{x=1}$

Harmonic reverse vertex polynomial

$H(G,x) = 2 \sum_{uv \in E(G)} x^{cu+cv-1}$

$H(G) = \frac{\partial H(G,x)}{\partial x} /_{x=1}$

.

The corresponding Harmonic Revan vertex degree, Harmonic reverse vertex degree polynomials are defined from degree-based Harmonic polynomial and Harmonic index. It is interesting to see what happens to Harmonic polynomial and Harmonic indices in terms of Revan vertex degree and reverse vertex degree. All the molecular graphs considered in this paper are simple, connected, loopless and without multiple edges. The notations used in this paper are standard and mainly taken from the standard books of graph theory [24-27].We are interested to see that what happens to Harmonic indices under the study of Revan vertex degree and inverse vertex degree for branched hydrocarbon, nanocone and carbon nanotube. In this paper degree, inverse degree and revan vertex degree based Harmonic polynomials for molecular graphs of 2, 2, 3-trimethyl pentane, carbon nanocone C5 □2□ and $TUAC_6$[5, 9] nanotube [28, 29] are investigated.

Table 1. The edge partitions, Revan vertex degree, inverse vertex degree and vertex degree of molecular graphs armchair polyhex $TUAC_6$[5, 9] nanotube, carbon nanocone C_5 [2].

Molecular graph : $TUAC_6$ [5, 9] nanotube	$d_u, d_v \in E(G)$ vertex degree	(2,2)	(2,3)	(3,3)
	Revan vertex degree	(3,3)	(3,2)	(2,2)
	Inverse vertex degree	(2,2)	(2,1)	(1,1)
	Number of edges	2m	4m	3mn-2m
Carbon nanocone C_5[2]	Revan vertex degree	(3,3)	(3,2)	(2,2)
	Inverse vertex degree	(2,2)	(2,1)	(1,1)
	Number of edges	5	20	35

Table 2. The edge partitions, Revan vertex degree, inverse vertex degree and vertex degree in molecular graph of 2, 2, 3-trimethyl pentane.

Molecular graph: 2,2,3-trimethyl pentane	$d_u, d_v \in E(G)$ vertex degree	(1,4)	(1,3)	(2,3)	(3,4)	(1,2)
	Revan vertex degree	(4,1)	(4,2)	(3,2)	(2,1)	(4,3)
	Inverse vertex degree	(4,1)	(4,2)	(3,2)	(2,1)	(4,3)
	Number of edges	(3)	(1)	(1)	(1)	(1)

Table 3. The Harmonic polynomials and Harmonic indices of $TUAC_6$ [5, 9], C_5 [2] and 2, 2, 3-trimethyl pentane.

Molecular graph	Degree	Harmonic polynomial	Harmonic index
$TUAC_6$[5,9]	Vertex degree	$4mx^3+8mx^4+2(3mn-2m)x^5$	44m+10(3mn-2m)
	Revan vertex degree	$2(3mn-2m)x^3+8mx^4+4mx^5$	52m+6(3mn-2m)
	Inverse vertex degree	$2(3mn-2m)x+8mx^2+4mx^3$	28m+2(3mn-2m)
C_5[2]	Vertex degree	$10x^3+40x^4+70x^5$	540
	Revan vertex degree	$70x^5+40x^4+10x^5$	420
	Inverse vertex degree	$40x^2+10x^3+70x^{5s}$	460
2,2,3-trimethyl pentane	Vertex degree	$2x^2 + 2x^3+8x^4+2x^6$	54

	Revan vertex degree	$2x^2 + 8x^4+2x^5+2x^6$	58
	Inverse vertex degree	$2x^2+8x^4+2x^5$	46

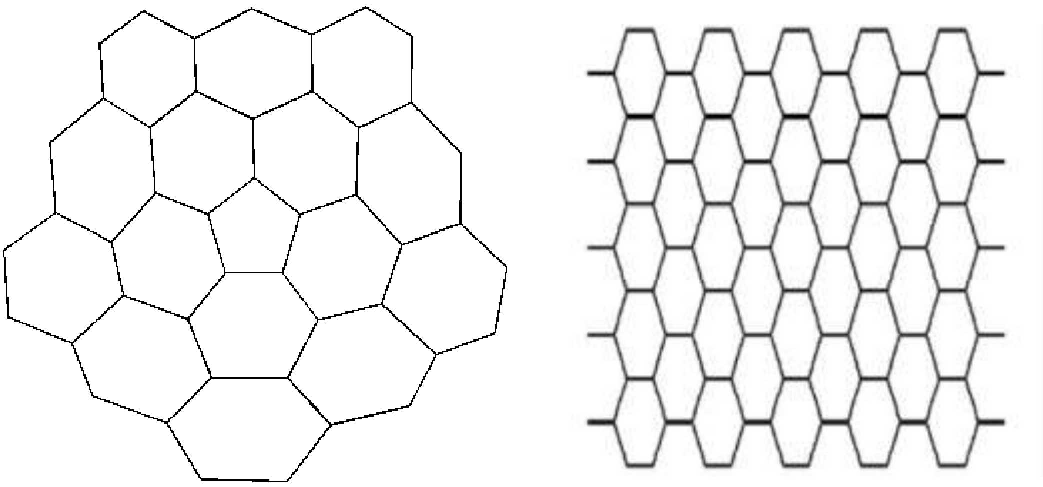

Figure 1. Graph of pentagonal nanocones C_5 □2□ with its first two layers and armchair polyhex TUAC6[5, 9].

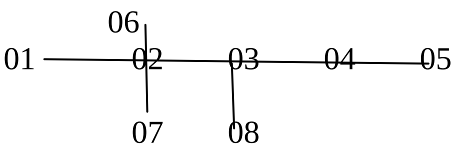

Figure 2. Molecular graph of 2, 2, 3- trimethyl pentane.

3. Results and Analysis

The molecular graph of $TUAC_6[5,9]$ and $C_5[2]$ are shown in figure 1.The maximum and minimum degree for $TUAC_6[5, 9]$ and $C_5[2]$ are 3 and 2 respectively.In the armchair polyhex nanotube G = TUAC $_6$ [m, n],where m denotes number of hexagons in first row and n denotes number of rows. There are 2m, 4m and 2(3mn-2m) edges.The hydrogen suppressed molecular graph of 2, 2, 3-trimethyl pentane is shown in figure 2. In this molecular graph maximum degree is 4 for vertex 2 and minimum degree is 1 for the pendent vertex. It is observed from figure 1 that edges uv are 3x(1,4),1x(1,3),1x(3,4),1x(2,3) and 1x(1,2) as there are 5 pendent vertices. The number of edges, vertex degree, Revan vertex degree and inverse vertex degrees for $TUAC_6[5,9]$, $C_5[2]$ and 2,2,3-trimethyl pentane computed on figures 1-2 and are used in computing the Harmonic polynomials and Harmonic indices of $TUAC_6[5,9]$,$C_5[2]$ and 2,2,3-trimethyl pentane. The Harmonic polynomial and Harmonic index for $TUAC_6[5,9]$ computed as,

Harmonic vertex degree polynomial,

$H(G,x) = 2 \sum_{u v \in E(G)} x^{d(u)+d(v)-1}$.= $4mx^3+8mx^4+2(3mn-2m)x^5$.

Where m and n denotes number of hexagons in first row and n denotes number of rows.

$H(G) = \frac{\partial H(G,x)}{\partial x}/_{x=1}$ = 44m+10(3mn-2m).

Harmonic Revan vertex degree polynomial,

$H(G,x) = 2 \sum_{u v \in E(G)} x^{r(u)+r(v)-1} = 2(3mn-2m)x^3+8mx^4+4mx^5$.

$H(G) = \frac{\partial H(G,x)}{\partial x}/_{x=1}$ = 52m+6(mn-2m).

Harmonic reverse vertex degree polynomial,

$H(G,x) = 2 \sum_{u v \in E(G)} x^{cu+cv-1} = 2(3mn-2m)x+8mx^2+4mx^3$.

$H(G) = \frac{\partial H(G,x)}{\partial x}/_{x=1}$ = 28m+2(3mn-2m).

The edge partition, Revan vertex degree, inverse vertex degree and vertex degree of molecular graph of

$TUAC_6[5,9]$, $C_5[2]$, 2,2, 3-trimethyl pentane are given in table 1-2. The Harmonic polynomials and

Harmonic indices for $C_5[2]$ and 2,2,3-trimethyl pentane are computed by using vertex degree, Revan

vertex degree, inverse vertex degree and edge partitions on respective molecular graphs.

The Harmonic polynomials and Harmonic indices of $TUAC_6$ [5, 9], $C_5[2]$ and 2,2,3-trimethyl pentane are represented in table 3.

4. Conclusion

The Harmonic polynomials and Harmonic indices are studied in terms of Revan vertex degree, inverse vertex degree and vertex degree for Molecular graphs of 2,2,3-trimethyl pentane,$C_5[2]$ and $TUAC_6$.The Harmonic polynomials and indices are different for Revan vertex degree, inverse vertex degree,vertex degree in 2,2,3-trimehyl pentane , $C_5[2]$ and $TUAC_6$.

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