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IRREGULARITY TOPOLOGICAL INDEX OF A NANOROD GRAPH

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Introduction

Nanostructures have revolutionized modern science and technology, offering novel properties and applications in electronics, medicine, energy storage and catalysis. One way to model and analyze the structural properties of nanomaterials is through graph theory. In particular, topological indices derived from graph representations of nanostructures provide valuable insights into their chemical reactivity, stability and other physicochemical properties. In recent years, irregularity indices have gained prominences an important class of topological indices. These indices quantify the deviation from regularity in a graph, which can be linked to molecular instability or asymmetry in nanostructures. The discovery of fullerenes and carbon nanotubes (CNTs) led to the irregular molecular graphs [5]. Various irregularity indices such as Albertson's irregularity index, variance of degrees, total irregularity, IRL and IRM indices have been proposed and studied extensively in graph theory and mathematical chemistry.Quantifying the irregularity of graphs is a fundamental concept in numerous scientific disciplines, including chemistry and network theory. Admidst the different proposed irregularity measures, the Albertson irregularity index has received great interest due to its widespread applications [1]. The entire Albertson and entire sigma indices exhibited excellent correlations with the boiling point (BP) and π-electronic energy (E^{π}) of benzenoid hydrocarbons [2]. Tamas Reti et.al., determined the irregularity index for 18 set of isomers [8]. Arroyo et al.introduced the IRL and IRM indices, which further refine the concept of irregularity by incorporating linear and multiplicative relationships between vertex degrees. Recent work by Ghalavand et al. (2022) and others has focused on computing irregularity indices for various nanostructure families, including armchair polyhex nanotubes and other cylindrical nanostructures [3]. Shunguang kang et al., discusses the irregularity indices for neural networks [6]. Studies on nanostructure constructed from rectangular tessellations of hexagons, squares or other polygonal units have revealed patterns in irregularity indices that correlate with their size and structural configuration [4]. However the size of the non-metal oxide nano-structured system is not analyzed using these irregularity indices.

The present study builds on this foundation by deriving analytical expressions for several irregularity indices-including Albertson's irregularity index,irregularity based topological index, $IRA(G_{Nr})$, $IRLF(G_{Nr})$ and $IRLA(G_{Nr})$ for the nanorod graph. The results elucidate into how topological features influence the irregularity of nanostructures and pave the way for applications in materials design and nanotechnology. We investigate the irregularity topological indices of this graph to quantify its structural irregularity and to derive analytical expressions for these indices. The results contribute to the growing database of topological descriptors useful in nanoscience and support the development of quantitative structural property relationships (QSPR) for engineered nanomaterials. we aim to develope mathematical relationships that can further aid in understanding the influence of topology on nanorod-based materials. The author Sonia et al. [7] previously investigated the bioactivity of CuO Nanorods prepared under various concentrations of NaOH. The degree of vertex u, indicated by d_u, is the number of edges that are incident to u.

Albertson introduced the concept of irregularity index in 1997 [1]. Albertson irregularity index defined as

$$AL(G)=\sum_{uv\in E(G)}|d_u-d_v)$$

Li and Gutman were described as $IRA(G)$ in 2006 [9]. $IRA(G)$ defined as

$$IRA(G)=\sum_{uv\in E(G)}\left(\frac{1}{\sqrt{d_u}}-\frac{1}{\sqrt{d_v}}\right)^2$$

The irreegularity based topological index defined as [9]

$$IRB(G)=\sum_{uv\in E(G)}\left(\sqrt{d_u}-\sqrt{d_v}\right)^2$$

$IRLF(G)$ and $IRLA(G)$ are defined as [9]

$$IRLF(G)=\sum_{uv\in E(G)}\frac{|d_u-d_v)}{\sqrt{d_u d_v}} \text{ and } IRLA(G)=2\sum_{uv\in E(G)}\frac{|d_u-d_v)}{d_u+d_v}$$

Structure of the article

This reseearch elucidates the Nanorod graph for the first time as a method for analyzing the optical properties of CuO nanostructures. Additionally, the study also predict the irregular topological indices of the Nanorod graph, including the Albertson irregularity index, irregularity based topological index, $IRA(G_{Nr})$, $IRLF(G_{Nr})$ and $IRLA(G_{Nr})$ for various values of k and estimating the numerical values for generated Nanorod graphs. The present study on irregularity indices leads to + determine the size of the nanoparticle.

Nanorod graph

The Nanorod graph, represented as G_{Nr} is a simple connected graph with a vertex set $V(G)=\{v_1,v_2,v_3,\ldots,v_n\}$ and an edge set $E(G)$. In G_{Nr}, each vertex represents a different NaOH concentrations, and an edge is formed between two vertices if they correspond to the UV spectrum parameters (pH, temperature, time, volume of solvent in a given ratio) associated with those NaOH concentrations. To construct the family of Nanorod graphs, various step values are used from the range 0 to $[NaOH)_{max}$. In this study, we employ ten step values of $'k'(denotedby\,yk=0.1,0.09,0.08,0.07,0.06,0.05,0.04,0.03,0.02,0.01)$. The order of the Nanorod graph, represented as ’$^{p}[p=/\frac{0.5}{k}+1$¿¿]’, corresponds to the number of vertices, while the size is denoted by ’q’ and the reaction time is ’t’. Without loss of generality, we set $t=2$ hours to calculate the topological indices. This article aims to find the various irregularity based topological indices of the Nanorod graph G_{Nr}, considering its order (p) and reaction time (t)

Definition 1. Let $V(G_{Nr})$ represents the vertex set, which consists of the concentration of the NaOH solution. Specifically, $V(G)=\{v_1,v_2,v_3,\cdots/0.5\le v_i\le 2,\$\backslash\backslash\$ i=1,2,3,\cdots\}$.
Two vertices v_i and v_j are adjacent in G_{Nr} if

$$200\le\frac{\left[\left\{\left(v_i+v_j\right)Sol.1+Sol.2(C.S)\right)t+pH+R.T\right)}{Min\left(v_i,v_j\right)}\le 400$$

where, $R.T=30^{\circ}C$, $pH=12$, $t=2$hrs , Sol.1=Solvent 1= 25[Used to prepare aqueous NaOH solution],Sol.2= Solvent 2=50[Used to prepare aqueous copper acetate solution], C.S =Copper Source = copper acetate =0.2Mol.

Example 2. Figure 3.1 illustrates a Nanorod graph G_{Nr} with the step value $k=0.1$
In this graph, $V(G_{Nr})=\{v_1,v_2,\cdots;v_{16}\}$,(i.e) $V(G_{Nr})=\{0.5,0.6,0.7,0.8,\cdots;2\}$ and $E(G_{Nr})=\{e_1,e_2,\cdots;e_{59}\}$. According to definition 3.1,the vertices v_1 and v_2 are adjacent in G_{Nr}.Since $\frac{[(0.5+0.6)25+50(0.2))2+12+30}{Min(0.5,0.6)}=234$, which verifies the condition $200\le 234\le 400$.
Also, the vertices v_3 and v_4 are not adjacent in G_{Nr} as $\frac{[(0.7+0.8)25+50(0.2))2+12+30}{Min(0.7,0.8)}=195$, which does not lie in the required limit. Similarly, the adjacency of other vertex pairs in G_{Nr} can be determined by using the Definition 3.1. If the result falls within the range $200\le value\le 400$, then v_i and v_j are adjacent; otherwise, they are not.

Irregularity topological index of a Nanorod graph

In this section, we determine the Irregularity indices, including the Albertson irregularity index,Irregularity based index, $IRA(G_{Nr})$, $IRLF(G_{Nr})$ and $IRLA(G_{Nr})$ for a Nanorod Graph. We assume that $n=t-1,t,t+1,t+2$.

Theorem 3. *For any Nanorod Graph* G_{Nr}*,the Albertson irrugularity index* $AL(G_{Nr})$ *is*

$$\left\{\begin{array}{c} 82n+342 \; if\; k=0.1, n=t-1 \; and \; k=0.09, n=t \\ 4n^2+127n+4pn+17p+124 \; if \; k=0.08, n=t-1 \; and \; k=0.07, n=t \\ -47.6667n^5+320.3611n^4+163.5n^3-745.3889n^2+11828.6667n- \\ 10.8333pn^3+36.5pn^2-146.6667pn+131p-8432 \; if \; k=0.06, n=t-1, \\ k=0.05, n=t, k=0.04, n=t+1 \; and \; k=0.03, n=t+2 \\ 8340n^2+252788n-123pn+782p-264167 \; if \; k=0.02, n=t-1 \\ and \; k=0.01, n=t \end{array}\right)$$

Proof. *Let* G_{Nr} *be a Nanorod Graph*
We know that, the Albertson irregularity index is

$$AL(G_{Nr})=\sum_{uv\in E(G_{Nr})}|d_u-d_v)$$

Case (i) *When* $k=0.1, n=t-1$ *and* $k=0.09, n=t$

$$\sum_{uv\in E(G_{Nr})}|d_u-d_v)=|(p-1)-(p-1))+2|(p-1)-(p-2))+2\vee(p-1)- \quad \$\backslash\backslash\$$$

$$(p-5)|+2)(p-1)-(p-7)|+(-4n+12))(p-1)-(p-10)|+(6n-4))(p-1)- \quad \$\backslash\backslash\$\$(p-13)|+6|(p-1)-(p-11)|+6|(p-1)-(p-12)|+|(p-2)-(p-7)|+\backslash\backslash(-2n+6)|(p-2)-(p-10)|+(3n-2)|(p-2)-(p-13)|+3|(p-2)-(p-12)|+3|(p-2)-(p-11)|+3|(p-5)-(p-12)|+3|(p-5)-(p-11)|+(-2n+5)\backslash\backslash|(p-5)-(p-10)|+3|(p-7)-(p-11)|+(-2n+5)|(p-7)-(p-10)|+(-2n+5)|(p-10)-(p-10)|+(3n-3)|(p-5)-(p-13)|+(3n-3)|(p-7)-(p-12)|+(3n-3)|(p-10)-(p-11)|+(n-1)|(p-13)-(p-10)|\$.$$

On Simplification, we get

$$AL(G_{Nr})=\sum_{uv\in E(G_{Nr})}|d_u-d_v)=82n+342$$

Case(ii) *When* $k=0.08, n=t-1$ *and* $k=0.07, n=t$

$$\sum_{uv\in E(G_{Nr})}|d_u-d_v)=3|(p-1)-(p-1))+3|(p-1)-(p-3))+3\vee(p-1) \quad \$\backslash\backslash\$$$

On Simplification, we get

$$AL(G_{Nr})=\sum_{uv\in E(G_{Nr})}|d_u-d_v)=4n^2+127n+4pn+17p+124$$

The same procedure is used for Case (iii) and (iv) also. Thus,

Case (iii) *When* $k=0.06, n=t-1, k=0.05, n=t, k=0.04, n=t+1$ *and* $k=0.03, n=t+2$

$$AL(G_{Nr})=\sum_{uv\in E(G_{Nr})}|d_u-d_v)=-47.6667n^5+320.3611n^4+163.5n^3-745.3889n^2+11828.6667n-10.8333pn^3+36.5pn^2$$

Similarly,

Case(iv) *When* $k=0.02, n=t-1$ *and* $k=0.01, n=t$

$$AL(G_{Nr})=\sum_{uv\in E(G_{Nr})}\left|d_u-d_v\right)=8340n^2+252788n-123pn+782p-264167$$

Theorem 4. *Let* G_{Nr} *be a Nanorod Graph.Then the Irregualrity index* $IRA(G_{Nr})$ *is*

Proof. *Let* G_{Nr} *be a Nanorod Graph*
We know that, the Irregularity index is

$$IRA(G_{Nr})=\sum_{uv\in E(G_{Nr})}\left(\frac{1}{\sqrt{d_u}}-\frac{1}{\sqrt{d_v}}\right)^2$$

(i.e) $IRA(G_{Nr})=\sum_{uv\in E(G_{Nr})}\frac{d_u+d_v-2}{d_ud_v}$

Case (i) *When* $k=0.1,n=t-1$ *and* $k=0.09,n=t$

Simplifying the above expression, we get

$$\sum_{uv\in E(G_{Nr})}(d_u+d_v-2)=-39n+7pn+52p-131 \quad ...(1)$$

On Simplication, we get

$$\sum_{uv\in E(G_{Nr})}(d_ud_v)=943n+7p^2n-154pn+52p^2-610p+224 \quad ...(2)$$

From (1) and (2), $IRA(G_{Nr})=\frac{-168n+14pn+104p-714}{943n+7p^2n-154pn+52p^2-610p+224}$

$$IRA(G_{Nr})=(-168n+14pn+104p-714)(943n+7p^2n-154pn+52p^2-610p+224)^{-1}$$

Case(ii) *When* $k=0.08,n=t-1$ *and* $k=0.07,n=t$

$$\sum_{uv\in E(G_{Nr})}(d_u+d_v-2)=3[(p-1)+(p-1)-2]+3[(p-1)+(p-3)-2]+3[(p-1)+(p-6)-2]+3[(p-1)+(p-9)-2]+(-3n+9)[(p-1)+(p-11)-2]+12[(p-1)+(p-14)-2]+(6n-3)[(p-1)+(p-15)-2]+(-6n+15)[(p-1)+(p-13)-2]+9[(p-1)+(-n+8)-2]+(-n+3)[(p-3)+(p-11)-2]+4[(p-3)+(p-14)-2]+(2n-1)[(p-3)+(p-15)-2]+(-2n+5)[(p-3)+(p-13)-2]+3[(p-3)+(-n+8)-2]+3[(p-6)+(p-14)-2]+(-2n+5)[(p-6)+(p-13)-2]+3[(p-6)+7-2]+(2n-1)[(p-6)+(-2n+10)-2]+(-2n+5)[(p-9)+(p-13)-2]+3[(p-9)+7-2]+(2n-1)[(p-9)+8-2]+3[(p-11)+7-2]+(2n-1)$$

Simplifying the above expression, we get

$$\sum_{uv\in E(G_{Nr})}(d_u+d_v-2)=-4n^2-477n+42pn+117p-491 \quad ...(3)$$

On Simplication, we get

$$\sum_{uv\in E(G_{Nr})}(d_ud_v)=24n^2+602n-4pn^2+19p^2n-346pn+44p^2-310p-517 \quad ...(4)$$

From (3) and (4), $IRA(G_{Nr})=\frac{-4n^2-477n+42pn+117p-491}{24n^2+602n-4pn^2+19p^2n-346pn+44p^2-310p-517}$

$$IRA(G_{Nr})=(-4n^2-477n+42pn+117p-491)(24n^2+602n-4pn^2+19p^2n-346pn+44p^2-310p-517)^{-1}$$

The same method is used for Case (iii) and (iv) also. Thus,

Case(iii) *When* $k=0.06,n=t-1,k=0.05,n=t,k=0.04,n=t+1$ *and* $k=0.03,n=t+2$

$$\sum_{uv\in E(G_{Nr})}(d_u+d_v-2)=-7.8056n^6+50.9999n^5-309.1111n^4-1324.8333n^3+12960.3333n^2-25570.6666n+49.16$$

...(5)

$$\sum_{uv\in E(G_{Nr})}(d_ud_v)=1.5833n^6-133.3333n^5+524.3611n^4+17681.9999n^3-103823n^2+201366.667n-7.75pn^6+47.3$$

...(6)

From (5) and (6),

Similarly,

Case(iv) *When* $k=0.02, n=t-1$ *and* $k=0.01, n=t$

$$\sum_{uv\in E(G_{Nr})}(d_u+d_v-2)=-16445n^2-438851n+7768pn-6139p+457298$$ *...(7)*

$$\sum_{uv\in E(G_{Nr})}(d_ud_v)=-139987n^3+1133153n^2+7164254n-15469pn^2-411029pn+3627p^2n-3264p^2+424663p-$$

...(8)

From (7) and (8),

$$IRA(G_{Nr})=\frac{-16445n^2-438851n+7768pn-6139p+457298}{-139987n^3+1133153n^2+7164254n-15469pn^2-411029pn+3627p^2n-3264p^2+424663p-828}$$

Therefore,

$$IRA(G_{Nr})=(-16445n^2-438851n+7768pn-6139p+457298)(-139987n^3+1133153n^2+7164254n-15469p$$

Theorem 5. *For any Nanorod graph* G_{Nr}*, the Irrugularity Based index* $IRB(G_{Nr})$ *is*

Proof. *Let* G_{Nr} *be a Nanorod Graph*

We know that, the Irrugularity Based index is

$$IRB(G_{Nr})=\sum_{uv\in E(G_{Nr})}\left(\sqrt{d_u}-\sqrt{d_v}\right)^2$$

(i.e) $$IRB(G_{Nr})=\sum_{uv\in E(G_{Nr})}(d_u+d_v-2d_ud_v)$$

Case (i) *When* $k=0.1, n=t-1$ *and* $k=0.09, n=t$

$$\sum_{uv\in E(G_{Nr})}(d_u)=(p-1)+2(p-1)+2(p-1)+2(p-1)+[-4n+12)(p-1)+[6n-4)(p-1)+6(p-1)+6(p-1)+(p-2)+[$$

Simplifying the above expression, we get

$$\sum_{uv\in E(G_{Nr})}(d_u)=-39n+7pn+52p-131 \quad ...(1)$$

$$\sum_{uv\in E(G_{Nr})}(d_v)=(p-1)+2(p-2)+2(p-5)+2(p-7)+[-4n+12)(p-10)+[6n-4)(p-13)+6(p-11)+6(p-12)+(p-$$

Simplifying the above expression, we get

$$\sum_{uv\in E(G_{Nr})}(d_v)=-115n+7pn+52p-479 \quad ...(2)$$

By Theorem 4.2, $\sum_{uv\in E(G_{Nr})}(d_ud_v)=943n+7p^2n-154pn+52p^2-610p+224$ *...3)*

From (1),(2) and
(3),

$$IRB(G_{Nr})=-39n+7pn+52p-131-115n+7pn+52p-479-2(943n+7p^2n-154pn+52p^2-610p+224)$$

Therefore,

$$IRB(G_{Nr})=(-154n+14pn+104p-610)-2(943n+7p^2n-154pn+52p^2-610p+224)$$

Case(ii) *When* $k=0.08, n=t-1$ *and* $k=0.07, n=t$

Simplifying the above expression, we get

$$\sum_{uv\in E(G_{Nr})}(d_u)=-155n+17pn+61p-116 \quad ...(4)$$

Simplifying the above expression, we get

$$\sum_{uv\in E(G_{Nr})}(d_v)=-4n^2-272n+17pn+44p-259 \quad ...(5)$$

By Theorem 4.2, $\sum_{uv\in E(G_{Nr})}(d_ud_v)=24n^2+602n-4pn^2+19p^2n-346pn+44p^2-310p-517$ *...6)*

From (4),(5) and
(6),

$$IRB(G_{Nr})=-155n+17pn+61p-116-4n^2-272n+17pn+44p-259-2(24n^2+602n-4pn^2+19p^2n-346p$$

Therefore,

$$IRB(G_{Nr})=(-4n^2-427n+34pn+105p-375)-2(24n^2+602n-4pn^2+19p^2n-346pn+44p^2-310p-517)$$

The same method is used for Case (iii) and (iv) also. Thus,

Case (iii) *When* $k=0.06, n=t-1, k=0.05, n=t, k=0.04, n=t+1$ *and* $k=0.03, n=t+2$

$$\sum_{uv\in E(G_{Nr})}(d_u)=-248.3333n^3+5604n^2-3122.5n+11.3889pn^3-183.5pn^2+304.8333pn+24p+168$$

...(7)

$$\sum_{uv\in E(G_{Nr})}(d_v)=-6.6944n^6+74.3333n^5-426.0278n^4-803.0833n^3+8530n^2-18450.3056n+45.6667pn^3-274p$$

...(8)

By Theorem 4.2,

$$\sum_{uv\in E(G_{Nr})}(d_ud_v)=1.5833n^6-133.3333n^5+524.3611n^4+17681.9999n^3-103823n^2+201366.667n-7.75pn^6+47.3$$

...(9)

From (7),(8) and (9),

Therefore,

Case(iv) *When* $k=0.02, n=t-1$ *and* $k=0.01, n=t$

$$\sum_{uv\in E(G_{Nr})}(d_u)=-3634n^2-92625n+3704pn-2625p-94648 \quad ...(10)$$

$$\sum_{uv\in E(G_{Nr})}(d_v)=-12107n^2-337116n+3848pn-3433p+350859 \quad ...(11)$$

By Theorem 4.2,

$$\sum_{uv\in E(G_{Nr})}(d_ud_v)=-139987n^3+1133153n^2+7164254n-15469pn^2-411029pn+3627p^2n-3264p^2+424663p-$$

...(12)

From (7),(8) and
(9),

$$IRB(G_{Nr})=-3634n^2-92625n+3704pn-2625p-94648-12107n^2-337116n+3848pn-3433p+350859-$$

Therefore,

$$IRB(G_{Nr})=(-15741n^2-429741n+7552pn-6058p+256211)-2(-139987n^3+1133153n^2+7164254n-1546$$

Theorem 6. *Let* G_{Nr} *be a Nanorod Graph.Then the Irrugularity index* $IRLF(G_{Nr})$ *is*

¿ ***Proof.*** *Let* G_{Nr} *be a Nanorod Graph*

We know that, the Irrugularity index is

$$IRLF(G_{Nr})=\sum_{uv\in E(G_{Nr})}\frac{|d_u-d_v)}{\sqrt{d_ud_v}}$$

Case (i) *When* $k=0.1, n=t-1$ *and* $k=0.09, n=t$

By Theorem 4.1, $\sum_{uv\in E(G_{Nr})}|d_u-d_v)=82n+342$ *...(1)*

By Theorem 4.2, $\sum_{uv\in E(G_{Nr})}(d_ud_v)=943n+7p^2n-154pn+52p^2-610p+224$

$$\sum_{uv\in E(G_{Nr})}(\sqrt{d_ud_v})=\sqrt{943n+7p^2n-154pn+52p^2-610p+224} \quad ...(2)$$

From (1) and (2), $IRLF(G_{Nr})=\dfrac{82n+342}{\sqrt{943n+7p^2n-154pn+52p^2-610p+224}}$

Therfore, $IRLF(G_{Nr})=(82n+342)(943n+7p^2n-154pn+52p^2-610p+224)^{-\frac{1}{2}}$

Case(ii) *When* $k=0.08, n=t-1$ *and* $k=0.07, n=t$

By Theorem 4.1, $\sum_{uv\in E(G_{Nr})}|d_u-d_v)=4n^2+127n+4pn+17p+124$ *...(3)*

By Theorem 4.2, $\sum_{uv\in E(G_{Nr})}(d_ud_v)=943n+7p^2n-154pn+52p^2-610p+224$

$$\sum_{uv\in E(G_{Nr})}\left(\sqrt{d_ud_v}\right)=\sqrt{24n^2+602n-4pn^2+19p^2n-346pn+44p^2-310p-517}$$ *...(4)*

From (3) and (4), $IRLF(G_{Nr})=\frac{4n^2+127n+4pn+17p+124}{\sqrt{24n^2+602n-4pn^2+19p^2n-346pn+44p^2-310p-517}}$

Therfore,

$$IRLF(G_{Nr})=\left(4n^2+127n+4pn+17p+124\right)\left(24n^2+602n-4pn^2+19p^2n-346pn+44p^2-310p-517\right)^{-\frac{1}{2}}$$

Case(iii) *When* $k=0.06,n=t-1,k=0.05,n=t,k=0.04,n=t+1$ *and* $k=0.03,n=t+2$

By Theorem 4.2,

$$\sum_{uv\in E(G_{Nr})}\left(d_ud_v\right)=1.5833n^6-133.3333n^5+524.3611n^4+17681.9999n^3-103823n^2+201366.667n-7.75pn^6+47.3$$

$\sum_{uv\in E(G_{Nr})}\left(\sqrt{d_ud_v}\right)=\sqrt{1.5833n^6-133.3333n^5+524.3611n^4+17681.9999n^3}$ *$\\$*

$\sqrt{-103823n^2+201366.667n-7.75pn^6+47.3333pn^5-347pn^4-1450.8333pn^3+}$¿*$\\$*

$\sqrt{12751.5pn^2-24696pn+46.6667p^2n^3-266p^2n^2+465p^2n-188.5p^2+13940p-108630}$ *...(5)*

By Theorem 4.1,

$$\sum_{uv\in E(G_{Nr})}\left|d_u-d_v\right|=-47.6667n^5+320.3611n^4+163.5n^3-745.3889n^2+11828.6667n-10.8333pn^3+36.5pn^2-14$$

...(6)

From (5) and (6),Therfore,

Similarly,

Case (iv) *When* $k=0.02,n=t_1$ *and* $k=0.01,n=t$

By Theorem 4.2,

$$\sum_{uv\in E(G_{Nr})}\left(d_ud_v\right)=-139987n^3+1133153n^2+7164254n-15469pn^2-411029pn+3627p^2n-3264p^2+424663p-$$

$\sum_{uv \in {E(G_{Nr})}}(\sqrt{d_ud_v})=\\ \sqrt{-139987n^3+1133153n^2+7164254n-15469pn^2-411029pn+3627p^2n-3264p^2+}$$\\$$\sqrt{424663p-828825}$ *...(7)*

By Theorem 4.1, $\sum_{uv\in E(G_{Nr})}\left|d_u-d_v\right|=8340n^2+252788n-123pn+782p-264167$ *...(8)*

From (7) and (8),

$$IRLF(G_{Nr})=\frac{8340n^2+252788n-123pn+782p-264167}{\sqrt{-139987n^3+1133153n^2+7164254n-15469pn^2-411029pn+3627p^2n-3264p^2+424663p-}}$$

Therfore,

$$IRLF(G_{Nr})=\left(8340n^2+252788n-123pn+782p-264167\right)\left(-139987n^3+1133153n^2+7164254n-15469pn^2-\right.$$

Theorem 7. *For any Nanorod graph* G_{Nr}*, the Irregularity index* $IRLA(G_{Nr})$ *is*

¿ ***Proof.*** *Let* G_{Nr} *be a Nanorod Graph*

We know that, the Irrugularity index is

$$IRLF(G_{Nr})=\sum_{uv\in E(G_{Nr})} 2\frac{|d_u-d_v)}{d_u+d_v}$$

Case (i) *When* $k=0.1, n=t-1$ *and* $k=0.09, n=t$

By Theorem 4.1, $\sum_{uv\in E(G_{Nr})}|d_u-d_v)=82n+342$ *...(1)*

On Simplification, we get

$$\sum_{uv\in E(G_{Nr})}(d_u+d_v)=-154n+14pn+104p-610$$ *...(2)*

From (1) and (2), $IRLF(G_{Nr})=2\frac{82n+342}{-154n+14pn+104p-610}$

Therfore, $IRLF(G_{Nr})=2(82n+342)(-154n+14pn+104p-610)^{-1}$

Case(ii) *When* $k=0.08, n=t-1$ *and* $k=0.07, n=t$

By Theorem 4.1, $\sum_{uv\in E(G_{Nr})}|d_u-d_v)=4n^2+127n+4pn+17p+124$ *...(1)*

Simplifying the above expression, we get

$$\sum_{uv\in E(G_{Nr})}(d_u+d_v)=-4n^2-435n+42pn+117p-358$$ *...(2)*

From (1) and (2), $IRLF(G_{Nr})=2\frac{4n^2+127n+4pn+17p+124}{-4n^2-435n+42pn+117p-358}$

Therfore, $IRLF(G_{Nr})=2(4n^2+127n+4pn+17p+124)(-4n^2-435n+42pn+117p-358)^{-1}$

The same Method is used for Case (iii) and (iv) also. Thus,

Case(iii) *When* $k=0.06, n=t-1, k=0.05, n=t, k=0.04, n=t+1$ *and* $k=0.03, n=t+2$

$$\sum_{uv\in E(G_{Nr})}(d_u+d_v)=-7.8056n^6+65.6667n^5-313.2778n^4-1161.6667n^3+11922.1667n^2-17873n+69pn^3-392p$$

...(1)

By Theorem 4.1,

$$\sum_{uv\in E(G_{Nr})}|d_u-d_v)=-47.6667n^5+320.3611n^4+163.5n^3-745.3889n^2+11828.6667n-10.8333pn^3+36.5pn^2-14$$

...(2)

From (1) and (2),$IRLF(G_{Nr})=\\2\frac{-47.6667n^5+320.3611n^4+163.5n^3-745.3889n^2+11828.6667n-10.8333pn^3+36.5pn^2-146.6667pn+131p-8432}{-7.8056n^6+65.6667n^5-313.2778n^4-1161.6667n^3+11922.1667n^2-17873n+69pn^3-392pn^2+623pn-144p+12550}$

Therfore,

$$IRLF(G_{Nr})=2(-47.6667n^5+320.3611n^4+163.5n^3-745.3889n^2+11828.6667n-10.8333pn^3+36.5pn^2-146.$$

Similarly,

Case (iv) *When* $k=0.02, n=t_1$ *and* $k=0.01, n=t$

$$\sum_{uv\epsilon E(G_{Nr})}(d_u+d_v)=-16445n^2-429961n+7768pn-6139p+446995 \quad ...(1)$$

By Theorem 4.1, $\sum_{uv\in E(G_{Nr})}|d_u-d_v|=8340n^2+252788n-123pn+782p-264167 \quad ...(2)$

From (1) and (2), $IRLF(G_{Nr})=2\frac{8340n^2+252788n-123pn+782p-264167}{-16445n^2-429961n+7768pn-6139p+446995}$

Therfore,

$IRLF(G_{Nr})=2(8340n^2+252788n-123pn+782p-264167)(-16445n^2-429961n+7768pn-6139p+446995$

Numerical Assessment

Table 1 depicts the numerical values of various Irregularity topological indices for the Nanorod graph G_{Nr} corresponding to different step values of $k=0.1,0.09,0.08,0.07,0.06,0.05,0.04,0.03,0.02,0.01$. The indices considered include Albertson irregularity index irregularity based index, $IRA(G_{Nr})$, $IRLF(G_{Nr})$, $IRLA(G_{Nr})$.

The values diverge significantly, ranging from moderate to extremely large values, with some indices reaching exceptionally high magnitudes. Direct comparison and visualization of these values can be challenging due to the vast range of magnitudes. Hence the large index values in Table 1, is obtained using the formula:

$$NormalizedValue=\frac{OriginalValue}{max|OriginalValue)}\times 100$$

Revised Table

This transformation scales of all values relative to the maximum absolute value in the original dataset, converting them into dimensionless percentages. As a result, the revised values become easier to interpret and compare, emphasizing relative differences without being overwhelmed by large magnitudes. Negative values are preserved in their relative form, maintaining the direction of change while reducing their absolute impact. This scaling effectively manages a wide range of values, enhancing the visibility of trends and patterns. However, extremely small values with minimal influence can be excluded from the graph to avoid clutter and improve visual clarity.

Visualization using Cartesian plot

Plotting the original values directly would hinder effective visualization due to the wide range of magnitudes. In contrast,the scaled values enable clear comparative analysis and facilitate the identification of trends and behaviors patterns. Values that are close to zero in the revised data set can be considered negligible and may be omitted when plotting to enhance clarity.

figure 7.1

An Illustrate using six indices is presented in figure 7.1, where the maximum convergence of data points at $(0.045,-0.008)$ has been utilized to determine the size of the nanostructures. The size of the nanostructures is obtained by calculating the ratio of the Albertson irregularity index to the sum of all nodal intersection points and the entire expression is then divided by 10.

Conclusion

In this paper, various irregularity measures-namely the Albertson irregularity index, irregularity based topological index, $IRA(G_{Nr})$, $IRLF(G_{Nr})$ and $IRLA(G_{Nr})$, were analytically determined for different classes of Nanorod graphs. These indices provide insight into the structural diversity and vertex degree distribution within these molecular graph models, which are representative of nanomaterials with specific topologies. The derived closed-form expressions help in quantifying the extent of irregularity across different graph structures and highlight how the reaction parameters affect the degree-based properties. The findings are expected to contribute to the chemical graph theory framework and facliltate future studies in nanostructure modeling, ntopological characterization and design of new nanometrials with tailored properties.

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