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DEGREE BASED INDICES OF $g - C_3N_5$

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Abstract. A huge quantity of research in chemical graph theory divulges the significance about the relationship between molecular structures of chemical compound and its characteristics. The study on degree based topological invariants of chemical compounds helps to analyse its characteristics. Carbon nitrides are most curious graphite sheet type materials with different controlled structural properties. C_3N_5 is one such compound with interesting structural network of different C/N ratio. In this paper, few degree based indices of C_3N_5 is brought out further, the geometric interpretation and comparision is made which helps to understand its chemical features.

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1. Introduction

Carbon nitrides (CNs) are one of the most competent scaffolds in the advancing research field of material chemistry. Owing to the Carbon-Nitrogen structural framework of these materials, composition and crystallinity, a wide-range of properties are noticeable such as semi-conductivity, high hardness, intrinsic basicity, intercalating and adsorption. In recent years, the studies on various graphitic-carbon nitrides (g-CNs) have enticed the interest of chemists and physicists majorly to lessen the band gap and attain improvised chemical and physical properties (See [13]). In general, with an increase in the number of nitrogen atoms in the unit cell of C_3N_3, C_3N_4 and C_3N_5 it is observed that the electronic band gap decreases in the order 3.24 eV(C_3N_3) $\geq 2\ 0.81eV(C_3N_4) \geq 2\ 0.19eV(C_3N_5)$ of these graphitic carbon nitrides (See [28]). Also in comparison, the g-C_3N_5 class of molecules with a higher nitrogen content than g-C_3N_4 provides excellent electronic properties, such as a smaller band gap and catalytic properties, and other properties (See [32]) . Accordingly, several experiments have shown pronouncing results for photocatalytic, photovoltaic and adsorbent applications (See [4]).

The last few decades have witnessed the rise of semiconducting, all-organic polymers as excellent metal-free and visible light-active materials for various optoelectronic and energy harvesting applications.

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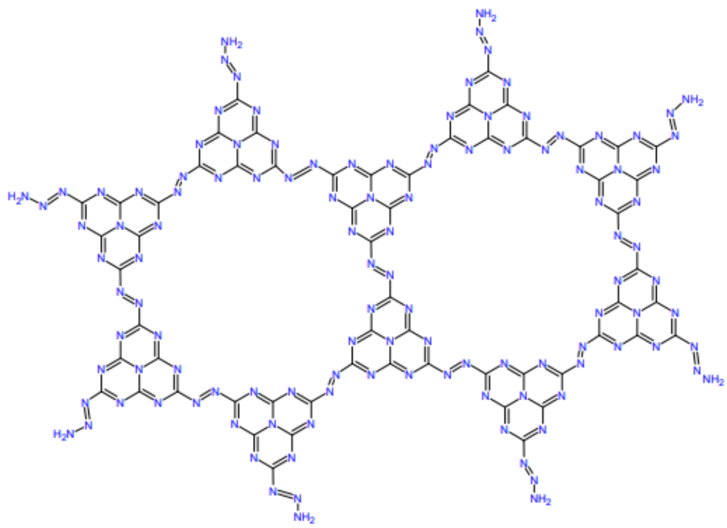

Figure 1. Structure of $g - C_3N_5$

Recently, an azo-linked carbon nitride C_3N_5 which behaves as a flat graphitic 2D crystal (named as g-C_3N_5 hereafter), was successfully synthesized via thermal decomposition of the melem hydrazine precursor for the first time. In this structure, two s-heptazine units are bridged together with an azo linkage. Due to its narrow band gap, it can be used as a high temperature resistant semiconductor in the field of optoelectronics. Since this new g-C_3N_5 was synthesized very recently, few works have been reported in [2]. Before the experiment, one theoretical work predicted a similar g-C_3N_5 structure and investigated its electronic and catalytic properties.

In past decade, the synthesis of a novel modified C_3N_5 is demonstrated for thermal deammoniation of the melem hydrazine precursor with an electronic bandgap of $1.76eV$. C_3N_5 with biaxial strain in the range of 12-14 percentage are predicted as remarkable photocatalyst in overall water-splitting with excellent optical absorption in the visible light spectrum. Evidently, the variation of core heteroatoms in C_3N_5 with extended $\pi - conjugation$ and low band gap function as a shuttle to extract carriers and excitons in nanostructured heterojunctions, enhance performance in optoelectronic devices and offers controlled reaction mechanism in photocatalysis [5]. The porous C_3N_5 nanosheet are known to possess unique electronic and topological properties. Carbon nitride nanoribbons (C_3NNRs) with distinct edge stabilities and variable semiconducting capacity bear potential applications in the fields of solar energy and nanodevices.

Among the topological indices of molecular graphs, the former most is Zagreb indices that became apparent in 1972 to enumerate the total electron energy of alternating hydrocarbons on the basis of connection number (degree of vertices at distance 2). The first and second Zagreb indices were brought out by Gutman and Trianjstic [10, 11]. The first Zagreb index $M_1(G)$ and the second Zagreb index $M_2(G)$ is exemplified as

$$M_1(G) = \sum_{pq \in E(G)} (d_p + d_q),$$

$$M_2(G) = \sum_{pq \in E(G)} (d_p \times d_q).$$

Fath-Tabar derived the third Zagreb index of a graph G [9] as

$$ZG_3(G) = \sum_{pq \in E(G)} |d_p - d_q|.$$

The Atom bond connectivity index is contributed by Estrada et al. [6]. It is exemplified as

$$ABC(G) = \sum_{pq \in E(G)} \sqrt{\frac{d_p + d_q - 2}{d_p \cdot d_q}}.$$

The Geometric-arithmetic index of a graph is established by Vukicevic et al. [33]. It is defined as

$$GA(G) = \sum_{pq \in E(G)} \frac{2\sqrt{d_p \cdot d_q}}{d_p + d_q}.$$

The inverse invariant of Geometric-arithmetic index is Arithmetic-geometric index introduced in [27], as

$$AG(G) = \sum_{pq \in E(G)} \frac{d_p + d_q}{2\sqrt{d_p \cdot d_q}}.$$

In [8], Furtula and Gutman introduced the Forgotten index as

$$F(G) = \sum_{pq \in E(G)} ({d_p}^2 + {d_q}^2).$$

Gao and Wang presented the general Harmonic index [7] as

$$H_k(G) = \sum_{pq \in E(G)} \left(\frac{2}{d_p + d_q}\right)^k$$

taking $k = 1$ the normal Harmonic index is given as

$$H(G) = \sum_{pq \in E(G)} \frac{2}{(d_p + d_q)}.$$

Ballobas and Erdos introduced the general Randic index in 1998 [26] as

$$R_\alpha(G) = \sum_{pq \in E(G)} (d_p \cdot d_q)^\alpha.$$

Many degree, distance and stress based topological indices have been defined and studied by several authors [1, 3, 12, 14–25, 29–31].

2. Degree based indices of $g - C_3N_5$

The motivation of this section is to exhibit various degree based indices of C_3N_5. Carbon nitrides are fasinating materials with unique properties. According to the C/N ratio of CN materials ranging from 0.4 to 3, the denomination of CN materials is distinguished as C_3N_7, C_3N_6, C_3N_5, C_3N_4, $C_{10}N_3$, C_3N_2, C_3N and so on. Clearly C_3N_5 has $32mn + 2(m + n)$ vertices and $39mn + m + n$ edges.

Vertex partition and edge partition are the main techniques used in the study to derive the desired results. Now, we procure the required results.

Table 1. Vertex partition of $g - C_3N_5$ structure based on degree.

degree	corresponding frequency
1	$2(m + n)$
2	$18mn$
3	$14mn$

Table 2. Edge partition of $g - C_3N_5$ structure

(d_p, d_q)	number of edges	Edge set
$(1, 2)$	$2(m + n)$	E_1
$(2, 2)$	$3mn - m - n$	E_2
$(2, 3)$	$30mn$	E_3
$(3, 3)$	$6mn$	E_4

Theorem 2.1. *The first, second and third Zagreb index of molecular graph $g - C_3N_5$ is given by,*

(i) $M_1(g - C_3N_5) = 198mn + 2m + 2n$
(ii) $M_2(g - C_3N_5) = 228mn$
(iii) $ZG_3(g - C_3N_5) = 30mn + 2m + 2n.$

Proof:

(i) First Zagreb index of $g - C_3N_5$ is

$$[M_1(g - C_3N_5) = \sum_{pq \in E(G)} (d_p + d_q)]$$
$$= \sum_{pq \in E_1(G)} (d_p + d_q) + \sum_{pq \in E_2(G)} (d_p + d_q) + \sum_{pq \in E_3(G)} (d_p + d_q) + \sum_{pq \in E_4(G)} (d_p + d_q)$$
$$= 2(m + n)(1 + 2) + (3mn - m - n)(2 + 2) + 30mn(2 + 3) + 6mn(3 + 3)$$
$$= 198mn + 2m + 2n.$$

(ii) The second Zagreb index of $g-C_3N_5$ is

$$M_2(g-C_3N_5) = \sum_{pq\in E(G)} (d_p \times d_q)$$
$$= \sum_{pq\in E_1(G)} (d_p \times d_q) + \sum_{pq\in E_2(G)} (d_p \times d_q) + \sum_{pq\in E_3(G)} (d_p \times d_q)$$
$$+ \sum_{pq\in E_4(G)} (d_p \times d_q)$$
$$= 2(m+n)(1\cdot 2) + (3mn-m-n)(2\cdot 2) + 30mn(2\cdot 3) + 6mn(3\cdot 3)$$
$$= 228mn.$$

(iii) The third zagreb index of the $g-C_3N_5$ is

$$ZG_3(g-C_3N_5) = \sum_{pq\in E(G)} |d_p - d_q|$$
$$= \sum_{pq\in E_1(G)} |d_p - d_q| + \sum_{pq\in E_2(G)} |d_p - d_q| + \sum_{pq\in E_3(G)} |d_p - d_q|$$
$$+ \sum_{pq\in E_4(G)} |d_p - d_q|$$
$$= 2(m+n)|1-2| + (3mn-m-n)|2-2| + 30mn|2-3| + 6mn|3-3|$$
$$= 30mn + 2m + 2n.$$

Theorem 2.2. *The ABC index, GA and AG index of $g-C_3N_5$ is,*

(i) $ABC(g-C_3N_5) = 29.334mn + 2.121m + 2.121n$

(ii) $GA(g-C_3N_5) = 38.393mn + 2.656m + 2.656n$

(iii) $AG(g-C_3N_5) = 39.618mn + 1.121m + 1.121n.$

Proof:

(i) The Atom-bond connectivity index of $g-C_3N_5$ is

$$ABC(g-C_3N_5) = \sum_{pq\in E(G)} \sqrt{\frac{d_p+d_q-2}{d_p\cdot d_q}}$$
$$= \sum_{pq\in E_1(G)} \sqrt{\frac{d_p+d_q-2}{d_p\cdot d_q}} + \sum_{pq\in E_2(G)} \sqrt{\frac{d_p+d_q-2}{d_p\cdot d_q}} + \sum_{pq\in E_3(G)} \sqrt{\frac{d_p+d_q-2}{d_p\cdot d_q}}$$
$$+ \sum_{pq\in E_4(G)} \sqrt{\frac{d_p+d_q-2}{d_p\cdot d_q}}$$
$$= 2(m+n)\sqrt{\frac{1+2-2}{1\cdot 2}} + (3mn-m-n)\sqrt{\frac{2+2-2}{2\cdot 2}} + 30mn\sqrt{\frac{2+3-2}{2\cdot 3}}$$
$$+ 6mn\sqrt{\frac{3+3-2}{3\cdot 3}}$$
$$= \frac{m+n}{\sqrt{2}} + \frac{3mn-m-n}{\sqrt{2}} + \frac{30mn}{\sqrt{2}} + 4mn$$
$$= 29.334mn + 2.121m + 2.121n.$$

(ii) The Geometric arithmetic mean of $g - C_3N_5$ is

$$\begin{aligned}
GA(g - C_3N_5) &= \sum_{pq \in E(G)} \frac{2\sqrt{d_p \cdot d_q}}{d_p + d_q} \\
&= \sum_{pq \in E_1(G)} \frac{2\sqrt{d_p \cdot d_q}}{d_p + d_q} + \sum_{pq \in E_2(G)} \frac{2\sqrt{d_p \cdot d_q}}{d_p + d_q} + \sum_{pq \in E_3(G)} \frac{2\sqrt{d_p \cdot d_q}}{d_p + d_q} \\
&+ \sum_{u,v \in E_4(G)} \frac{2\sqrt{d_p \cdot d_q}}{d_p + d_q} \\
&= 2(m+n)\frac{2\sqrt{1 \cdot 2}}{1+2} + (3mn - m - n)\frac{2\sqrt{2 \cdot 2}}{2+2} + 30mn\frac{2\sqrt{2 \cdot 3}}{2+3} \\
&+ 6mn\frac{2\sqrt{3 \cdot 3}}{3+3} \\
&= (9 + 12\sqrt{6})mn + (4\sqrt{2} - 3)m + (4\sqrt{2} - 3)n \\
&= 38.393mn + 2.656m + 2.656n.
\end{aligned}$$

(iii) The Arithmetic geometric index of $g - C_3N_5$ is

$$\begin{aligned}
AG(g - C_3N_5) &= \sum_{pq \in E(G)} \frac{d_p + d_q}{2\sqrt{d_p \cdot d_q}} \\
&= \sum_{pq \in E_1(G)} \frac{d_p + d_q}{2\sqrt{d_p \cdot d_q}} + \sum_{pq \in E_2(G)} \frac{d_p + d_q}{2\sqrt{d_p \cdot d_q}} + \sum_{pq \in E_3(G)} \frac{d_p + d_q}{2\sqrt{d_p \cdot d_q}} \\
&+ \sum_{pq \in E_4(G)} \frac{d_p + d_q}{2\sqrt{d_p \cdot d_q}} \\
&= 2(m+n)\frac{1+2}{2\sqrt{1 \cdot 2}} + (3mn - m - n)\frac{2+2}{2\sqrt{2 \cdot 2}} + 30mn\frac{2+3}{2\sqrt{2 \cdot 3}} \\
&+ 6mn\frac{3+3}{2\sqrt{3 \cdot 3}} \\
&= 2(m+n)\frac{1+2}{2\sqrt{1 \cdot 2}} + (3mn - m - n)\frac{2+2}{2\sqrt{2 \cdot 2}} + 30mn\frac{2+3}{2\sqrt{2 \cdot 3}} \\
&+ 6mn\frac{3+3}{2\sqrt{3 \cdot 3}} \\
&= 39.618mn + 1.121m + 1.121n.
\end{aligned}$$

Theorem 2.3. *The Harmonic index and Forgotten index of $g - C_3N_5$ are:*

(i) $H(g - C_3N_5) = 15.5mn + 0.833m + 0.833n$
(ii) $F(g - C_3N_5) = 522mn + 2m + 2n.$

Proof:

(i) The harmonic index of $g-C_3N_5$ is given by

$$
\begin{aligned}
H(g-C_3N_5) &= \sum_{pq\in E(G)} \frac{2}{(d_p+d_q)} \\
&= \sum_{pq\in E_1(G)} \frac{2}{(d_p+d_q)} + \sum_{pq\in E_2(G)} \frac{2}{(d_p+d_q)} + \sum_{pq\in E_3(G)} \frac{2}{(d_p+d_q)} \\
&+ \sum_{pq\in E_4(G)} \frac{2}{(d_p+d_q)} \\
&= 2(m+n)\frac{2}{1+2} + (3mn-m-n)\frac{2}{2+2} + 30mn\frac{2}{2+3} \\
&+ 6mn\frac{2}{3+3} \\
&= 15.5mn + 0.833m + 0.833n.
\end{aligned}
$$

(ii) The forgotten index of $g-C_3N_5$ is given by:

$$
\begin{aligned}
F(g-C_3N_5) &= \sum_{pq\in E(G)} [{d_p}^2+{d_q}^2] \\
&= \sum_{pq\in E_1(G)} [{d_p}^2+{d_q}^2] + \sum_{pq\in E_2(G)} [{d_p}^2+{d_q}^2] + \sum_{pq\in E_3(G)} [{d_p}^2+{d_q}^2] \\
&+ \sum_{pq\in E_4(G)} [{d_p}^2+{d_q}^2] \\
&= 2(m+n)(1+4) + (3mn-m-n)(4+4) + 30mn(4+9) + 6mn(9+9) \\
&= 522mn + 2m + 2n.
\end{aligned}
$$

Theorem 2.4. *The Randic indices of $g-C_3N_5$ for $\alpha = 1, -1, \frac{1}{2}, \frac{-1}{2}$ are given by:*

(i) $R_1(g-C_3N_5) = 228mn$
(ii) $R_{-1}(g-C_3N_5) = 6.416mn + 0.75m + 0.75n$
(iii) $R_{\frac{1}{2}}(g-C_3N_5) = 97.484mn + 0.828m + 0.828n$
(iv) $R_{\frac{-1}{2}}(g-C_3N_5) = 11.747mn + 1.914m + 1.914n.$

Proof:

(i) For $\alpha = 1$,

$$
\begin{aligned}
R_1(g-C_3N_5) &= \sum_{pq\in E(G)} (d_p\cdot d_q) \\
&= \sum_{pq\in E_1(G)} (d_p\cdot d_q) + \sum_{pq\in E_2(G)} (d_p\cdot d_q) + \sum_{pq\in E_3(G)} (d_p\cdot d_q) \\
&+ \sum_{pq\in E_4(G)} (d_p\cdot d_q) \\
&= 2(m+n)(1\cdot 2) + (3mn-m-n)(2\cdot 2) + 30mn(2\cdot 3) + 6mn(3\cdot 3) \\
&= 228mn.
\end{aligned}
$$

(ii) For $\alpha = -1$,

$$R_{-1}(g - C_3N_5) = \sum_{pq \in E(G)} \frac{1}{d_p \cdot d_q}$$

$$\sum_{pq \in E_1(G)} \frac{1}{d_p \cdot d_q} + \sum_{pq \in E_2(G)} \frac{1}{d_p \cdot d_q} + \sum_{pq \in E_3(G)} \frac{1}{d_p \cdot d_q}$$

$$+ \sum_{pq \in E_4(G)} \frac{1}{d_p \cdot d_q}$$

$$= 2(m+n)\frac{1}{1 \cdot 2} + (3mn - m - n)\frac{1}{2 \cdot 2} + 30mn\frac{1}{2 \cdot 3} + 6mn\frac{1}{3 \cdot 3}$$

$$= 6.416mn + 0.75m + 0.75n$$

(iii) For $\alpha = \frac{1}{2}$,

$$R_{\frac{1}{2}}(g - C_3N_5) = \sum_{pq \in E(G)} \sqrt{d_p \cdot d_q}$$

$$= \sum_{pq \in E_1(G)} \sqrt{d_p \cdot d_q} + \sum_{pq \in E_2(G)} \sqrt{d_p \cdot d_q} + \sum_{pq \in E_3(G)} \sqrt{d_p \cdot d_q}$$

$$+ \sum_{pq \in E_4(G)} \sqrt{d_p \cdot d_q}$$

$$= 2(m+n)\sqrt{1 \cdot 2} + (3mn - m - n)\sqrt{2 \cdot 2} + 30mn\sqrt{2 \cdot 3} + 6mn\sqrt{3 \cdot 3}$$

$$= 97.484mn + 0.828m + 0.828n.$$

(iv) For $\alpha = \frac{-1}{2}$,

$$R_{\frac{-1}{2}}(g - C_3N_5) = \sum_{pq \in E(G)} \frac{1}{\sqrt{d_p \cdot d_q}}$$

$$= \sum_{pq \in E_1(G)} \frac{1}{\sqrt{d_p \cdot d_q}} + \sum_{pq \in E_2(G)} \frac{1}{\sqrt{d_p \cdot d_q}} + \sum_{pq \in E_3(G)} \frac{1}{\sqrt{d_p \cdot d_q}}$$

$$+ \sum_{pq \in E_4(G)} \frac{1}{\sqrt{d_p \cdot d_q}}$$

$$= 2(m+n)\frac{1}{\sqrt{1 \cdot 2}} + (3mn - m - n)\frac{1}{\sqrt{2 \cdot 2}} + 30mn\frac{1}{\sqrt{2 \cdot 3}} + 6mn\frac{1}{\sqrt{3 \cdot 3}}$$

$$= 11.747mn + 1.914m + 1.914n.$$

3. Graphical and Numerical Comparison

Topological indices has proved to be effective molecular descriptor in QSPR/QSAR studies of a chemical compound. The degree based indices computed in this article help to predict the physio chemical properties of $g - C_3N_5$. In this section, we presented the numerical values for degree based TI's for the structure of $g - C_3N_5$ which provides an input on analysis between statistical and biological behaviour.

TABLE 3. Numerical Comparison of M_1, M_2 and ZG_3 of $g - C_3N_5$.

$[m, n]$	M_1	M_2	ZG_3
$[1, 1]$	202	228	34
$[2, 2]$	800	912	128
$[3, 3]$	1794	2052	282
$[4, 4]$	3184	3648	496
$[5, 5]$	4970	5700	770
$[6, 6]$	7152	8208	1104
$[7, 7]$	9730	11172	1498
$[8, 8]$	12704	14592	1498
$[9, 9]$	16074	18468	2466
$[10, 10]$	19840	22800	3040

TABLE 4. Numerical Comparison of ABC, GA, AG of $g - C_3N_5$.

$[m, n]$	ABC	GA	AG
$[1, 1]$	33.57	43.70	41.86
$[2, 2]$	125.82	164.20	162.95
$[3, 3]$	276.02	361.48	363.28
$[4, 4]$	486.32	635.55	642.85
$[5, 5]$	754.75	986.41	1001.66
$[6, 6]$	1081.49	1414.05	1439.70
$[7, 7]$	1467.08	1918.49	1956.98
$[8, 8]$	1911.34	2499.71	2553.49
$[9, 9]$	2414.27	3157.72	3229.24
$[10, 10]$	2975.87	3892.51	3984

TABLE 5. Numerical Comparison of H, F of $g - C_3N_5$.

$[m, n]$	H	F
$[1, 1]$	17.16	526
$[2, 2]$	65.33	2096
$[3, 3]$	144.49	4744
$[4, 4]$	254.66	8368
$[5, 5$	395.83	13070
$[6, 6]$	567.99	18816
$[7, 7]$	771.16	25606
$[8, 8]$	1005.32	33440
$[9, 9]$	1270.49	42318
$[10, 10]$	1566.66	52240

TABLE 6. Numerical Comparison of $R_1, R_{-1}, R_{\frac{1}{2}}$, $R_{\frac{-1}{2}}$ of $g - C_3N_5$.

$[m, n]$	R_1	R_{-1}	$R_{\frac{1}{2}}$	$R_{\frac{-1}{2}}$
$[1, 1]$	228	7.91	99.14	15.57
$[2, 2]$	912	28.66	393.24	54.64
$[3, 3]$	2052	62.24	881.85	117.20
$[4, 4]$	3648	108.65	1565.74	203.26
$[5, 5]$	5700	167.90	2444.60	312.815
$[6, 6]$	8208	239.97	3518.42	445.86
$[7, 7]$	11172	324.88	4787.21	602.39
$[8, 8]$	14592	422.62	6250.97	782.43
$[9, 9]$	18468	533.19	7909.70	985.95
$[10, 10]$	22800	656.60	9763.40	1212.98

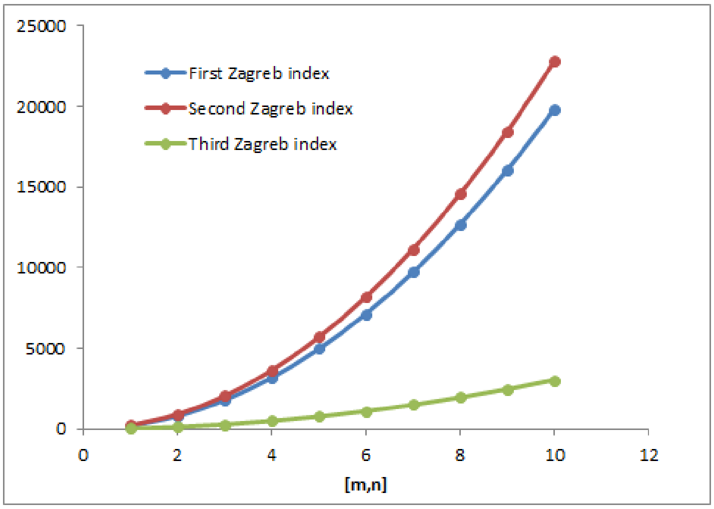

FIGURE 2. Graphical representation of First, Second and Third zagreb indices of $g-C_3N_5$

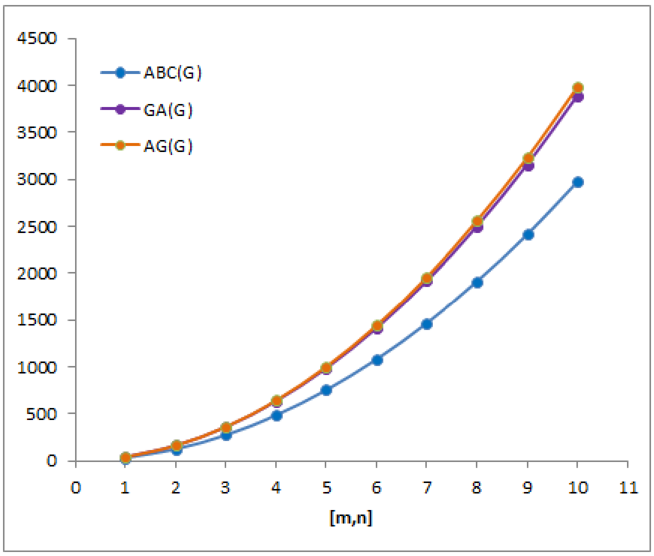

FIGURE 3. Graphical representation of ABC, GA, and AG of $g-C_3N_5$

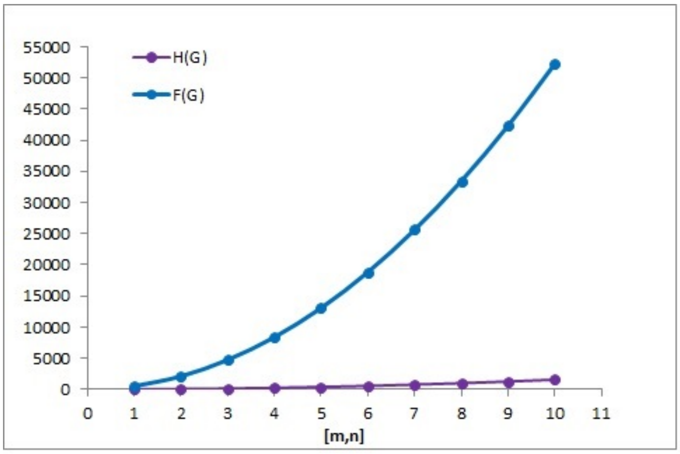

FIGURE 4. Graphical representation of Harmonic and Forgotten indices of $g - C_3N_5$

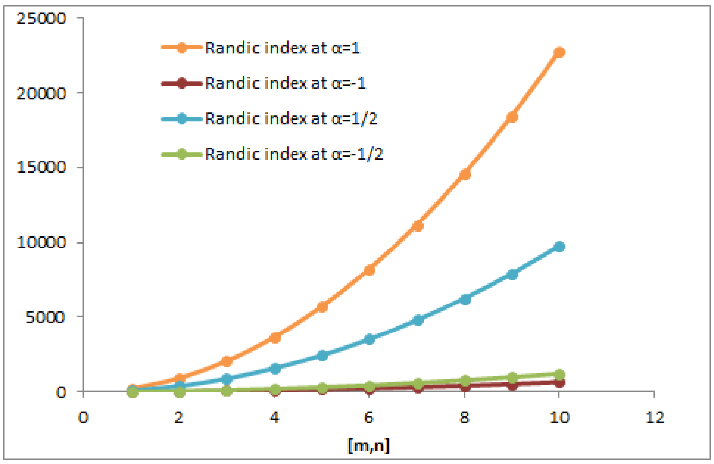

FIGURE 5. Graphical representation of Randic indices of $g - C_3N_5$

4. Conclusions and Discussion

In this work we computed few topological indices for $g-C_3N_5$ compound, decoded topological indices helps to understand the chemical and structural properties of molecular structure. We can observe from **Tables** 3 to 6 all the indices are in mounting order as per the n value. The graphical representation of derived topological indices are portrayed in **Figures** 2 to 5 for definite n values. This results provide the insights regraded to properties of compound. Entropy measures play a vital role in delivering valuable enlightenment into the nature of information content of molecular structures. These decoded topological descriptors are used to depict the entropy measures of $g - C_3N_5$ in our forthcoming research article.

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