A study of Indium phosphide and line graph of subdivision graph of H-naphtalenic nano-sheet via irregularity indices

Iftikhar Ali^{1™} , Muhammad Haroon Aftab^{2™} and Ali Akgül^{3,4,5}

¹Department of Mathematics, Baba Guru Nanak University, Nankana Sahib 39100, Pakistan
²Department of Mathematics and Statistics, The University of Lahore, Lahore 54000, Pakistan
³Department of Computer Science and Mathematics, Lebanese American University, Beirut 11022801, Lebanon
⁴Department of Mathematics, Art and Science Faculty, Siirt University, Siirt 56100, Turkey
⁵Department of Mathematics, Mathematics Research Center, Near East University, Near East Boulevard
PC: 99138, Nicosia /Mersin 10, Turkey

Corresponding author: iftikhar462@gmail.com; ORCID: https://orcid.org/0009-0006-5933-5317 haroonuet@gmail.com; ORCID: https://orcid.org/0000-0001-6441-2133

Received: 8 November 2024; revised: 14 April 2025; accepted: 29 April 2025

ABSTRACT

In this article, we have taken the molecular graph of indium phosphide InP[m,n] and line graph of subdivision graph of H-naphtalenicnano-sheet L(S(H(r,s))). Irregularity indices play an important role to describe the quantitative characterization of the non-regular graphs. In various problems and applications, particularly in subject of chemistry and material engineering irregular indices have so many uses, thus it is very important to know about the irregularity of a molecular structure. Moreover, the evaluation of the irregularity of graphs is an important not only for QSPR and QSAR but also very effective for the measuring the entropy, melting and boiling points, enthalpy of vaporization and toxicity. We have also discussed the graphical behaviors of the above indicated structures.

Keywords: Topological indices, irregular indices, indium phosphide, H-naphtalenic, molecular structure

INTRODUCTION

Corona virus 2 (SARS-CoV-2) is a contagious and caused form submicroscopic infectious agent virus [1-3]. Basically, nano-sheets are found in 2D nano-structures having thickness from 1 to 100 nm [1-4]. Nano-sheets having wonderful, physical, biological, electronic and chemical characteristics that are very effective for catalysis, storage, nano-bio-technology, electronics, optical and dielectric-associated problems. Thus, it is very important to describe these nano-structures to get understanding in the topology and increase their physical characteristics. Modern technologies depend upon the nano-materials/naphtalenic nano-sheet are very good in controlling the problems in usual drug transportation namely: weakly solubility, poison and weakly deliver design of drugs. The physical and chemical characteristics of these nano-sheets rely on their structure. H-Naphtalenic nano-sheet is denoted by (H(r,s)) and it contains alternating hexagons C_6 , C_4 and octagons C_8 . The number of vertices in (H(r,s)) is 10 rs, where r denotes the number of paired hexagons in every alternate row with C₄ cycle, and s denotes the number of rows consisting C₄. TIs of H-Naphtalenic nano-sheet are studied in [5]. In the present calculations, we employed edge partition and vertex partition tools of graph theory [6]. The graph of H-Naphtalenic nano-sheet is denoted by H(r,s), and line graph of subdivision graph is denoted by L(S(H(r, s))). Indium phosphide, is denoted by InP lie in group IIIA-VA, a semiconductor and its decomposing into bomb calorimeter give us two types of phosphorous i.e. red and black [7]. Crystallizes form of Inp is cubic form which is shown in Fig.1. InP is used commercially from so many years due to having band gap 1.35 Ev. complete composition, low toxic nature, shape and solution development potential. Inp nano-crystal has no cadmium and less-toxic nano-crystal with excellent characteristics like top thermal conductivity, stokes shift emission [8], near IR emitter, and best PL quantum turnout [9]. Inp is also used in the photo electro chemistry because it has band gap 1.35 Ev which is capture from the solar radiation by lowering the reflection of photons, resulting in separating of water in solar. Moreover,

© The Author(s). 2025 **Open access**. This article is distributed under the terms of the Creative Commons Attribution 4.0 International License (http://creativecommons.org/licenses/by/4.0/), which permits unrestricted use, distribution, and reproduction in any medium, provided you give appropriate credit to the original author(s) and the source, provide a link to the Creative Commons license, and indicate if changes were made.

by using InP nano-wire arrays on Si give excellent behavior in this field because of less cost, top surface area, and catalytic characteristics [10]. Nano-structured of InP indicate its incoming applications in the field of nano-photonic and optoelectronic devices as its excellent performance in harvesting and energy saving characteristics [11]. An extensible fabricated synapse based on InP was shown for upcoming applications with neuromorphic developments [8].

Equations work: In this section, used some equations to determine the irregular indices for the molecular graph of indium phosphide InP[m,n] and line graph of subdivision graph of H-naphtalenic nano-sheet L(S(H(r,s))). The irregular indices based on vertex degree are given below from Eq. 1.1 to Eq 1.16 respectively [14, 15-24].

$$VAR(G) = \frac{M_1(G)}{k} - \left(\frac{2l}{k}\right)^2 \tag{1.1}$$

$$AL(G) = \sum_{gh \in E(G)} |d_g - d_h| \tag{1.2}$$

$$IR1(G) = F(G) - \frac{2l}{k}M_1(G)$$
 (1.3)

$$IR2(G) = \sqrt{\frac{M_2(G)}{l} - \frac{2l}{k}}$$
 (1.4)

$$IRF(G) = F(G) - 2M_2(G)$$
 (1.5)

$$IRFW(G) = \frac{IRF(G)}{M_2(G)}$$
 (1.6)

$$IRA(G) = \sum_{gh \in E(G)} \left(d_g^{-\frac{1}{2}} - d_h^{-\frac{1}{2}} \right)^2$$
 (1.7)

$$IRA(G) = \sum_{gh \in E(G)} (d_g^{1/2} - d_h^{1/2})^2$$
 (1.8)

$$IRA(G) = \sum_{\mathbf{g} \mid \mathbf{h} \in \mathcal{B}(G)} \frac{\sqrt{d_{\mathbf{g}} d_{h}}}{l} - \frac{2l}{k}$$
 (1.9)

$$IRDIF(G) = \sum_{\substack{dh \in E(G) \\ d_h}} \left| \frac{d_g}{d_h} - \frac{d_h}{d_g} \right|$$
 (1.10)

$$IRL(G) = \sum_{gh \in E(G)} |lnd_g - lnd_h|$$
 (1.11)

$$IRLU(G) = \sum_{gh \in E(G)} \frac{|d_g - d_h|}{min(d_g, d_g)}$$
 (1.12)

$$IRLF(G) = \sum_{\substack{gh \in E(G)}} \frac{|d_g - d_h|}{\sqrt{d_g d_h}}$$
 (1.13)

$$IRLA(G) = \sum_{\substack{1 \le n \le G}} \frac{|d_g - d_h|}{d_g + d_h}$$
(1.14)

$$IRDI(G) = \sum_{gh \in E(G)} ln\{1 + |d_g - d_h|\}$$
 (1.15)

$$IRGA(G) = \sum_{gh \in E(G)} \frac{\ln(d_g + d_h)}{2\sqrt{d_g d_h}}$$
 (1.16)

Moreover, first and second Zagreb indices are defined as [25]

$$M_1(G) = \sum_{gh \in E(G)} \left(d_g + d_h\right),$$

$$M_2(G) = \sum_{gh \in E(G)} (d_g \times d_h).$$

Forgotten index, is defined as [26]

$$F(G) = \sum_{gh \in E(G)} (d_g^2 + d_h^2).$$

RESULTS AND DISCUSSIONS

Results on indium phosphide InP[m,n]: In this section, we compute some results on irregular indices for indium phosphide InP[m,n] which will be very effective to analyze the graphical behaviors of InP[m,n].

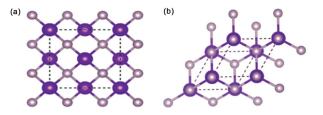


Fig. 1. Structural cell of indium phosphide InP[m,n]: (a) front view and (b) general view

Table1. Edge partition of InP[m,n]

Types of edges (d_g, d_h)	Count of edges
(1,4)	4m + 4n - 4
(2,4)	4mn+4m+4n
(4,4)	8 <i>mn-</i> 4 <i>m-</i> 4 <i>n</i>

Theorem

Let G denote InP[m,n], where InP[m,n] represent indium phosphide, then we compute the followings indices:

$$=\frac{36m^2 - 36n^2 + 384m^2n + 144n^2m - 36m - 84n + 880m^2n^2 - 24mn - 40}{(10mn + 3m + 3n + 2)^2}$$

(2)
$$AL(G) = -20m - 20n - 8mn + 12$$

$$= \frac{60m^2 + 60n^2 + 824m^2n + 1592n^2m - 164m - 164n + 544m^2n^2 + 752mn - 136}{(10mn + 3m + 3n + 2)}$$

(4)
$$IR2(G) = \sqrt{\frac{-m-n+10mn-1}{mn} - \frac{32mn}{10mn+3m+3n+2}}$$

$$(5) IRF(G) = 52m + 52n + 16mn - 36.$$

Proof:

(1) Using Eq. 1.1 and Table 1, we get

$$VAR(G) = \frac{M_1(G)}{k} - \left(\frac{2l}{k}\right)^2$$

$$= \frac{12m - 12n + 88mn - 20}{(10mn + 3m + 3n + 2)} - \left(\frac{32mn}{10mn + 3m + 3n + 2}\right)^2$$

$$= \frac{(12m - 12n + 88mn - 20)(3m + 3n + 10mn + 2) - 32mn}{(10mn + 3m + 3n + 2)^2}$$

$$= \frac{36m^2 - 36n^2 - 384m^2n - 144mn^2 - 36m - 84n + 880m^2n^2 - 24mn}{(10mn + 3m + 3n + 2)^2}$$

(2) Using Eq. 1.2 and Table 1, we get

$$AL(G) = \sum_{gh \in E(G)} |d_g - d_h|$$

$$= |1 - 4|(4m + 4n - 4) + |2 - 4|(4mn + 4m + 4n) + |4 - 4|(8mn - 4m)|$$

$$= -20m - 20n - 8mn + 12.$$

(3) Using Eq. 1.3 and Table 1, we have

$$IR1(G) = F(G) - \frac{2l}{k}M_1(G)$$

$$= (20m + 20n + 336mn - 68) - \frac{2(16mn)}{(10mn + 3m + 3n + 2)} (12m - 12n + 88mn - 20)$$

$$= \frac{60m^2 + 60n^2 + 824m^2n + 1592n^2m - 164m - 164n + 544m^2n^2 + 752mn - 136}{(10mn + 3m + 3n + 2)}$$

(4) Using Eq. 1.4 and Table 1, we conclude

$$\begin{split} &IR2(G) \ = \sqrt{\frac{M_2(G)}{l} - \frac{2l}{k}} \\ &= \sqrt{\frac{-16mn - 16n + 160mn - 16}{16mn} - \frac{32mn}{(10mn + 3m + 3n + 2)}} \\ &= \sqrt{\frac{-mn - n + 10mn - 1}{mn}} - \frac{32mn}{(10mn + 3m + 3n + 2)} \;. \end{split}$$

(5) Using Eq. 1.5 and Table 1, we get

$$IRF(G) = F(G) - 2M_2(G)$$

$$= (20m + 20n + 336mn - 68) - 2(-16mn - 16n + 160mn - 16)$$

$$= 52m + 52n + 16mn - 36.$$

Theorem

Suppose G denote InP[m,n], where InP[m,n] represent indium phosphide, then we compute the followings indices:

$$(1) IRFW(G) = \frac{13m + 13n + 4mn - 9}{-4m - 4n + 40mn - 4}$$

$$(2) IRA(G) = \left(4 - \frac{4}{\sqrt{2}}\right)m + \left(4 - \frac{4}{\sqrt{2}}\right)n + \left(-3 - \frac{4}{\sqrt{2}}\right)mn + 1$$

$$(3) IRB(G) = \left(28 - 16\sqrt{2}\right)m + \left(24 - 16\sqrt{2}\right)mn + \left(28 - 16\sqrt{2}\right)n - 4$$

$$(4) IRC(G)$$

$$= \frac{(-24 + 4\sqrt{8})m + \left(32 + 4\sqrt{8}\right)mn + \left(-24 + 4\sqrt{8}\right)n - 8}{16mn}$$

$$- \frac{32mn}{10mn + 3m + 3n + 2}$$

(5) IRDIF(G) = -27m - 27n - 12mn + 15.

Proof:

(1) Using Eq. 1.6 and Table 1, we have

$$IRFW(G) = \frac{IRF(G)}{M_2(G)}$$

$$= \frac{52m + 52n + 16mn - 36}{-16mn - 16n + 160mn - 16}$$

$$= \frac{13m + 13n + 4mn - 9}{-4m - 4n + 40mn - 4}$$

(2) Using Eq. 1.7 and Table 1, we have

$$\begin{split} & IRA(G) = \sum_{gh \in E(G)} \left(d_g^{-1/2} - d_h^{-1/2} \right)^2 \\ & = \left(1 - \frac{1}{\sqrt{4}} \right)^2 \left(4m + 4n - 4 \right) + \left(\frac{1}{\sqrt{2}} - \frac{1}{\sqrt{4}} \right)^2 \left(4mn + 4m + 4n \right) \\ & + \left(\frac{1}{\sqrt{4}} - \frac{1}{\sqrt{4}} \right)^2 \left(8mn - 4m - 4n \right) \\ & = \left(4 - \frac{4}{\sqrt{2}} \right) m + \left(4 - \frac{4}{\sqrt{2}} \right) n + \left(-3 - \frac{4}{\sqrt{2}} \right) mn + 1 \end{split}$$

(3) Using Eq. 1.8 and Table 1, we get

$$\begin{split} & IRB(G) = \sum_{gh \in E(G)} \left(d_g^{-1/2} - d_h^{-1/2} \right)^2 \\ & = \left(\sqrt{1} - \sqrt{4} \right)^2 (4m + 4n - 4) \\ & + \left(\sqrt{2} - \sqrt{4} \right)^2 (4mn + 4m + 4n) \\ & + \left(\sqrt{4} - \sqrt{4} \right)^2 (8mn - 4m - 4n) \\ & = \left(28 - 16\sqrt{2} \right) m + \left(24 - 16\sqrt{2} \right) mn + \left(28 - 16\sqrt{2} \right) n - 4 \end{split}$$

(4) Using Eq. 1.9 and Table 1, we conclude

$$IRC(G) = \sum_{gh \in E(G)} \frac{\sqrt{d_g d_h}}{l} - \frac{2l}{k}$$

$$=\frac{\left(\sqrt{1\times4}\right)(4m+4n-4)+\left(\sqrt{2\times4}\right)(4mn+4m+4n)+\left(\sqrt{4\times4}\right)(8mn-4m-4n)}{16mn}$$

$$=\underbrace{2(16mn)}$$

$$\begin{split} &-\frac{2(16mn)}{10mn+3m+3n+2}\\ &=\frac{\left(-24+4\sqrt{8}\right)m+\left(32+4\sqrt{8}\right)mn+\left(-24+4\sqrt{8}\right)n-8}{16mn}\\ &-\frac{32mn}{10mn+3m+3n+2}. \end{split}$$

(5) Using Eq. 1.10 and Table 1, we have

$$= \left| \frac{1}{4} - \frac{4}{1} \right| (4m + 4n - 4)$$

$$+ \left| \frac{2}{4} - \frac{4}{2} \right| (4mn + 4m + 4n)$$

$$+ \left| \frac{4}{4} - \frac{4}{4} \right| (8mn - 4m - 4n)$$

$$= -27m - 27n - 12mn + 15.$$

 $IRDIF(G) = \sum_{\substack{d \in G(G)}} \left| \frac{d_g}{d_h} - \frac{d_h}{d_g} \right|$

Theorem

Let G denote InP[m,n], where InP[m,n] represent indium phosphide, then we compute the followings indices:

(1)
$$IRL(G) = 8.3164m + 8.3164n + 2.772mn - 5.544$$

(2)
$$IRLU(G) = 16m + 16n + 4mn - 12$$

(3)
$$IRLF(G) = (6 + \sqrt{8})m + (6 + \sqrt{8})n + \sqrt{8}mn - 4$$

(4)
$$IRLA(G) = \frac{56}{15}m + \frac{56}{15}n + \frac{4}{3}mn - 4$$

(5)
$$IRDI(G) = 9.9384m + 9.9384n + 4.3944mn - 5.544$$

(6)
$$IRGA(G) = 1.1275m + 1.1275n + 0.2355mn - 0.892$$

Proof:

(1) Using Eq. 1.11 and Table 1, we have

$$\begin{split} & IRL(G) = \sum_{gh \in E(G)} \left| lnd_g - lnd_h \right| \\ & = \left| ln1 - ln4 \right| (4m + 4n - 4) \\ & + \left| ln2 - ln4 \right| (4mn + 4m + 4n) \\ & + \left| ln4 - ln4 \right| (8mn - 4m - 4n) \end{split}$$

(2) Using Eq. 1.12 and Table 1, we have

= 8.3164m + 8.3164n + 2.772mn - 5.544

$$IRLU(G) = \sum_{gh \in E(G)} \frac{|d_g - d_h|}{\min(d_g, d_g)}$$

$$= \frac{|1 - 4|}{\min(1, 4)} (4m + 4n - 4)$$

$$+ \frac{|2 - 4|}{\min(2, 4)} (4mn + 4m + 4n)$$

$$+ \frac{|4 - 4|}{\min(4, 4)} (8mn - 4m - 4n)$$

$$= 16m + 16n + 4mn - 12.$$

(3) Using Eq. 1.13 and Table 1, we get

$$IRLF(G) = \sum_{gh \in E(G)} \frac{|d_g - d_h|}{\sqrt{d_g d_h}}$$

$$= \frac{|1 - 4|}{\sqrt{1 \times 4}} (4m + 4n - 4)$$

$$+ \frac{|2 - 4|}{\sqrt{2 \times 4}} (4mn + 4m + 4n)$$

$$+ \frac{|4 - 4|}{\sqrt{4 \times 4}} (8mn - 4m - 4n)$$

$$= (6 + \sqrt{8})m + (6 + \sqrt{8})n + \sqrt{8}mn - 4.$$

(4) Using Eq. 1.14 and Table 1, we conclude

$$IRLA(G) = \sum_{gh \in E(G)} \frac{|d_g - d_h|}{d_g + d_h}$$

$$= \frac{|1 - 4|}{1 + 4} (4m + 4n - 4)$$

$$+ \frac{|2 - 4|}{2 + 4} (4mn + 4m + 4n)$$

$$+ \frac{|4 - 4|}{4 + 4} (8mn - 4m - 4n)$$

$$= \frac{56}{15}m + \frac{56}{15}n + \frac{4}{3}mn - 4.$$

(5) Using Eq. 1.15 and Table 1, we have

$$IRDI(G) = \sum_{gh \in E(G)} ln\{1 + |d_g - d_h|\}$$

$$= ln\{1 + |1 - 4|\}(4m + 4n - 4)$$

$$+ ln\{1 + |2 - 4|\}(4mn + 4m + 4n)$$

$$+ ln\{1 + |4 - 4|\}(8mn - 4m - 4n)$$

$$= 9.9384m + 9.9384n + 4.3944mn - 5.544.$$

(6) Using Eq. 1.16 and Table 1, we get

$$IRGA(G) = \sum_{gh \in E(G)} \frac{ln(d_g + d_h)}{2\sqrt{d_g d_h}}$$

$$IRGA(G) = \frac{\ln(1+4)}{2\sqrt{1\times4}} (4m+4n-4)$$

$$+ \frac{\ln(2+4)}{2\sqrt{2\times4}} (4mn+4m+4n)$$

$$+ \frac{\ln(4+4)}{2\sqrt{4\times4}} (8mn-4m-4n)$$

$$= 0.16328r + 0.08164s - 0.16328.$$

Results on L(S(H(r,s)))

In this section, we compute some results on L(S(H(r,s))) by using irregular indices and the graphical behaviors of L(S(H(r,s))) is shown at the end.

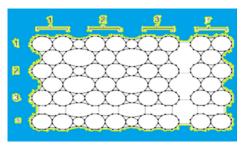


Fig. 2. Line graph of subdivision graph of H-naphtalenic nano-sheet L(S(H(r, s)))

Table 2. Edge partition of L(S(H(r, s)))

Types of edges $(d_{g'}, d_h)$	Count of edges
(1,4)	4r + 6s + 4
(2,4)	8r + 4s - 8
(4,4)	45rs - 22r - 20s + 4

Theorem

Let G denoteL(S(H(r,s))), where L(S(H(r,s)) be the line graph of subdivision graph of H-naphtalenicnano-sheet, then we compute the followings indices:

$$=\frac{304r^2+304s^2-3360r^2s-1080rs^2-20r-20s+8100r^2s^2-1672rs}{(30rs-4r-4s)^2}$$

(2)
$$AL(G) = 8r + 4s - 8$$

$$(3) \ IR1(G) \ = \frac{6360 \, r^2 - 480 \, s^2 - 29940 \, r^2 \, s \ - 13200 \, r \, s^2 + 24300 \, r^2 \, s^2 + 5880 \, r \, s}{(30 \, r \, s - 4 \, r - 4 \, s)}$$

(4)
$$IR2(G) = \sqrt{\frac{-134r - 132s + 405rs + 4}{45rs - 10r - 10s}} - \frac{90rs - 20r - 20s}{30rs - 4r - 4s}$$

(5)
$$IRF(G) = 4r + 524s - 8$$

Proof:

(1) From Eq. 1.1 and Table 2, we have

$$VAR(G) = \frac{M_1(G)}{k} - \left(\frac{2l}{k}\right)^2$$

$$= \frac{-76r - 76ss + 270rs}{30rs - 4r - 4s} - \left(\frac{2(45rs - 10r - 10s)}{30rs - 4r - 4s}\right)^2$$

$$= \frac{(-76r - 76s + 270rs)(30rs - 4r - 4s) - (90rs - 20r - 20s)}{(30rs - 4r - 4s)^2}$$

$$= \frac{304r^2 + 304s^2 - 3360r^2s - 1080rs^2 - 20r - 20s + 8100r^2s^2 - 1672rs}{(30rs - 4r - 4s)^2}$$

(2) From Eq. 1.2 and Table 2, we get

$$\begin{split} AL(G) &= \sum_{gh \in E(G)} \left| d_g - d_h \right| \\ &= |2 - 2|(4r + 6s + 4) + |2 - 3|(8r + 4s - 8) + |3 - 3|(45rs - 22r - 20s + 4) \\ &= 8r + 4s - 8. \end{split}$$

(3) From Eq. 1.3 and Table 2, we conclude

$$IR1(G) = F(G) - \frac{2l}{k} M_1(G)$$

$$= (-260r - 260s + 810rs)$$

$$- \frac{2(45rs - 10r - 10s)}{(30rs - 4r - 4s)} (-76r - 76s + 270rs)$$

$$= \frac{6360r^2 - 480s^2 - 29940r^2s - 13200rs^2 + 24300r^2s^2 + 5880rs}{(30rs - 4r - 4s)}$$

(4) From Eq. 1.4 and Table 2, we have

$$\begin{split} &IR2(G) = \sqrt{\frac{M_2(G)}{l}} - \frac{2l}{k} \\ &= \sqrt{\frac{-134r - 132s + 450rs + 4}{45rs - 10r - 10s}} - \frac{2(45rs - 10r - 10s)}{30rs - 4r - 4s} \\ &= \sqrt{\frac{-134r - 132s + 450rs + 4}{45rs - 10r - 10s}} - \frac{90rs - 20r - 20s}{30rs - 4r - 4s} \end{split}$$

(5) From Eq. 1.5 and Table 2, we get

$$IRF(G) = F(G) - 2M_2(G)$$

$$= -260r - 260s + 810rs - 2(-134r - 132s + 450rs + 4)$$

$$= 4r + 524s - 8.$$

Theorem

Suppose G represent L(S(H(r,s))), where L(S(H(r,s))) be the line graph of subdivision graph of H-naphtalenic nano-sheet, then we determine the followings indices:

$$(1) IRFW(G) = \frac{4r + 524s - 8}{405rs - 134r - 132s + 4}$$

$$(2) IRA(G) = \left(\frac{20}{3} - \frac{8\sqrt{2}}{\sqrt{3}}\right)r + \left(\frac{10}{3} - \frac{\sqrt{2}}{\sqrt{3}}\right)s + \left(-\frac{20}{3} + \frac{8\sqrt{2}}{\sqrt{3}}\right)$$

$$(3) IRB(G) = (40 - 16\sqrt{6})r + (20 - 8\sqrt{6})s + (16\sqrt{6} - 40)$$

$$(4) IRC(G) = \frac{(-58 + 6\sqrt{8})r + (-48 + 4\sqrt{6})s + 135rs}{45rs - 10r - 10s} - \frac{45rs - 10r - 10s}{15rs - 2r - 2s}$$

$$(5) IRDIF(G) = \frac{20}{3}r + \frac{10}{3}s - \frac{20}{3}$$

Proof:

(1) From Eq. 1.6 and Table 2, we have

$$IRFW(G) = \frac{IRF(G)}{M_2(G)}$$

$$= \frac{4r + 524s - 8}{405rs - 134r - 132s + 4}$$

$$= \frac{4r + 524s - 8}{405rs - 134r - 132s + 4}.$$

(2) From Eq. 1.7 and Table 2, we get

$$\begin{split} & IRA(G) = \sum_{gh \in E(G)} \left(d_g^{-1/2} - d_h^{-1/2}\right)^2 \\ &= \left(\frac{1}{\sqrt{2}} - \frac{1}{\sqrt{2}}\right)^2 \left(4r + 6s + 4\right) + \left(\frac{1}{\sqrt{2}} - \frac{1}{\sqrt{3}}\right)^2 \left(8r + 4s - 8\right) \\ &+ \left(\frac{1}{\sqrt{3}} - \frac{1}{\sqrt{3}}\right)^2 \left(45rs - 22r - 20s + 4\right) \\ &= \left(\frac{20}{3} - \frac{8\sqrt{2}}{\sqrt{3}}\right)r + \left(\frac{10}{3} - \frac{\sqrt{2}}{\sqrt{3}}\right)s + \left(-\frac{20}{3} + \frac{8\sqrt{2}}{\sqrt{3}}\right) \end{split}$$

(3) From Eq. 1.8 and Table 2, we conclude

$$\begin{split} IRB(G) &= \sum_{gh \in E(G)} \left(d_g^{1/2} - d_h^{1/2}\right)^2 \\ &= \left(\sqrt{2} - \sqrt{2}\right)^2 \left(4r + 6s + 4\right) + \left(\sqrt{2} - \sqrt{3}\right)^2 (8r + 4s - 8) \\ &\quad + \left(\sqrt{3} - \sqrt{3}\right)^2 (45rs - 22r - 20s + 4) \\ &= \left(40 - 16\sqrt{6}\right)r + \left(20 - 8\sqrt{6}\right)s + \left(16\sqrt{6 - 40}\right). \end{split}$$

(4) From Eq. 1.9 and Table 2, we have

$$\begin{split} & IRB(G) = \sum_{gh \in E(G)} \left(d_g^{-1/2} - d_h^{-1/2}\right)^2 \\ & = \left(\sqrt{2} - \sqrt{2}\right)^2 \left(4r + 6s + 4\right) + \left(\sqrt{2} - \sqrt{3}\right)^2 (8r + 4s - 8) \\ & \quad + \left(\sqrt{3} - \sqrt{3}\right)^2 (45rs - 22r - 20s + 4) \\ & = \left(40 - 16\sqrt{6}\right)r + \left(20 - 8\sqrt{6}\right)s + \left(16\sqrt{6} - 40\right). \end{split}$$

(5) From Eq. 1.10 and Table 2, we get

$$\begin{split} & IRDIF(G) = \sum_{gh \in E(G)} \left| \frac{d_g}{d_h} - \frac{d_h}{d_g} \right| \\ & = \left| \frac{2}{2} - \frac{2}{2} \right| (4r + 6s + 4) \\ & + \left| \frac{2}{3} - \frac{3}{2} \right| (8r + 4s - 8) \\ & + \left| \frac{3}{3} - \frac{3}{3} \right| (45rs - 22r - 20s + 4) \\ & = \left(\frac{20}{3} r - \frac{10}{3} s - \frac{20}{3} \right). \end{split}$$

Theorem

Suppose G represent L(S(H(r,s))), where L(S(H(r,s))) be the line graph of subdivision graph of H-naphtalenic nano-sheet, then we determine the followings indices:

(1)
$$IRL(G) = 3.2436r + 1.6218s - 3.2436$$

(2)
$$IRLU(G) = 4r + 2s - 4$$

(3)
$$IRLF(G) = \frac{1}{\sqrt{6}}(8r + 4s - 8)$$

(4)
$$IRLA(G) = \frac{1}{5}(8r + 4s - 8)$$

$$(5) IRDI(G) = 5.5448r + 2.7724s - 5.5448$$

(6)
$$IRGA(G) = 0.16328r + 0.08164s - 0.16328$$
.

Proof:

(1) From Eq. 1.11 and Table 2, we have

$$\begin{split} & IRL(G) = \sum_{gh \in E(G)} \left| lnd_g - lnd_h \right| \\ & = \left| ln2 - ln2 \right| (4r + 6s + 4) \\ & + \left| ln2 - ln3 \right| (8r + 4s - 8) \\ & + \left| ln3 - ln3 \right| (45rs - 22r - 20s + 4) \\ & = (3.2436r + 1.6218s - 3.2436). \end{split}$$

(2) From Eq. 1.12 and Table 2, we get

$$\begin{split} & \mathit{IRDLU(G)} = \sum_{gh \in E(G)} \frac{|d_g - d_h|}{\min(d_g, d_g)} \\ & = \frac{|2 - 2|}{\min(2, 2)} (4r + 6s + 4) \\ & + \frac{|2 - 3|}{\min(2, 3)} (8r + 4s - 8) \\ & + \frac{|3 - 3|}{\min(4, 4)} (45rs - 22r - 20s + 4) \\ & = (4r + 2s - 4). \end{split}$$

(3) From Eq. 1.13 and Table 2, we deduce

$$IRDLF(G) = \sum_{gh \in E(G)} \frac{|d_g - d_h|}{\sqrt{d_g d_h}}$$

$$= \frac{|2 - 2|}{2 + 2} (4r + 6s + 4)$$

$$+ \frac{|2 - 3|}{2 + 3} (8r + 4s - 8)$$

$$+ \frac{|3 - 3|}{3 + 3} (45rs - 22r - 20s + 4)$$

$$= \frac{1}{\sqrt{6}} (8r + 4s - 8).$$

(4) From Eq. 1.14 and Table 2, we have

$$\begin{split} & IRLA(G) = \sum_{gh \in E(G)} \frac{\left| d_g - d_h \right|}{d_g + d_h} \\ & = \frac{\left| 2 - 2 \right|}{2 + 2} (4r + 6s + 4) \\ & + \frac{\left| 2 - 3 \right|}{2 + 3} (8r + 4s - 8) \\ & + \frac{\left| 3 - 3 \right|}{3 + 3} (45rs - 22r - 20s + 4) \\ & = \frac{1}{6} \left(8r + 4s - 8 \right). \end{split}$$

(5) From Eq. 1.15 and Table 2, we get

$$\mathit{IRDI(G)} = \sum_{gh \in \mathit{E(G)}} ln\{1 + \left|d_g - d_h\right|\}$$

$$= ln\{1 + |2 - 2|\}(4r + 6s + 4)$$

$$+ ln\{1 + |2 - 3|\}(8r + 4s - 8)$$

$$+ ln\{1 + |3 - 3|\}(45rs - 22r - 20s + 4)$$

$$= 0.16328r + 0.08164s - 0.16328$$

(6) From Eq. 1.16 and Table 2, we conclude

$$\begin{split} & \operatorname{IRGA}(G) = \sum_{gh \in E(G)} \frac{\ln(d_g + d_h)}{2\sqrt{d_g d_h}} \\ & = \frac{\ln(2+2)}{2\sqrt{2\times 2}} \left(4r + 6s + 4\right) \\ & + \frac{\ln(2+3)}{2\sqrt{2\times 3}} \left(8r + 4s - 8\right) \\ & + \frac{\ln(3+3)}{2\sqrt{3\times 3}} \left(45rs - 22r - 20s + 4\right) \\ & = 0.16328r + 0.08164s - 0.16328. \end{split}$$

We have sketched the irregular indices graphically for the indium Phosphide InP[m,n] and line graph of subdivision graph of H-naphtalenicnano-sheet L(S(H(r,s))) and quantitative comparison is shown in Fig. 3 (a) to (j). It indicates how the irregular indices change its behavior with the increase in network size and structure. Graphical representation of irregular indices for some InP[m,n] and L(S(H(m,n))) is shown below.

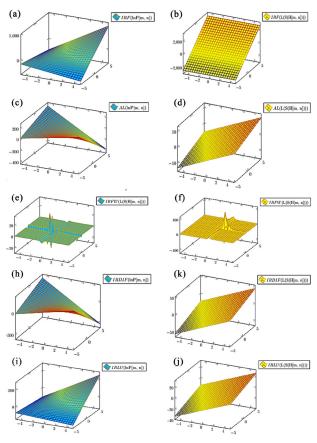


Fig. 3. (a) to (j) Irregular indices for Indium Phosphide (InP[m,n] and the line graph of the subdivision graph of H-naphtalenic nanosheet L(SH(r,s)))

CONCLUSIONS

We have determined the irregular indices of indium Phosphide InP[m,n] and line graph of subdivision graph of H-Naphtalenic nano-sheet L(S(H(r,s))) and quantitative comparison is shown in figures. The results show which properties have most effective on invariants. Molecular characteristics like: flash point, boiling point, critical pressure and polarization etc. can be computed by using topological indices. We have also investigated different indices for indium Phosphide InP[m,n] and line graph of subdivision graph of H-Naphtalenic nano-sheet L(S(H(r,s))) such as VAR(G), AL(G), IR1(G), IR2(G), IRF(G), IRF(G), IRA(G), IRB(G), IRC(G), IRDIF(G), IRL(G), IRLU(G), IRLF(G), IRLA(G), IRDI(G), IRGA(G). Graphical behaviors of InP[m,n] and L(S(H(r,s)))have also been discussed at the end.

AUTHOR CONTRIBUTIONS:

All authors contributed equally to this study.

ACKNOWLEDGMENT

All authors are grateful to those who supported this work.

FUNDING STATEMENT:

No specific funding available.

CONFLICT OF INTEREST:

The authors declare no conflict of interest.

DATA AVAILABILITY:

All data used are included inside the article.

REFERENCES

- Coleman J N., Lotya M., O'Neill A et al. (2011) Two-dimensional nano sheets produced by liquid exfoliation of layered materials. Science, 331, 568– 571. https://doi.org/10.1126/science.1194975
- Guo, S., & Dong, S. (2011) Graphene nanosheet: synthesis, molecular engineering, thin flm, hybrids, and energy and analytical applications. *Chem. Soc. Rev.*, 40, 2644–2672. http://doi.org/10.1126/science.1194975
- Garcia, JC., de Lima DB., Assali LVC., & Justo JF. (2011) Group IV Graphene and Graphane-Like Nanosheets. J. Phys. Chem. C., 115, 13242– 13246.
 - https://pubs.acs.org/doi/10.1021/jp203657w
- Khan I., Saeed, K. Khan I. (2019) Nano particles Properties, applications and toxicities. *Arab. J. Chem.*, 12, 908–931. https://doi.org/10.1016/j.arabjc.2017.05.011
- Deng, F., Zhang, X., Alaeiyan, M., Mehboob, A., & Farahani, MR. (2019) Topological Indices of the Pent-Heptagonal Nano sheets VC5C7 and HC5C7. Adv. Mater. Sci. Eng., 2019:9594549., 1-13. https://doi.org/10.1155/2021/4863993
- 6. García, I., Fall, Y., & Gómez, G. (2010) Using

- topological indices to predict anti-Alzheimer and anti-parasitic GSK-3 inhibitors by multi-target QSAR in silicoscreening. *Molecules*, **15**(8), 5408-5422. https://doi.org/10.3390/molecules15085408
- 7. Vasil'ev, V.P., &Gachon, J.C. (2006) Thermodynamic properties of III–V compounds. *Inorganic materials*, **42**, 1176-1187. http://doi.org/10.1134/S0020168506110021
- Lin, Q., Sarkar, D., Lin, Y et al. (2017) Scalable indium phosphide thin-film nanophotonics platform for photovoltaic and photo electrochemical devices. ACS Nano., 11(5), 5113–5119. https://doi.org/10.1021/acsnano.7b02124
- Sadeghi, S., Bahmani Jalali, H., Melikov, R., Ganesh Kumar, B., Mohammadi Aria, M., Ow-Yang, C. W., & Nizamoglu, S. (2018) Stokes-shiftengineered indium phosphide quantum dots for efficient luminescent solar concentrators. ACS applied materials & interfaces, 10(15), 12975-12982. http://.doi.org/10.1021/acsami.7b19144
- Britto, Reuben J., Jesse D. Benck., James L. Young., Christopher Hahn., Todd G. Deutsch.,& Thomas F. Jaramillo.(2016) Molybdenum disulfide as a protection layer and catalyst for gallium indium phosphide solar water splitting photocathodes. *The journal of physical chemistry letters* 7, 11, 2044-2049. https://pubs.acs.org/doi/abs/10.1021/acs.jpclett.6b00563
- Kornienko, N., Gibson, N. A., Zhang, H et al. (2016) Growth and photo electrochemical energy conversion of quartzite indium phosphide nanowire arrays. ACS Nano, 10(5), 5525–5535. https://doi.org/10.1021/acsnano.6b02083
- 12. Bonchev, D. (1991) Chemical graph theory: Introduction and fundamentals, (1). *CRC Press*. https://doi.org/10.1201/9781315139104
- Wiener H. (1947) Structural determination of paraffin boiling points. *Journal of the American Chemical Society*, 69(1), 17-20. https://doi.org/10.1021/ja01193a005
- Shirakol, S., Kalyanshetti, M., &Hosamani, S. M. (2019) QSPR analysis of certain distance based topological indices. *Applied Mathematics and Nonlinear Sciences*, 4(2), 371-386. https://doi.org/10.2478/AMNS.2019.2.00032
- Konsalraj, J., Padmanabhan, V., & Perumal, C. (2021) Topological analysis of PAHs using Irregularity based indices. *Biointerface research* in applied chemistry, 12(3), 2970-2987. https://doi.org/10.33263/BRIAC123.29702987
- Ahmad, A. (2020) Upper bounds of irregularity indies of categorical product of two connected graphs. *Palestine Journal of Mathematics*, 9(1), 26-30.
- Kang, S., Chu, Y. M., Virk, A. u. R., Nazeer, W., & Jia, J. (2020) Computing irregularity indices for probabilistic neural network. *Frontiers in Physics*, 8, 1-5. https://doi.org/10.3389/fphy.2020.00359

- Sardar, M. S., Zafar, S., Zahid, Z, Farhani, M. R., Wang, S., &Naduvath., S. (2020) Certain topological indices of line graph of Dutch Windmill graphs. Southeast Asian Bulletin of Mathematics, 44, 119-129.
- Danish, M., Ali, M. A., Tasleem, M. W., Rajpoot, S. R., Tasleem, S., & Shahzad, M. (2021) Computation of certain degree-based topological indices of propranolol (C16H21NO2). *International Journal of Research Publication and Reviews*, 2, 531-541.
- Kang, S. M., Asghar, A., Ahmad, H., & Kwun Y. C. (2019) Irregularity of Sierpinski graph. Journal of Discrete Mathematical Sciences and Cryptography, 22(7), 1269-1280. https://doi.org/10.1080/09720529.2019.1698186
- 21. Dimitrov, D., & Reti, R. (2014) Graphs with equal irregularity indices. *Acta Polytech. Hung.*, 11,41-57. https://www.researchgate.net/publication/261703990 Graphs with Equal Irregularity Indices

- 22. Reti, T., &Toth-Laufer, E. (2017) On the construction and comparison of graph irregularity indices. *Kragujevac J. Sci.*, **39**, 53-75.
- 23. Gutman, I. (2016) Irregularity of molecular graphs. Kragujevac J. Sci., 38, 71-78. http://doi.org/10.5937/KgJSci1638071G
- 24. Sardar, M. S., Ali, M. A; Mehdi Alaeiyan, M. R.F&Cancan, M. (2023) Analysis of certain silicon carbide graphs by using irregularity, Eur. Chem. Bull., **13**(5), 51-68. https://www.researchgate.net/publication/370479328
- 25. Gutman, I., &Trinajstic, N. (1972) Graph theory and molecular orbits. Total -electron energy of alternant hydrocarbons. *Chemical Physics Letters*, **17**(4), 535-538. https://doi.org/10.1016/0009-2614(72)85099-1
- 26. Furtula, B., & Gutman, I. (2015) A forgotten topological index. *Journal of Mathematical Chemistry*, 1184-1190. http://doi.org/10.1007/s10910-015-0480-z