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Irregularity molecular descriptors of $VC_5C_7[m,n]$ and $HC_5C_7[m,n]$ nanotubes

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Scientific organizations are creating carbon nanotube-based composites like $VC_5C_7[m,n]$ and $HC_5C_7[m,n]$, which indicate significant response against voltage. Imbalance-based irregularity indices determine the degree of irregularity of a certain molecular structure and, as a result, determine the properties of a molecular substance. In this article, we aim to compute irregularity indices of two nanotubes, $VC_5C_7[m,n]$ and $HC_5C_7[m,n]$. We produce formulas for the irregularity of these two nanotubes, which are functions depending on the parameters of the structure m and n. We compare our results graphically and conclude that $VC_5C_7[m,n]$ is more irregular than $HC_5C_7[m,n]$.

KEYWORDS

irregularity index, $VC_5C_7[m,n]$ and HC_5C_7 $[m,n]$, nanotubes, imbalance-based irregularity measure, molecular computing

Introduction

The chemical graph theory is rich with novel developments of functions and polynomials to foresee physiochemical aspects of chemical structures without using tools of quantum mechanics. One type of such a function is imbalance-based irregularity indices which determine the molecular complexity of the chemical substance under discussion. Carbon nanotubes are allotropes of carbon with a cylindrical-shaped nanostructure. These cylindrical-shaped carbon particles have amazing properties, which are significant for nanotechnology, optics, electronics, and various fields of material science and development [1–3].

Regarding flexible modulus and elasticity, carbon nanotubes are the stiffest and most grounded materials individually. This quality results from the covalent sp_2 bonds framed between the carbon atoms. A multi-walled carbon nanotube was analyzed in 2000, which has a tensile strength of 63 gigapascals. The adaptability and quality of carbon nanotubes make them of potential use in controlling other nanoscale structures, which suggests that they will have a basic activity in nanotechnology building [4–7]. Molecular topologists are interested in studying the complexity, pattern, combinatorial properties, and irregularities of molecular structures. A basic tool is the conversion of the molecular structure into a graph theoretic model, where vertices are used as toms and edges are used as bonds.

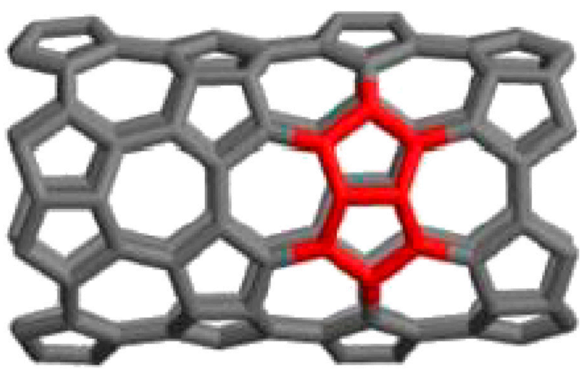

FIGURE 1
Molecular graph of VC_5C_7.

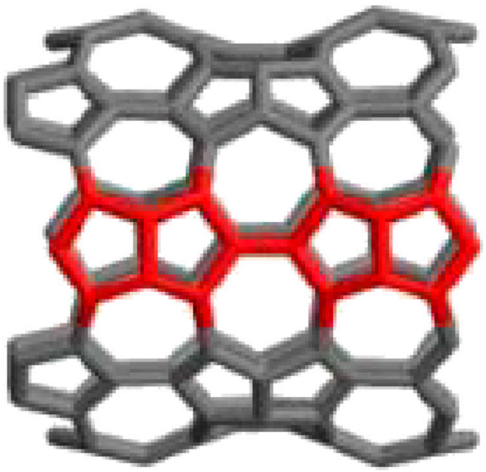

FIGURE 2
Molecular graph of HC_5C_7.

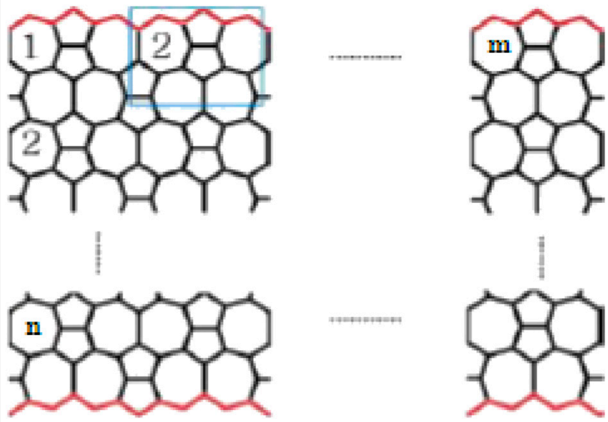

FIGURE 3
Two-dimensional lattice of VC_5C_7.

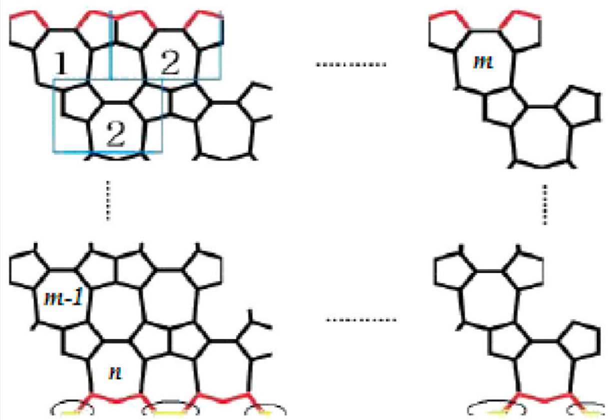

FIGURE 4
Two-dimensional lattice of HC_5C_7.

In this article, we aim to compute the imbalance-based degree of irregularity of carbon nanotubes. The molecular graphs of carbon nanotubes $VC_5C_7[m,n]$ and $HC_5C_7[m,n]$ are shown in Figures 1, 2, respectively. One is interested to know the degree of the molecular complexity of these tubes comparatively so that an overview of the properties depending upon the molecular complexity can be understood. By using linear regression, a stochastic relationship can be established between the aforementioned irregularity indices and different properties such as standard enthalpy of vaporization, boiling point, entropy, and acentric factor. The structures of these nanotubes consist of cycles C_5 and C_7 (C_5C_7 net which is a trivalent decoration constructed by alternating C_5 and C_7) by different compounds. It can cover either a cylinder or a torus.

The two-dimensional lattice of $VC_5C_7[m,n]$ is shown in Figure 3, and the two-dimensional lattice of $HC_5C_7[m,n]$ is shown in Figure 4.

In order to proceed with our main objective, we have to be a bit familiar with some notions and notations of the graph theory. We consider only a simple and connected graph G with vertex V, edge set E, and *du* and *dv*, the degree of vertices u and v, respectively. A topological invariant is an isomorphism of the graph that preserves the topology of the graph. A graph is said to be regular if every vertex of the graph has the same degree. A

TABLE 1 Edge partition of the $VC_5C_7[m,n]$ nanotube.

Number of edges (d_u, d_v)	Number of indices
$(2,3)$	$[24mn - 6m]$
$(3,3)$	$12m$

topological invariant is called an irregularity index if this index vanishes for a regular graph and is non-zero for a non-regular graph. Regular graphs have been extensively investigated, particularly in mathematics. Their applications in the chemical graph theory initiated the discovery of nanotubes and fullerenes. Paul Erdos stressed the study of irregular graphs for the first time in history in [8]. In the Second Krakow Conference on Graph Theory (1994), Erdos officially posed an open problem as "the determination of extreme size of highly irregular graphs of given order" [9]. Since then, irregular graphs and the degree of irregularity have become one of the core open problems of the graph theory.

A graph in which each vertex has a different degree than the other vertices is known as a perfect graph. The authors of [10] demonstrated that no graph is perfect. The graphs lying in between are called quasi-perfect graphs, in which all except two vertices have different degrees [9]. Simplified ways of expressing irregularities are irregularity indices. These irregularity indices have been studied recently in a novel way [11, 12]. The first such irregularity index was introduced in [13]. Most of these indices used the concept of the imbalance of an edge defined as $\boldsymbol{imball_{uv}} = |\boldsymbol{du} - \boldsymbol{dv}|$ [14, 15]. The Albertson index, AL(G), was defined by Albertson in [15] as $\boldsymbol{AL(G)} = \sum_{UV \in E} |d_u - d_v|$. In this index, the imbalance of edges is computed. The irregularity indices IRL(G) and IRLU(G) are introduced by Vukicevic and Gasparov [16], as $\boldsymbol{IRL(G)} = \sum_{UV \in E} |\ln d_u - \ln d_v|$ and $\boldsymbol{IRLU(G)} = \sum_{UV \in E} \frac{|d_u - d_v|}{\min(d_u, d_v)}$, respectively. Recently, Abdoo et al. have introduced a new term "total irregularity measure of a graph G," which is defined as [17–19] $\boldsymbol{IRR_t(G)} = \frac{1}{2} \sum_{UV \in E} |d_u - d_v|$. Recently, Gutman et al. have introduced the IRF(G) irregularity index of the graph G, which is described as $\boldsymbol{IRF(G)} = \sum_{UV \in E} (d_u - d_v)^2$ in [20]. The Randic index itself is directly related to an irregularity measure, which is described as $\boldsymbol{IRA(G)} = \sum_{UV \in E} (d_u^{-1/2} - d_v^{-1/2})^2$ in [21]. Further irregularity indices of similar nature can be traced in [21] in detail. These indices are given as $\boldsymbol{IRDIF(G)} = \sum_{UV \in E} |\frac{d_u}{d_v} - \frac{d_v}{d_u}|$, $\boldsymbol{IRLF(G)} = \sum_{UV \in E} \frac{|d_u - d_v|}{\sqrt{(d_u d_v)}}$, $\boldsymbol{LA(G)} = 2 \sum_{UV \in E} \frac{|d_u - d_v|}{(d_u + d_v)}$, $\boldsymbol{IRD1} = \sum_{UV \in E} \ln\{1 + |d_u - d_v|\}$,

TABLE 2 Test values for the irregularity indices of the nanotube $VC_5C_7[m,n]$.

Irregularity indices for the $VC_5C_7[m,n]$ nanotube

Irregularity index	$m=1$ $n=1$	$m=2$ $n=2$	$m=3$ $n=3$	$m=4$ $n=4$	$m=5$ $n=5$
$IRDIF(G) = \sum_{UV \in E} \lvert\frac{d_u}{d_v} - \frac{d_v}{d_u}\rvert$	15	70	165	300	475
$IRR(G) = \sum_{UV \in E} \lvert d_u - d_v\rvert$	20	88	204	368	580
$IRL(G) = \sum_{UV \in E} \lvert\ln d_u - \ln d_v\rvert$	7.29837	34.05906	80.28207	145.9674	231.1150
$IRLU(G) = \sum_{UV \in E} \frac{\lvert d_u - d_v\rvert}{\min(d_u, d_v)}$	9	42	99	180	285
$IRLU(G) = \sum_{UV \in E} \frac{\lvert d_u - d_v\rvert}{\sqrt{(d_u d_v)}}$	7.348469	34.2928	80.8331	146.9693	232.7015
$\sigma(G) = \sum_{UV \in E} (d_u - d_v)^2$	18	84	198	360	570
$IRLA(G) = 2 \sum_{UV \in E} \frac{\lvert d_u - d_v\rvert}{(d_u + d_v)}$	7.2	33.6	79.2	144	228
$IRD1 = \sum_{UV \in E} \ln\{1 + \lvert d_u - d_v\rvert\}$	12.4766	58.2243	137.2431	249.5329	395.094
$IRA(G) = \sum_{UV \in E} (d_u^{-1/2} - d_v^{-1/2})^2$	0.3031	1.4143	3.3336	6.0612	9.5969
$IRGA(G) = \sum_{UV \in E} \ln \frac{d_u + d_v}{2\sqrt{(d_u d_v)}}$	0.3673	1.7145	4.0414	7.3479	11.6343
$IRB(G) = \sum_{UV \in E} (d_u^{1/2} - d_v^{1/2})^2$	1.8184	8.4857	20.0021	36.3674	57.5817
$IRR_t(G) = \frac{1}{2} \sum_{UV \in E} \lvert d_u - d_v\rvert$	9	42	99	180	285

TABLE 3 Edge partition of the $C_5C_7[m,n]$ nanotube.

Number of edges (d_u, d_v)	Number of indices
(2,2)	m
(3,3)	$8m$
(2,3)	$(12mn - 4m)$

$IRGA(G) = \sum_{UV\in E} ln(\frac{d_u+d_v}{2\sqrt{(d_u d_v)}})$, and $IRB(G) = \sum_{UV\in E} (d_u^{\frac{1}{2}} - d_v^{\frac{1}{2}})^2$. Further details are given in [21–32]. There were various attempts to quantify the irregularity of a graph, of which the Collatz–Sinogowitz index, Bell index, Albertson index, and total irregularity are the best known [13–15]. It has been mathematically proven that no two of these irregularity measures are mutually consistent, namely, that for any two such measures, irrX and irrY, there exist pairs of graphs G1 and G2, such that irrX (G1) > irrX (G2) but irrY (G1) < irrY (G2). People working in related fields have used the aforementioned indices to capture the irregularity of chemical graphs, and occasionally, these indices depict properties such as symmetry and stability of isomers [21].

These irregularity indices have applications in determining the properties of alkane isomers [21]. These applications pushed others to think in this direction. Most recently, authors have computed irregularity indices of chemical substances [33–36]. Hussain et al. established closed forms of the aforementioned irregularity indices for some benzenoid systems in [35] and some nanostar dendrimers in [36]. The present article can be treated as a continuation of the articles [35, 36].

The main results

In this section, we present our main results about the theoretical computation of irregularity indices of the aforementioned nanotubes.

Theorem 1: For $m, n > 0$, the irregularity measures of $VC_5C_7[m,n]$ are

1 $IRDIF(VC_5C_7[m,n]) = 20mn - 5m$;
2 $IRR(VC_5C_7[m,n]) = 24mn - 4m$;
3 $IRL(VC_5C_7[m,n]) = 9.73116mn - 2.43279m$;
4 $IRLU(VC_5C_7[m,n]) = 12mn - 3m$;
5 $IRLU(VC_5C_7[m,n]) = 4\sqrt{6}mn - \sqrt{6}m$;
6 $\sigma(VC_5C_7[m,n]) = 24mn - 6m$;
7 $IRLA(VC_5C_7[m,n]) = 9.6mn - 2.4m$;

TABLE 4 Test values for the irregularity indices of the nanotube $HC_5C_7[m,n]$.

Irregularity indices for the $HC_5C_7[m,n]$ nanotube

Irregularity index	$m = 1$ $n = 1$	$m = 2$ $n = 2$	$m = 3$ $n = 3$	$m = 4$ $n = 4$	$m = 5$ $n = 5$
$IRDIF(G) = \sum_{UV\in E} \lvert\frac{d_u}{d_v} - \frac{d_v}{d_u}\rvert$	6.667	33.334	80.001	146.668	233.335
$IRR(G) = \sum_{UV\in E} \lvert d_u - d_v\rvert$	8	40	96	176	280
$IRL(G) = \sum_{UV\in E} \lvert lnd_u - lnd_v\rvert$	3.2437	16.2186	38.9246	71.3618	113.5302
$IRLU(G) = \sum_{UV\in E} \frac{\lvert d_u - d_v\rvert}{min(d_u,d_v)}$	4	20	48	88	140
$IRLU(G) = \sum_{UV\in E} \frac{\lvert d_u - d_v\rvert}{\sqrt{(d_u d_v)}}$	3.26598	16.3299	39.1918	71.8516	114.3095
$\sigma(G) = \sum_{UV\in E} (d_u - d_v)^2$	8	40	96	176	280
$IRLA(G) = 2\sum_{UV\in E} \frac{\lvert d_u - d_v\rvert}{(d_u + d_v)}$	3.2	16.0	38.4	70.4	112.0
$IRD1 = \sum_{UV\in E} ln\{1 + \lvert d_u - d_v\rvert\}$	5.54517	27.7258	66.54213	121.9939	194.0812
$IRA(G) = \sum_{UV\in E} (d_u^{-\frac{1}{2}} - d_v^{-\frac{1}{2}})^2$	0.13469	0.67347	1.616328	2.963268	4.71429
$IRGA(G) = \sum_{UV\in E} ln\frac{d_u + d_v}{2\sqrt{(d_u d_v)}}$	0.163287	0.81644	1.95945	3.592335	5.715079
$IRB(G) = \sum_{UV\in E} (d_u^{\frac{1}{2}} - d_v^{\frac{1}{2}})^2$	0.80816	4.04082	9.697969	17.7796	28.2857
$IRR_t(G) = \frac{1}{2}\sum_{UV\in E} \lvert d_u - d_v\rvert$	4	20	48	88	140

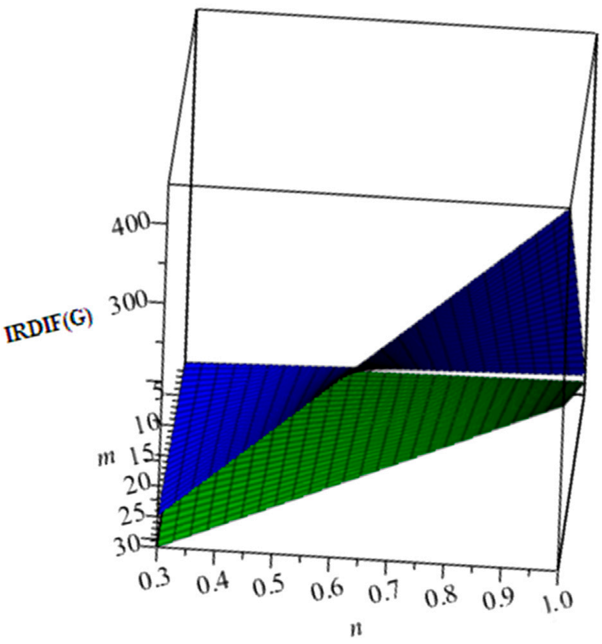

FIGURE 5
Demonstration of IRDIF.

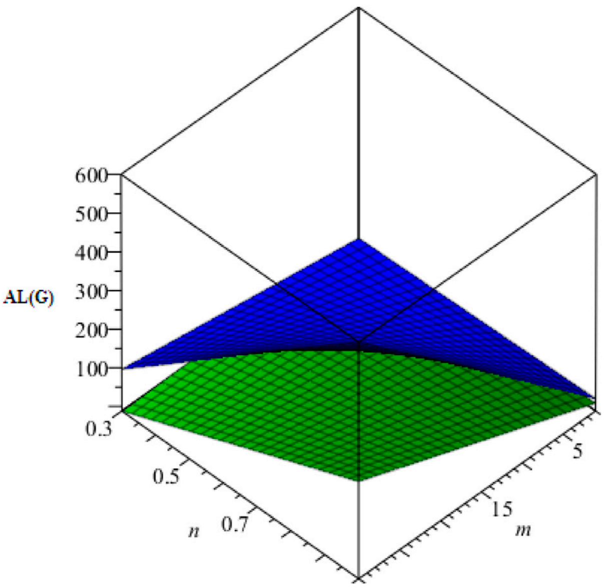

FIGURE 6
Demonstration of AL.

8 $IRD1\,(VC_5C_7\,[m, n]) = 16.635528mn - 4.158882m$;
9 $IRA\,(VC_5C_7\,[m, n]) = 0.4040820576mn - 0.1010205145m$;
10 $IRGA\,(VC_5C_7\,[m, n]) = 0.4898639342mn$
$-0.1224659836m$;

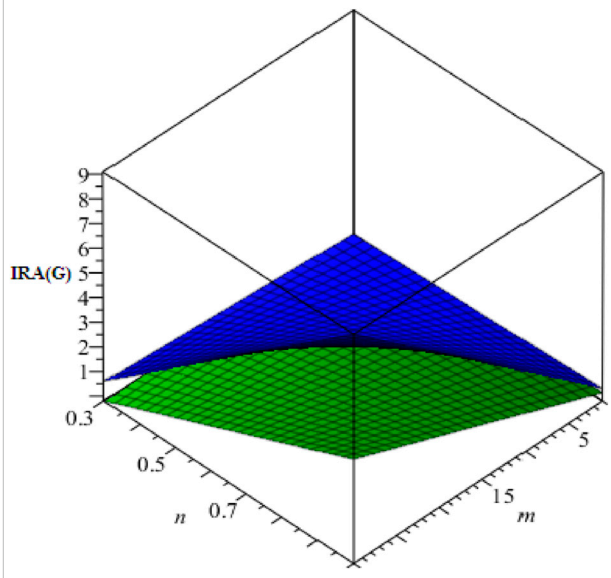

FIGURE 7
Demonstration of IRA.

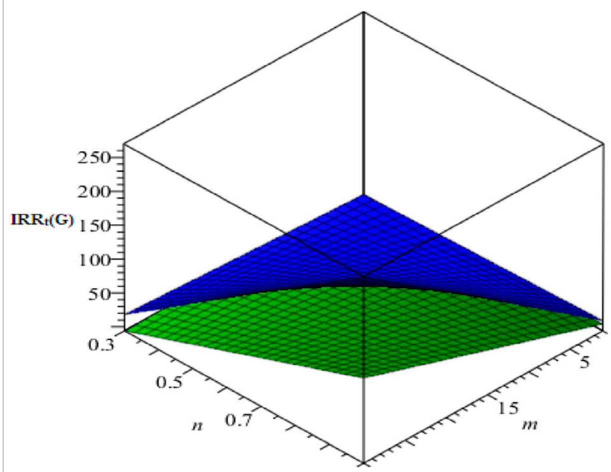

FIGURE 8
Demonstration of IRR_t.

11 $IRB\,(VC_5C_7\,[m, n]) = 2.424492346mn - 0.6061230864m$;
12 $IRR_t\,(VC_5C_7\,[m, n]) = 12mn - 3m$.

Proof:

In order to prove the aforementioned theorem, we have to consider Figures 1, 3. Table 1 shows the mathematical distribution of the types of edges into two different classes.

Now using Table 1 and the aforementioned definitions, we have

1. $IRDIF(G) = \sum_{UV \in E} |\frac{d_u}{d_v} - \frac{d_v}{d_u}|$

$$IRDIF(VC_5C_7[m,n]) = 12m|\frac{3}{3} - \frac{3}{3}| + [24mn - 6m]|\frac{3}{2} - \frac{2}{3}|$$
$$= 12m|0| + [24mn - 6m]|\frac{3}{2} - \frac{2}{3}| = [24mn - 6m]|\frac{3}{2} - \frac{2}{3}|;$$

2. $IRR(G) = \sum_{UV \in E} |d_u - d_v|$

$$IRR(VC_5C_7[m,n]) = 12m|3-3| + [24mn - 6m]|3-2|$$
$$= 12m|3-3| + [24mn - 6m]|3-2| = [24mn - 6m];$$

3. $(G) = \sum_{UV \in E} |lnd_u - lnd_v|$

$$IRL(VC_5C_7[m,n]) = 12m|ln\,3 - ln\,3| + [24mn - 6m]|ln\,3 - ln\,2|$$
$$= 12m|ln\,1| + [24mn - 6m]|ln\,3 - ln\,2|$$
$$= [24mn - 6m]\,ln\,\frac{3}{2};$$

4. $IRLU(G) = \sum_{UV \in E} \frac{|d_u - d_v|}{min(d_u d_v)}$

$$IRLU(VC_5C_7[m,n]) = 12m\frac{|3-3|}{3} + [24mn - 6m]\frac{|3-2|}{2}$$
$$= 12m\frac{|0|}{3} + [24mn - 6m]\frac{|3-2|}{2}$$
$$= [24mn - 6m]\frac{1}{2} = 12mn - 3m;$$

5. $IRLU(G) = \sum_{UV \in E} \frac{|d_u - d_v|}{\sqrt{(d_u d_v)}}$

$$IRLU(VC_5C_7[m,n]) = 12m\frac{|3-3|}{\sqrt{9}} + [24mn - 6m]\frac{|3-2|}{\sqrt{6}}$$
$$= 12m\frac{|0|}{\sqrt{9}} + [24mn - 6m]\frac{|1|}{\sqrt{6}} = \frac{24mn - 6m}{\sqrt{6}};$$

6. $\sigma(G) = \sum_{UV \in E} (d_u - d_v)^2$

$$\sigma(VC_5C_7[m,n]) = 12m(3-3)^2 + [24mn - 6m](3-2)^2$$
$$= 12m(0)^2 + [24mn - 6m](3-2)^2 = 24mn - 6m;$$

7. $IRLA(G) = 2\sum_{UV \in E} \frac{|d_u - d_v|}{(d_u + d_v)}$

$$IRLA(VC_5C_7[m,n]) = 2[12m\frac{|3-3|}{(9)} + [24mn - 6m]\frac{|3-2|}{(5)}]$$
$$= 2[12m\frac{|0|}{(9)} + [24mn - 6m]\frac{|1|}{(5)}] = \frac{48mn - 12m}{5};$$

8. $IRD1 = \sum_{UV \in E} ln\{1 + |d_u - d_v|\}$

$$IRD1 = 12mln\{1 + |3-3|\} + [24mn - 6m]\,ln\{1 + |3-2|\}$$
$$= 12mln\{1\} + [24mn - 6m]\,ln\{1+1\}$$
$$= [24mn - 6m]\,ln\,2 + 12\,ln\,1 = [24mn - 6m]\,ln\,2;$$

9. $IRA(G) = \sum_{UV \in E} (d_u^{-½} - d_v^{-½})^2$

$$IRA(VC_5C_7[m,n]) = 12m(\frac{1}{\sqrt{3}} - \frac{1}{\sqrt{3}})^2 + [24mn - 6m](\frac{1}{\sqrt{3}} - \frac{1}{\sqrt{2}})^2$$
$$= 12m(0)^2 + [24mn - 6m](\frac{1}{\sqrt{3}} - \frac{1}{\sqrt{2}})^2$$
$$= [24mn - 6m](\frac{1}{\sqrt{3}} - \frac{1}{\sqrt{2}})^2;$$

10. $RGA(G) = \sum_{UV \in E} ln\frac{d_u + d_v}{2\sqrt{(d_u d_v)}}$

$$IRGA(VC_5C_7[m,n]) = 12mln\frac{3+3}{2\sqrt{(9)}} + [24mn - 6m]\,ln\frac{3+2}{2\sqrt{(6)}}$$
$$= 12mln1 + [24mn - 6m]\,ln\frac{3+2}{2\sqrt{(6)}}$$
$$= [24mn - 6m]\,ln\frac{5}{2\sqrt{(6)}};$$

11. $IRB(G) = \sum_{UV \in E} (d_u^{½} - d_v^{½})^2$

$$IRB(VC_5C_7[m,n]) = 12m(\sqrt{3} - \sqrt{3})^2 + [24mn - 6m](\sqrt{3} - \sqrt{2})^2$$
$$= [24mn - 6m](\sqrt{3} - \sqrt{2})^2;$$

12. $IRR_t(G) = \frac{1}{2}\sum_{u,v \in V(G)} |d_u - d_v|$

$$IRR_t(VC_5C_7[m,n]) = \frac{1}{2}[12m|3-3| + [24mn - 6m]|3-2|]$$
$$= \frac{1}{2}[(24mn - 6m)|1| + 12m|0|] = 12mn - 3m;$$

Test values of the irregularity measures of the nanotube $VC_5C_7[m, n]$ has been given in Table 2. Now, we give our results about $HC_5C_7[m,n]$ for positive values of m and n.

Theorem 2: For $m, n > 0$, the irregularity measures of $HC_5C_7[m,n]$ are

1. $IRDIF(HC_5C_7[m,n]) = 10mn - 3.333m$;
2. $IRR(HC_5C_7[m,n]) = 12mn - 4m$;
3. $IRL(HC_5C_7[m,n]) = 4.865581297mn - 1.621860432m$;
4. $IRLU(HC_5C_7[m,n]) = 6mn - 2m$;
5. $IRLU(HC_5C_7[m,n]) = 2\sqrt{6}mn - \frac{2\sqrt{6}}{3}m$;
6. $\sigma(HC_5C_7[m,n]) = 12mn - 4m$;
7. $IRLA(HC_5C_7[m,n]) = 4.8mn - 1.6m$;
8. $IRD1(HC_5C_7[m,n]) = 8.317766167mn - 2.772588722m$;
9. $IRA(HC_5C_7[m,n]) = 0.2020410492mn - 0.06734700964m$;
10. $IRGA(HC_5C_7[m,n]) = 0.2449319671mn - 0.08164398904m$;
11. $IRB(HC_5C_7[m,n]) = 1.212246173mn - 0.4040820576m$;
12. $IRR_t(HC_5C_7[m,n]) = 6mn - 2m$.

Proof:

In order to prove the aforementioned theorem, we have to consider Figures 2, 4. Table 3 shows the distribution of edges into three different classes.

Now using Table 4 and the aforementioned definitions from Table 1, we have

1. $IRDIF(G) = \sum_{UV\in E} |\frac{d_u}{d_v} - \frac{d_v}{d_u}|$

$$IRDIF(HC_5C_7[m,n]) = m|\frac{2}{2} - \frac{2}{2}| + 8m|\frac{3}{3} - \frac{3}{3}| + (12mn - 4m)|\frac{3}{2} - \frac{2}{3}|$$
$$= m|0| + 8m|0| + (12mn - 4m)|\frac{3}{2} - \frac{2}{3}| = (12mn - 4m)|\frac{3}{2} - \frac{2}{3}|;$$

2. $IRR(G) = \sum_{UV\in E} |d_u - d_v|$

$$IRR(HC_5C_7[m,n]) = m|2-2| + 8m|3-3| + (12mn - 4m)|3-2|$$
$$= m|0| + 8m|0| + (12mn - 4m)|1| = (12mn - 4m)|1|;$$

3. $IRL(G) = \sum_{UV\in E} |lnd_u - lnd_v|$

$$IRL(HC_5C_7[m,n]) = m|ln\,2 - ln\,2| + 8m|ln\,3 - ln\,3| + (12mn - 4m)|ln\,3 - ln\,2|$$
$$= m|0| + 8m|0| + (12mn - 4m)|ln\,3 - ln\,2| = (12mn - 4m)\,ln\,\frac{3}{2};$$

4. $IRLU(G) = \sum_{UV\in E} \frac{|d_u - d_v|}{min(d_u d_v)}$

$$IRLU(HC_5C_7[m,n]) = m\frac{|2-2|}{2} + 8m\frac{|3-3|}{3} + (12mn - 4m)\frac{|3-2|}{2}$$
$$= m\frac{|0|}{2} + 8m\frac{|0|}{3} + (12mn - 4m)\frac{|1|}{2} = 6mn - 2m;$$

5. $IRLU(G) = \sum_{UV\in E} \frac{|d_u - d_v|}{\sqrt{(d_u d_v)}}$

$$IRLU(HC_5C_7[m,n]) = m\frac{|2-2|}{\sqrt{4}} + 8m\frac{|3-3|}{\sqrt{9}} + (12mn - 4m)\frac{|3-2|}{\sqrt{6}}$$
$$= m\frac{|0|}{\sqrt{4}} + 8m\frac{|0|}{\sqrt{9}} + (12mn - 4m)\frac{|1|}{\sqrt{6}} = \frac{(12mn - 4m)}{\sqrt{6}};$$

6. $\sigma(G) = \sum_{UV\in E} (d_u - d_v)^2$

$$\sigma(HC_5C_7[m,n]) = m(2-2)^2 + 8m(3-3)^2 + (12mn - 4m)(3-2)^2$$
$$= m(0)^2 + 8m(0)^2 + (12mn - 4m)(1)^2 = 12mn - 4m;$$

7. $IRLA(G) = 2\sum_{UV\in E} \frac{|d_u - d_v|}{(d_u + d_v)}$

$$IRLA(HC_5C_7[m,n]) = 2[m\frac{|2-2|}{(4)} + 8m\frac{|3-3|}{(9)} + (12mn - 4m)\frac{|3-2|}{(5)}]$$
$$= 2[m\frac{|0|}{(4)} + 8m\frac{|0|}{(9)} + (12mn - 4m)\frac{|1|}{(5)}] = \frac{2(12mn - 4m)}{(5)};$$

8. $IRD1 = \sum_{UV\in E} ln\{1 + |d_u - d_v|\}$

$$\text{IRD1} = mln\{1 + |2-2|\} + 8mln\{1 + |3-3|\} + (12mn - 4m)\,ln\{1 + |3-2|\}$$
$$= mln\{1 + |0|\} + 8mln\{1 + |0|\} + (12mn - 4m)\,ln\{1 + |1|\}$$
$$= mln1 + 8mln1 + (12mn - 4m)\,ln\,2 = (12mn - 4m)\,ln\,2;$$

9. $IRA(G) = \sum_{UV\in E} (d_u^{-½} - d_v^{-½})^2$

$$\text{IRA}(HC_5C_7[m,n]) = m(\frac{1}{\sqrt{2}} - \frac{1}{\sqrt{2}})^2 + 8m(\frac{1}{\sqrt{3}} - \frac{1}{\sqrt{3}})^2 + (12mn - 4m)(\frac{1}{\sqrt{3}} - \frac{1}{\sqrt{2}})^2$$
$$= m(0)^2 + 8m(0)^2 + (12mn - 4m)(\frac{1}{\sqrt{3}} - \frac{1}{\sqrt{2}})^2$$
$$= (12mn - 4m)(\frac{1}{\sqrt{3}} - \frac{1}{\sqrt{2}})^2;$$

10. $IRGA(G) = \sum_{UV\in E} ln\frac{d_u + d_v}{2\sqrt{(d_u d_v)}}$

$$IRGA(HC_5C_7[m,n]) = mln\frac{2+2}{2\sqrt{(4)}} + 8mln\frac{3+3}{2\sqrt{(9)}} + (12mn - 4m)\,ln\frac{3+2}{2\sqrt{(6)}}$$
$$= mln1 + 8mln1 + (12mn - 4m)\,ln\frac{5}{2\sqrt{(6)}}$$
$$= (12mn - 4m)\,ln\frac{5}{2\sqrt{(6)}};$$

11. $IRB(G) = \sum_{UV\in E} (d_u^{½} - d_v^{½})^2$

$$IRB(HC_5C_7[m,n]) = m(\sqrt{2} - \sqrt{2})^2 + (12mn - 4m)(\sqrt{3} - \sqrt{2})^2 + 8m(\sqrt{3} - \sqrt{3})^2$$
$$= m(0)^2 + (12mn - 4m)(0)^2 + 8m(\sqrt{3} - \sqrt{3})^2$$
$$= (12mn - 4m)(\sqrt{3} - \sqrt{2})^2;$$

12. $IRR_t(G) = \frac{1}{2}\sum_{u,v\in V(G)} |d_u - d_v|$

$$IRR_t(HC_5C_7[m,n]) = \frac{1}{2}[m|2-2| + 8m|3-3| + (12mn - 4m)|3-2|]$$
$$= \frac{1}{2}[m|0| + 8m|0| + (12mn - 4m)|1|]$$
$$= \frac{1}{2}[12mn - 4m] = 6mn - 2m.$$

Graphical analysis, discussions, and conclusion

In this section, we present our computational analysis of the irregularity of both of these nanotubes and compare the results obtained. We used 3D graphs in which the Z-axis represents the values of the irregularity indices and the other two axes are devoted to m and n. We used a BLUE graph to show the behavior irregularity indices of $VC_5C_7[m,n]$, and a GREEN graph shows the graphical behavior irregularity indices of $HC_5C_7[m,n]$. Following Figure 5 is the irregularity demonstration for the index IRDIF, which shows that $VC_5C_7[m,n]$ is more irregular than $HC_5C_7[m,n]$.

In Figure 6, we give a demonstration for the irregularity index AL. Again it can easily be concluded that $VC_5C_7[m,n]$ is more irregular than $HC_5C_7[m,n]$. It is evident from the graphs and the two tables where comparative values for the calculated indices are given. Values obtained by most irregularity indices for VC5C7 are higher than those for HC5C7 for the same values of parameters m and n. So, as far as computational irregularity is concerned, VC5C7 is more irregular than HC5C7. The same trends are shown by all other irregularity indices; please see Figures 7, 8. Based on the aforementioned comparative analysis, we conclude that $VC_5C_7[m,n]$ is more irregular than $HC_5C_7[m,n]$ for all irregularity indices discussed in this article. This conclusion can be useful in nano-engineering and electronics.

Data availability statement

The raw data supporting the conclusion of this article will be made available by the authors, without undue reservation.

Author contributions

MM conducted the computation and conceived the idea.

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Conflict of interest

The author declares that the research was conducted in the absence of any commercial or financial relationships that could be construed as a potential conflict of interest.

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