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Second Hyper-Zagreb Index of Titania Nanotubes and Their Applications

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ABSTRACT Topological index is a numerical descriptor of a molecule, based on a certain topological feature of the corresponding molecular graph, it is found that there is a strong correlation between the properties of chemical compounds and their molecular structure. In the other side, titania nanotube is a well-known semiconductor and has numerous technological applications such as biomedical devices, dye-sensitized solar cells, and etc. In this paper, the second Hyper-Zagreb index and their coindex of Titania nanotubes have been computed. Furthermore, strong correlation coefficients between second Hyper-Zagreb index and some physicochemical properties such as Density (DENS), Molar volume (MV), Acentric factor (Acenfac) and Entropy (S) have been Appeared.

INDEX TERMS Second hyper-Zagreb coindex, second hyper-Zagreb index, titania nanotube, Zagreb indices.

I. INTRODUCTION

Titania nanotubes are a semiconductor widely used in numerous technological applications. During the last two decades, titania nanotubes were systematically synthesized were carefully studied as prospective technological materials. Therefore, the study of titania nanotubes has received attention in both chemical and mathematical literature [1]. Recently, De [2] studied some topological indices such as F-index, reformulated first Zagreb index, and hyper-Zagreb index of titania nanotubes, Malik and Imran [3] studied the Zagreb indices and Nadeem and Shaker [4] studied the eccentric connectivity index of an infinite class of this type of nanotubes. Topological indices and their coindices are real numbers related to graphs, they have many applications as tools for modeling chemical and other properties of molecules. In practical applications, Zagreb Indices are among the best topological indices in applications to recognize the physical properties, chemical reactions, and biological activities [5], [6]. Throughout this paper, we consider a finite connected graph G that has no loops or multiple edges. The vertex and the edge sets of a graph G are denoted by $V(G)$ and $E(G)$, respectively. The degree of the vertex a is the number of edges joined with this vertex, denoted by $\delta(a)$.

The first Zagreb index $M_1(G)$, and the second Zagreb index $M_2(G)$ were firstly considered by Gutman and Trinajstic in 1972 [7]–[9]. They are defined as:

$$M_1(G) = \sum_{v\in V(G)} \delta_G{}^2(v) = \sum_{uv\in E(G)} \delta_G(u) + \delta_G(v)$$

$$M_2(G) = \sum_{uv\in E(G)} \delta_G(u)\,\delta_G(v)$$

In 2013, Shirdel and Sayadi [10], Milovanovic*et al.* [20] introduced distance-based Zagreb indices named Hyper-Zagreb index as:

$$HM(G) = \sum_{uv\in E(G)} (\delta_G(u) + \delta_G(v))^2$$

Furtula and Gutman in 2015 introduced a forgotten index (F-index) [11], [12] which defined as:

$$F(G) = \sum_{v\in V(G)} \delta_G{}^3(v) = \sum_{uv\in E(G)} \left(\delta_G{}^2(u) + \delta_G{}^2(v)\right)$$

Ghobadi and Ghorbaninejad in 2018 are computed exact formulas for the Zagreb and Hyper-Zagreb indices of Some Molecular Graphs [13]. They defined a new degree-based Zagreb index named Forgotten topological index or "Hyper F-index" defined as:

$$HF(G) = \sum_{uv\in E(G)} [\delta_G{}^2(u) + \delta_G{}^2(v)]^2$$

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A. Alameri et al in 2020, introduced Y-index [14] and Y-coindex [15] defined, respectively, as:

$$Y(G) = \sum_{u\in V(G)} \delta_G^4(u) = \sum_{uv\in E(G)} [\delta_G^3(u) + \delta_G^3(v)]$$
$$\overline{Y}(G) = (n-1)F(G) - Y(G)$$

In 2016, computed exact formulas for the Zagreb and Hyper-Zagreb indices of Carbon Nanocones $CNC_k[n]$ by Gao *et al.* They defined a new degree-based topological index named second Hyper-Zagreb index [16]. In this paper, we compute a new topological index and their coindices (such as second Hyper-Zagreb index, Y-index, and their coindices) of Titania nanotubes. Moreover, we will compare some topological indices with the second Hyper-Zagreb index by using the strong correlation coefficient acquired from the chemical graphs of octane isomers. In the next section, we will define the second Hyper-Zagreb index and their coindex, also we give some important equation to connect between the second Hyper-Zagreb index and their coindex. Any unexplained terminology is standard, typically as in [17], [18], [21], [22].

II. PRELIMINARIES

Definition 2.1: The second Hyper-Zagreb index of a graph G defined as:

$$HM_2(G) = \sum_{uv\in E(G)} [\delta_G(u)\,\delta_G(v)]^2 = \sum_{uv\in E(G)} {\delta_G}^2(u){\delta_G}^2(v)$$

Definition 2.2: The second Hyper-Zagreb coindex of a graph G defined as:

$$\overline{HM}_2(G) = \sum_{uv\notin E(G)} [\delta_G(u)\,\delta_G(v)]^2 = \sum_{uv\notin E(G)} {\delta_G}^2(u){\delta_G}^2(v)$$

Proposition 2.3: Let G be a graph with n vertices and m edges. Then:

$$\overline{HM}_2(G) = \{1/2\}M_1^2(G) - \{1/2\}Y(G) - HM_2(G).$$

Proof. By (Definitions 2.1, 2.2), and using a similar method as
(Theorem 2.1) in [19], we have:

$$\begin{aligned}
&HM_2(G) + \overline{HM}_2(G)\\
&= [\sum_{uv\in E(G),u\neq v} + \sum_{uv\notin E(G),u\neq v}](\delta_G(u)\delta_G(v))^2\\
&= \{1/2\}[\sum_{u\in V(G),u\neq v}\ \sum_{v\in V(G),u\neq v} (\delta_G(u)\delta_G(v))^2\\
&\quad - \sum_{v\in V(G),u=v} (\delta_G(u)\delta_G(v))^2]\\
&= \{1/2\}[\sum_{u\in V(G)} \delta_G^2(u) \sum_{v\in V(G)} \delta_G^2(v)\\
&\quad - \sum_{v\in V(G)} \delta_G^4(u)]\\
&= \{1/2\}[M_1^2(G) - Y(G)].
\end{aligned}$$

Thus,

$$\overline{HM}_2(G) = \{1/2\}M_1^2(G) - \{1/2\}Y(G) - HM_2(G).$$

III. MAIN RESULTS

Titania nanotubes are considered one of the most studied compounds in materials science. Owing to some outstanding properties, it is used, for instance, in photocatalysis, dye-sensitized solar cells, and biomedical devices. In the following section, we study the Y-index and the second Hyper-Zagreb index and their coindices of titania nanotubes $Tio_2[m,n]$ that has total $2n+2$ rows and m columns and is presented in Figure 1.

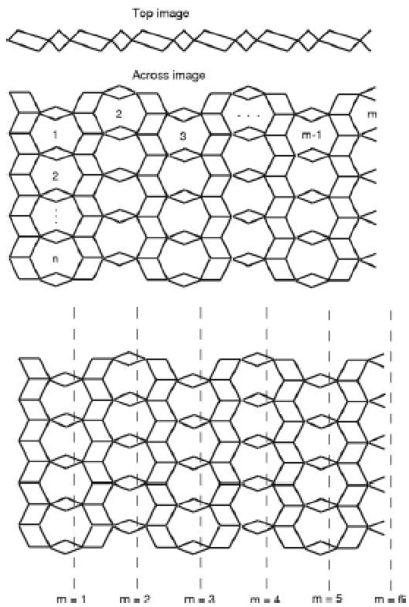

FIGURE 1. The molecular graph of $TiO_2[n,m]$ nanotube for m = 6 and n = 4.

Theorem 3.1: The Y-index of $TiO_2[n,m]$ nanotube is given by

$$Y(TiO_2[n,m]) = 1444mn + 576n.$$

Proof: By definition of the Y-index

$$Y(G) = \sum_{uv\in E(G)} \left(\delta_G^3(u) + \delta_G^3(v)\right),$$

and by replacing each G with TiO_2,which yields

$$Y(TiO_2) = \sum_{uv\in E(TiO_2)} \left(\delta_{TiO_2}^3(u) + \delta_{TiO_2}^3(v)\right).$$

The partitions of the vertex set and edge set $V(TiO_2)$, $E(TiO_2)$, of $TiO_2[n,m]$ nanotubes are given in (Tables 1,2) respectively [2].

TABLE 1. The vertex partition of $TiO_2[n,m]$ nanotubes.

Vertex partition	v_2	v_3	v_4	v_5
$Cardinality$	$2mn+4n$	$2mn$	$2n$	$2mn$

The edge set of TiO_2 is divided into three edge partitions based on the sum of degrees of the end vertices as:

$$E_6(TiO_2) = E_8^*$$
$$= \{e = uv \in E(TiO_2) : \delta(u) = 2, \delta(v) = 4\},$$

TABLE 2. **The edge partition of $TiO_2[n, m]$ nanotubes.**

Edge partition	$E_6 = E_8^*$	$E_7 = E_{10}^* \cup E_{12}^*$	$E_8 = E_{15}^*$	E_{12}^*	E_{10}^*
$Cardinality$	$6n$	$4mn + 4n$	$6mn - 2n$	$4mn + 2n$	$2n$

$$\begin{aligned} E_7(TiO_2) &= E_{10}^* \cup E_{12}^* \\ &= \{e = uv \in E(TiO_2) : \delta(u) = 2, \delta(v) = 5\} \\ &\cup \{e = uv \in E(TiO_2) : \delta(u) = 3, \delta(v) = 4\}, \\ E_8(TiO_2) &= E_{15}^* \\ &= \{e = uv \in E(TiO_2) : \delta(u) = 3, \delta(v) = 5\}. \end{aligned}$$

Thus:

$$\begin{aligned} Y(TiO_2) &= \sum_{uv \in E(TiO_2)} [\delta_{TiO_2}^3(u) + \delta_{TiO_2}^3(v)] \\ &= \sum_{uv \in E_6(TiO_2)} [\delta_{TiO_2}^3(u) + \delta_{TiO_2}^3(v)] \\ &\quad + \sum_{uv \in E_7(TiO_2)} [\delta_{TiO_2}^3(u) + \delta_{TiO_2}^3(v)] \\ &\quad + \sum_{uv \in E_8(TiO_2)} [\delta_{TiO_2}^3(u) + \delta_{TiO_2}^3(v)] \\ &= \sum_{uv \in E_8^*(TiO_2)} [\delta_{TiO_2}^3(u) + \delta_{TiO_2}^3(v)] \\ &\quad + \sum_{uv \in E_{10}^*(TiO_2)} [\delta_{TiO_2}^3(u) + \delta_{TiO_2}^3(v)] \\ &\quad + \sum_{uv \in E_{12}^*(TiO_2)} [\delta_{TiO_2}^3(u) + \delta_{TiO_2}^3(v)] \\ &\quad + \sum_{uv \in E_{15}^*(TiO_2)} [\delta_{TiO_2}^3(u) + \delta_{TiO_2}^3(v)] \\ &= 72|E_8^*(TiO_2)| + 133|E_{10}^*(TiO_2)| \\ &\quad + 91|E_{12}^*(TiO_2)| + 152|E_{15}^*(TiO_2)| \\ &= 1444mn + 576n. \end{aligned}$$

Corollary 3.2: The Y-coindex of $TiO_2[n, m]$ nanotube is given by:

$$\begin{aligned} &\overline{Y}(TiO_2[n, m]) \\ &\quad = 1920m^2\, n^2 + 2880mn^2 + 960n^2 - 900mn - 444n. \end{aligned}$$

Proof: We have

$$\begin{aligned} \overline{Y}(G) &= (n-1)F(G) - Y(G), \\ F(TiO_2) &= 320mn + 160n, \end{aligned}$$

given in [2],

$$Y(TiO_2) = 580mn + 284n$$

given in (Theorem 3.1) above. Thus

$$\begin{aligned} &\overline{Y}(TiO_2[n, m]) \\ &= [\sum |V(TiO_2)| - 1]F(TiO_2[n, m]) - Y(TiO_2[n, m]) \\ &= 1920m^2\, n^2 + 2880mn^2 + 960n^2 - 900mn - 444n. \end{aligned}$$

Theorem 3.3: The second Hyper-Zagreb index of $TiO_2[n, m]$ nanotube is given by:

$$HM_2(TiO_2[n, m]) = 1930mn + 362n.$$

Proof: By (Definition 2.1), we have

$$HM_2(TiO_2) = \sum_{uv \in E(TiO_2)} \left(\delta_{TiO_2}(u)\, \delta_{TiO_2}(v)\right)^2.$$

As (Theorem 3.1) the partitions of the vertex set and edge set $V(TiO_2)$, $E(TiO_2)$, of $TiO_2[n, m]$ nanotubes are given in (Table 1) and (Table 2) respectively. Thus

$$\begin{aligned} HM_2(TiO_2) &= \sum_{uv \in E(TiO_2)} [\delta_{TiO_2}(u)\delta_{TiO_2}(v)]^2 \\ &= \sum_{uv \in E_6(TiO_2)} [\delta_{TiO_2}(u)\delta_{TiO_2}(v)]^2 \\ &\quad + \sum_{uv \in E_7(TiO_2)} [\delta_{TiO_2}(u)\delta_{TiO_2}(v)]^2 \\ &\quad + \sum_{uv \in E_8(TiO_2)} [\delta_{TiO_2}(u)\delta_{TiO_2}(v)]^2 \\ &= \sum_{uv \in E_8^*(TiO_2)} [\delta_{TiO_2}(u)\delta_{TiO_2}(v)]^2 \\ &\quad + \sum_{uv \in E_{10}^*(TiO_2)} [\delta_{TiO_2}(u)\delta_{TiO_2}(v)]^2 \\ &\quad + \sum_{uv \in E_{12}^*(TiO_2)} [\delta_{TiO_2}(u)\delta_{TiO_2}(v)]^2 \\ &\quad + \sum_{uv \in E_{15}^*(TiO_2)} [\delta_{TiO_2}(u)\delta_{TiO_2}(v)]^2 \end{aligned}$$

Therefore.

$$\begin{aligned} HM_2(TiO_2) &= 64|E_8^*(TiO_2)| + 100|E_{10}^*(TiO_2)| \\ &\quad + 144|E_{12}^*(TiO_2)| + 225|E_{15}^*(TiO_2)| \\ &= 1930mn + 362n. \end{aligned}$$

Corollary 3.4 : The second hyper-Zagreb coindex of $TiO_2[n, m]$ nanotube is given by:

$$\overline{HM}_2(TiO_2[n, m]) = 8[19mn + 12n]^2 - 2652mn - 650n.$$

Proof: By replacing each G with TiO_2 in By (Proposition 2.3), we have

$$\overline{HM}_2(TiO_2) = \{1/2\}M_1^2(TiO_2) - \{1/2\}Y(TiO_2) - HM_2(TiO_2)$$

using $M_1(TiO_2) = 76mn + 48n$ given in(2015) [3], and by (Theorems 3.1, 3.3)

$$\begin{aligned} &\overline{HM}_2(TiO_2[n, m]) \\ &\quad = \{1/2\}M_1^2(TiO_2[n, m]) - \{1/2\}Y(TiO_2[n, m]) \\ &\quad - HM_2(TiO_2[n, m]) \\ &\quad = 8[19mn + 12n]^2 - 2652mn - 650n. \end{aligned}$$

IV. APPLICATIONS

In this section, we will compare some topological indices with each other by using strong or good correlation coefficients acquired from the chemical graphs of octane isomers. The dataset of octane isomers (first six columns of (Table 3) are taken from www.moleculardescriptors.eu and (the last four columns of Table 3) are computed from the definitions of forgotten index (F-index) $F(G)$, Hyper-forgotten index "HF-index" $HF(G)$, first Hyper-Zagreb index $HM_1(G)$ and second Hyper-Zagreb index $HM_2(G)$ respectively. The following physicochemical features have been modeled:

- Density (DENS)
- Molar volume (MV)
- Acentric factor (AcenFac)
- Entropy (S)

TABLE 3. Some physicochemical properties and topological indices of octane isomers.

MolID	AcenFac	S	MV	DENS	M_1	M_2	F	HM_1	HM_2	HF
01	0.3979	111.67	162.605	0.3979	26	24	50	98	88	370
02	0.3779	109.84	163.653	0.3779	28	26	62	114	106	586
03	0.3710	111.26	161.845	0.3710	28	27	62	116	121	616
04	0.3715	109.32	162.12	0.3715	28	27	62	116	121	616
05	0.3625	109.43	160.076	0.3625	28	28	62	118	136	646
06	0.3394	103.42	164.289	0.3394	32	30	92	152	124	1372
07	0.3482	108.02	160.413	0.3482	30	30	74	134	164	882
08	0.3442	106.98	163.093	0.3442	30	29	74	132	139	832
09	0.3568	105.72	164.715	0.3568	30	28	74	130	124	802
10	0.3226	104.74	160.887	0.3226	32	32	92	156	184	1492
11	0.3403	106.59	158.653	0.3403	30	31	74	136	179	912
12	0.3324	106.06	158.807	0.3324	30	31	74	136	179	912
13	0.3069	101.48	157.039	0.3069	32	34	92	160	220	1564
14	0.3008	101.31	159.517	0.3008	34	35	104	174	241	1786
15	0.3054	104.09	165.096	0.3054	34	32	104	168	166	1636
16	0.2932	102.06	157.298	0.2932	34	36	104	176	262	1828
17	0.3174	102.39	158.851	0.3174	32	33	86	152	257	1037
18	0.2553	93.06	138.598	0.2553	38	40	134	214	352	2758

In (Table 4). We select those physicochemical properties of octane isomers which give reasonably strong or good correlations, i.e., the absolute value of correlation coefficient between the second Hyper-Zagreb index and Acentric factor (AcenFac) is strong correlated $|r| = 0.92284$, and the absolute value of correlation coefficients between the second Hyper-Zagreb index and Entropy (S), Molar volume (MV) and Density (DENS), are good correlated larger than 0.80. we can say that the second Hyper-Zagreb index is possible tools for QSPR researches. Moreover, in (Table 5). We find that the correlation coefficient between the second Hyper-Zagreb index and some topological indices, then the correlation coefficient between the second Hyper-Zagreb index $HM_2(G)$ and the second Zagreb index $M_2(G)$ is strong correlated ($r = 0.96029 \geqslant 0.90$), and then the correlation coefficient between the second Hyper-Zagreb index and other topological indices as $M_1(G), F(G), HM_1(G)$ and $HF(G)$ are good correlated ($r \geqslant 0.80$). We will conclude this work with the following examples.

TABLE 4. The correlation coefficients between topological indices and some physicochemical properties of octane isomers.

Index	AcenFac	S	MV	DENS
M_1	-0.97306	-0.95429	-0.63445	0.639762
M_2	-0.98642	-0.94169	-0.74045	0.730287
F	-0.96505	-0.95272	-0.64212	0.648498
HM_1	-0.98291	-0.96143	-0.67739	0.679247
HM_2	-0.92284	-0.89933	-0.82728	0.814151
HF	-0.9514	-0.94259	-0.7035	0.708221

TABLE 5. The correlation coefficients between The second Hyper-Zagreb index and some topological indices of octane isomers.

r	M_1	M_2	F	HM_1	HM_2	HF
HM_2	0.86633	0.96029	0.85193	0.89258	1.00000	0.85576

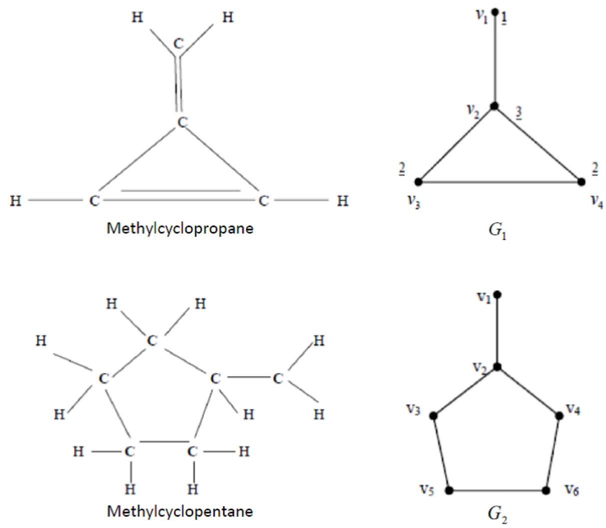

FIGURE 2. Graphs of Methylcyclopropane and Methylcyclopentane.

Example 4.1: Let G_1, G_2 be the four and six atoms of carbon from Chemical compounds: Methylcyclopropane and Methylcyclopentane, respectively, depicted in (Figure 2). Thus,

$$\begin{aligned} HM_2(G_1) &= \sum_{uv \in E(G_1)} \left(\delta_{G_1}(u)\delta_{G_1}(v)\right)^2 \\ &= ((1)(3))^2 + ((3)(2))^2 + ((3)(2))^2 + ((2)(2))^2 = 97. \\ HM_2(G_2) &= \sum_{uv \in E(G_2)} \left(\delta_{G_2}(u)\delta_{G_2}(v)\right)^2 \\ &= ((1)(3))^2 + 2((2)(3))^2 + 3((2)(2))^2 = 129. \end{aligned}$$

Example 4.2: The second Hyper-Zagreb index of spider graph $S_{m,n}$ (cf. Fig. 3) is given by

$$HM_2(S_{m,n}) = 2\,n(256\,m - 415)$$

It is good practice to explain the significance of the figure in the caption.

Example 4.3: Consider the dendrimer D as depicted in Figure 4. The vertex degrees of this graph are 1 and 3, thus, the vertices of every layer are in the same orbit under the action of automorphism graph on the set of vertices. This graph has $3+3(2)+3(2^2)+3(2^3)$ edges, there are $3(2^3)$ edges connected with end vertices where the degrees of this group are 1 but the others are 3. Hence, the second Hyper-Zagreb index of dendrimer D is given by

$$\begin{aligned} HM_2(S_{m,n}) &= (3^2)(3^2)[3 + 3(2) + 3(2^2)] + (3^2)(1^2)[3(2^3)] \\ &= 81[21] + 9[72] = 2349. \end{aligned}$$

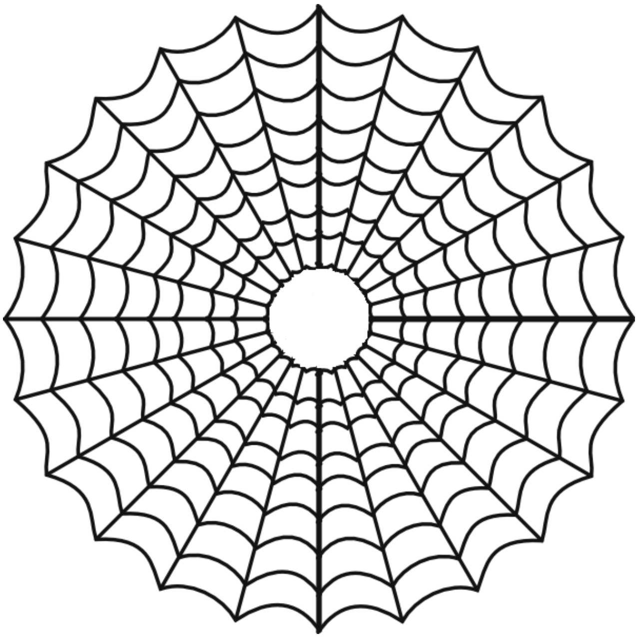

FIGURE 3. $S_{9,24}$.

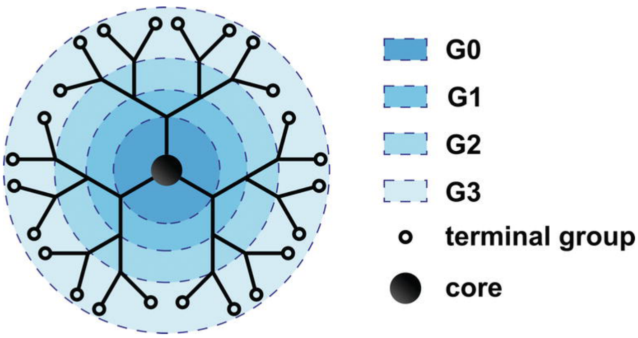

FIGURE 4. 2D Graph of Dendrimer D.

V. CONCLUDING REMARKS

In this paper, the expressions for some new topological indices and their coindices such as Y-index, Y-coindex, second Hyper-Zagreb index, and second Hyper-Zagreb coindex of titania $TiO2$ nanotubes have been derived. In applications the strong correlation coefficients between second Hyper-Zagreb index and some physicochemical properties as Density (DENS) have been Appeared. Much work still needs to be done, and here we mention some possible directions for future research as multiplicative second Hyper-Zagreb index.

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