One Study of Weighted Entropy Based on Topological Indices for Triazine-Based Dendrimer: A Mathematical Chemistry Approach

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Abstract:

Based on a series of previous experiments, there is a natural relationship between the molecular structures of various chemicals and drugs and their biomedical and pharmacological characteristics. Topological Indices are numerical descriptors that are computed for various molecular structures. These topological indices deal with many properties of molecular structure. A dendrimer is a nanometer-scale star-shaped macromolecule. Three components define dendrimers: a central core, an interior dendritic structure (branches), and an exterior surface. Medical and pharmaceutical fields have used topological indices that predict the biological features of new chemical compounds and drugs by calculating weighted entropies for molecular structures. In this paper, we compute the First (a, b) *K.A.* Index, Sombor Index, Modified Sombor Index, Reduced Sombor Index, Reduced modified Sombor Index, Reduced 1^{st} (a, b) *K.A.* Index, Reduced 2nd (a, b) *K.A.* Index for Triazine Based Dendrimer ($TBD - G_n$). Furthermore, we determine weighted entropies of $TBD - G_n$ by computing the topological properties such as the 1^{st} Zagreb index, 2^{nd} Zagreb index, Modified 2^{nd} Zagreb index, Augmented Zagreb Index, Hyper Zagreb 2^{nd} Index, Redefined 1st Zagreb Index, Redefined 2nd Zagreb Index and Redefined 3rd Zagreb Index.

Keywords: Entropy, Graph indices, weighted entropies of $\mathrm{TBD} - \mathrm{G_n}$, Dendrimer, Entropy of $\mathrm{TBD} - \mathrm{G_n}$, Triazine Based Dendrimer

Introduction:

Graph theory is an important branch of mathematics. This field deals with graphs in different fields like mathematics and computer science. There is a non-empty set in the field of graph theory, which is the collection of apexes and controls called graph G. It is signified as $G\ (V, E)$, where V denotes the vertex set and E denotes the edge set. Graph theory was first introduced in 1735 when a bridge problem was solved by a mathematician named Leonhard Euler [1]. To find the degree of vertices, we count the number of controls/edges connected through that vertex. To make modern communication and technological processes possible, we can use graphs underlying many computer programs. They donate to the development of thinking, both abstract and logical. For example, in a famous game like connecting the dots on a piece of paper to make a figure, a cat, or a dog, those connections are also graphs. Chemical graph theory is a field of graph theory that is essential. In Chemical graph theory, an atomic structure is represented by a graph where edges represent the bonding and vertices represent the atoms. The whole graph can be represented in this field by just one quantity, a chemical index, and chemical indexes are often related to chemical properties. An index's minimum or maximum values for any given graph topology are particularly significant. Many of these chemical indices are defined in terms of (topological) vertex degrees, distances between the vertices, or the spectra of matrices describing the graph (like the adjacency matrix) as in spectral graph theory [2].

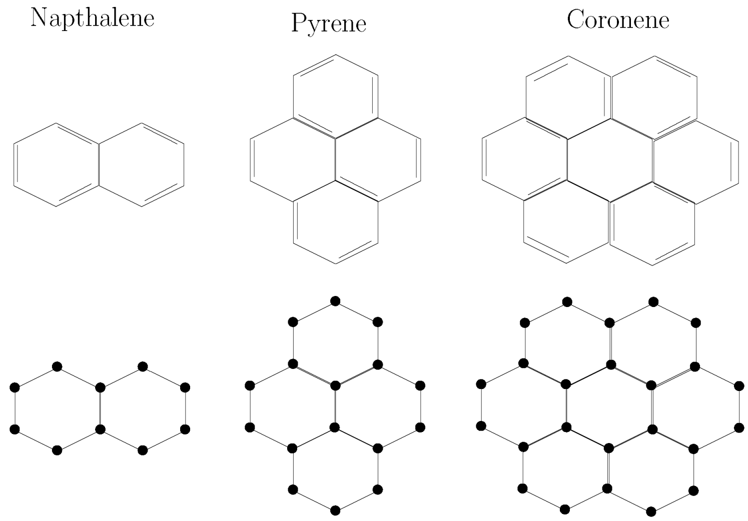
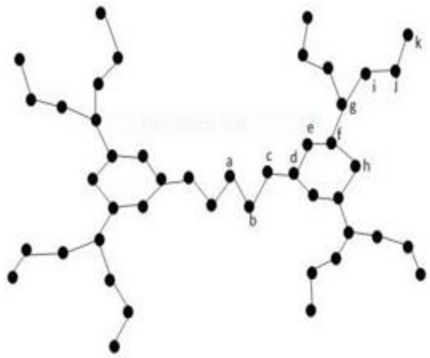


Figure 1: *Chemical Compound and Chemical Structure.*

Mathematical chemistry is a topological branch of chemical graph theory in which we use graph theory to model chemical events mathematically [3]. In recent years, chemical graph theory has fascinated increasing my research interest. In 1988, around 500 articles were produced annually by several researchers, each on chemical graph theory. In this area, many monographs have been written, and it also contains two volumes of a comprehensive text name, Chemical Graph Theory by Trinajstic that summarized the field up to the mid-1980s [4]. Proponents of the theory say that the properties of a chemical graph (i.e., the theoretical representation of a molecule graph) provide valuable insights into chemical phenomena. Some say that graphs play only a fringe role in chemical research [5]. In the mid-nineteenth century, theoretical chemists found useful information about many aspects of organic substances with molecular structure. Examining relevantly generated invariants of the underlying molecular graph yields these molecular structures. Topological indices are called invariants of the graph and are useful in chemistry. Quantitative structure-property relation, QSPR, and quantitative structure-activity relation, QSAR, are two significant topological indices to readers' study [6, 7, 8, 9, and 10]. Here property means some physical or chemical property, and structure means a molecular structure.

Dendrimers are repetitively branched molecules [11]. The word dendrimer derives from the word Dendron, which means tree. Fritz Vogtle introduced the first dendrimer in 1978. Dendrimers are nanosized, void-spaced, monodispersed macromolecules with a high degree of terminal functionality and branching [12, 13]. Due to these properties, dendrimers play a prospective role in the field of drug delivery [14], cancer therapy [15], and catalysis [16]. Dendrimers are monodispersing, homogeneous, and well-defined structures; Dendrimers consist of tree-like branches or arms [17]. Generally, Dendrimers have three elements that are (i) a core, (ii) a branched dendron, and (iii) a terminal group [18]. The core is the main part of dendrimers. Triazine trichloride is one of the most important dendrimers [19]. We can display orthogonally functional surfaces by designing Triazine dendrimers. These orthogonally functional surfaces can enable post-synthetic management such as supplement of the drug, PEGylation, and the fixing of ligands [20, 21].



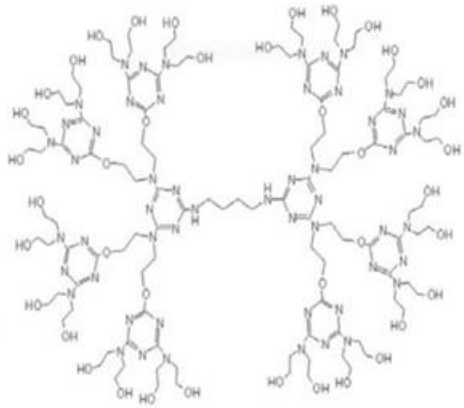


Figure 2: $TBD - G_n$ *of First-generation* **Figure 3:** $TBD - G_n$ *of the second generation*

Set of Edges	(d_s, d_t)	Frequency
E_1	(1,2)	$\frac{6 \times 2^{2n}}{3}$
E_2	(2,2)	$\frac{10 \times 2^{2n} - 4}{3}$
E_3	(2,3)	$\frac{22 \times 2^{2n} - 22}{3}$
E_4	(3,3)	$\frac{4 \times 2^{2n} - 4}{3}$

Table 1: *Edge partition of TBD-G_n.*

The molecular descriptor, another name for the topological index, is a mathematical formula that may be used to calculate and can be used on any graph representing a molecular structure. It is possible to examine mathematical values and explore various physical features of a molecule using this index. As a result, avoiding expensive and time-consuming laboratory tests is a good approach. In mathematical chemistry, molecular descriptors play an important function, especially in QSAR and QSPR investigations.

A topological descriptor is an example of a molecular descriptor. Many topological indices are available today, some of which are used in chemistry. This can be classified based on the graphs used to calculate the structural properties. For example, to calculate the Hosoya index, we count the nonincident edges in a graph. The Wiener index is one of the most used and familiar topological indices. In 1947, Harold Wiener described and utilized it to help him correlate the boiling temperatures of several alkane isomers. Since 1947, more than 3000 topological graph indices have been registered in Chemical DataBases. Chemists and mathematicians both study this field of research [22, 33-47]. There is a growing interest in this topic, hence the topology graph. Some topological indices are discussed here,

Definition 1.1: [23] The 1st Zagreb index $M_1(G)$ is stated as

$$M_1(G) = \sum_{st \in E(G)} (d_s + d_t)$$

Definition 1.2: [23] The 2nd Zagreb index $M_2(G)$ is stated as

$$M_2(G) = \sum_{st \in E(G)} (d_s . d_t)$$

Definition 1.3: [24] Modified 2nd Zagreb index $^{m}M_2(G)$ is stated as

$$Modified\ M_2(G) = \sum_{st \in E(G)} \frac{1}{d_s . d_t}$$

Definition 1.4: [25] Augmented Zagreb Index $AZI(G)$ is stated as

$$AZI(G) = \sum_{st \in E(G)} \left(\frac{d_s d_t}{d_s + d_t - 2}\right)^3$$

Definition 1.5: [26] Hyper Zagreb 2nd Index is $H_2(G)$ and states as

$$H_2(G) = \sum_{st \in E(G)} (d_s .\ d_t)^2$$

Definition 1.6: [27] Redefined 1st Zagreb Index is $ReZ\ G_1(G)$ and is stated as

$$ReZ\ G_1(G) = \sum_{st \in E(G)} \frac{d_s + d_s}{d_s . d_t}$$

Definition 1.7: [28] Redefined 2nd Zagreb Index is $ReZ\ G_2(G)$and stated as

$$ReZ\ G_2(G) = \sum_{st \in E(G)} \frac{d_s . d_t}{d_s + d_t}$$

Definition 1.8: [28] Redefined 3rd Zagreb Index is $ReZ\ G_3(G)$ and is stated as

$$ReZ\ G_3(G) = \sum_{st \in E(G)} ((d_s . d_t)(d_s + d_t))$$

Definition 1.9: [29] Suppose that we have a probability density function

$$P_{ij} = \frac{w(st)}{\sum W(st)}$$

Then the entropy for any graph *G* is defined as
$I(G, w) = -\sum P_{ij} \log{(P_{ij})}$

Definition 1.10: [30] The first $(a,b)-K.A.$ The index is introduced in [10] and defined as

$$KA^1_{(a,b)}(G) = \sum_{xy \in E(G)} [d_G(x)^a + d_G(y)^a]^b$$

Where $a, b \in$ R are chosen suitably.
Definition 1.11: [31], The Sombor Index is introduced in [11] and defined as

$$SO(G) = \sum_{xy \in E(G)} \sqrt{d_G(x)^2 + d_G(y)^2}$$

If at First $(a,b)-K.A.$ For the index, we take values $a = 2$ and $b = \frac{1}{2}$ then we get the sombor index.
Definition 1.12: [32], We define the modified sombor Index as $^{the\ mSO}$ (G), graph G as

$$Modified\ SO(G) = \sum_{xy \in E(G)} \frac{1}{\sqrt{d_G(x)^2 + d_G(y)^2}}$$

Definition 1.13: [32], We define the reduced sombor Index for a graph G as

$$RSO(G) = \sum_{xy \in E(G)} \sqrt{(d_G(x)-1)^2 + (d_G(y)-1)^2}$$

Definition 1.14: We define the reduced modified Sombor index for a graph G as

$$Modified\ RSO(G) = \sum_{xy \in E(G)} \frac{1}{\sqrt{(d_G(x)-1)^2 + (d_G(y)-1)^2}}$$

Definition 1.15: We define Reduced 1st $(a,b)-K.A.$ Index for a graph G as

$$RKA^1_{(a,b)}(G) = \sum_{xy \in E(G)} \left[(d_G(x)-1)^a + (d_G(y)-1)^a\right]^b$$

Definition 1.16: We define the Reduced 2nd $(a,b)-K.A.$ Index for a graph G as

$$\boldsymbol{RKA^2_{(a,b)}(G)} = \sum_{\boldsymbol{xy \in E(G)}} [\boldsymbol{(d_G(x)-1)^a (d_G(y)-1)^a}]^{\boldsymbol{b}}$$

Discussion and Results

First, we compute the First (*a*, *b*) *K.A.* Index, Sombor Index, Modified Sombor Index, Reduced Sombor Index, Reduced modified Sombor Index, Reduced 1st (*a*, *b*) *K.A.* Index, Reduced 2nd (*a*, *b*) *K.A.* Index for $TBD - G_n$. Then in the later part of this section, we determine weighted entropies of $\boldsymbol{TBD - G_n}$ by computing the topological properties such as the 1st Zagreb index, 2nd Zagreb index, Modified 2nd Zagreb index, Augmented Zagreb Index, Hyper Zagreb 2nd Index, Redefined 1st Zagreb Index, Redefined 2nd Zagreb Index and Redefined 3rd Zagreb Index. The general results for the computed indices and weighted entropies of $\boldsymbol{TBD - G_n}$ are computing are given as follows:

Theorem 1: The First (a,b)−K.A. index of $TBD-G_n$ is

$$K.A.^1(a,b)[TBD - G_n] = \frac{2^{2n}}{3}\begin{bmatrix} 6(1+2^a)^b + 5(2^{ab+b+1}) + \\ 22(2^a+3^a)^b + (2^{b+2}.3^{ab}) \end{bmatrix} - \frac{2}{3}\begin{bmatrix} 2^{ab+b+1} + 11(2^a+3^a)^b + \\ (2^{b+1}.3^{ab}) \end{bmatrix}$$

Proof: By using table 1 and definition 1.10. We have

$$K.A.^1(a,b)[TBD - G_n] = \sum_{xy \in E(G)} [d_G(u)^a + d_G(v)^a]^b$$

$$K.A.^1(a,b)[TBD - G_n] = \begin{bmatrix} \frac{6 \times 2^{2n}}{3}[1^a + 2^a]^b + \frac{10 \times 2^{2n} - 4}{3}[2^a + 2^a]^b + \\ \frac{22 \times 2^{2n} - 22}{3}[2^a + 3^a]^b + \frac{4 \times 2^{2n} - 4}{3}[3^a + 3^a]^b \end{bmatrix}$$

$$K.A.^1(a,b)[TBD - G_n] = \begin{bmatrix} \frac{6 \times 2^{2n}}{3}[1^a + 2^a]^b + \frac{10 \times 2^{2n}}{3}2^{ab+b} + \frac{22 \times 2^{2n}}{3}[2^a + 3^a]^b + \\ + \frac{4 \times 2^{2n}}{3}[2 \times 3^a]^b - \frac{4 \times 2^{ab+b}}{3} - \frac{22}{3}(2^a + 3^a)^b - \frac{4}{3}[2 \times 3^a]^b \end{bmatrix}$$

$$K.A.^1(a,b)[TBD - G_n] = \frac{2^{2n}}{3}\begin{bmatrix} 6(1+2^a)^b + 5(2^{ab+b+1}) + \\ 22(2^a+3^a)^b + (2^{b+2}.3^{ab}) \end{bmatrix} - \frac{2}{3}\begin{bmatrix} 2^{ab+b+1} + 11(2^a+3^a)^b + \\ (2^{b+1}.3^{ab}) \end{bmatrix}$$

Corollary 1: By using table 1 and definition 1.11. We have

$$SO[TBD - G_n] = \sum_{xy \in E(G)} \sqrt{d_G(u^2) + d_G(v^2)}$$

$$SO[\mathrm{TBD}-\mathrm{G_n}] = \left[\frac{6\times 2^{2n}\sqrt{5}}{3} + \frac{(10\times 2^{2n}-4)\,2\sqrt{2}}{3} + \frac{(22\times 2^{2n}-22)\sqrt{13}}{3} + \frac{(4\times 2^{2n}-4)\,3\sqrt{2}}{3}\right]$$

$$SO[\mathrm{TBD}-\mathrm{G_n}] = \left[\frac{6\times 2^{2n}\sqrt{5}}{3} + \frac{(20\times 2^{2n})\sqrt{2}}{3} - \frac{8\sqrt{2}}{3} + \frac{(22\times 2^{2n})\sqrt{13}}{3} - \frac{22\sqrt{13}}{3} + \frac{(12\times 2^{2n})\sqrt{2}}{3} - \frac{12\sqrt{2}}{3}\right]$$

$$SO[\mathrm{TBD}-\mathrm{G_n}] = \left[\frac{2^{2n}}{3}\left[6\sqrt{5}+20\sqrt{2}+22\sqrt{13}+12\sqrt{2}\right] - \frac{2}{3}\left[4\sqrt{2}+11\sqrt{13}+6\sqrt{2}\right]\right]$$

$$SO[\mathrm{TBD}-\mathrm{G_n}] = \left[\frac{2^{2n}}{3}\left[6\sqrt{5}+32\sqrt{2}+22\sqrt{13}\right] - \frac{2}{3}\left[10\sqrt{2}+11\sqrt{13}\right]\right]$$

Corollary 2: By using table 1 and definition 1.12. We have

$${}^{m}SO(TBD-G_n) = \left[\frac{|E_1|}{\sqrt{1^2+2^2}} + \frac{|E_2|}{\sqrt{2^2+2^2}} + \frac{|E_3|}{\sqrt{2^2+3^2}} + \frac{|E_4|}{\sqrt{3^2+3^3}}\right]$$

$${}^{m}SO(TBD-G_n) = \left[\frac{\frac{6\times 2^{2n}}{3}}{\sqrt{5}} + \frac{\frac{10\times 2^{2n}-4}{3}}{2\sqrt{2}} + \frac{\frac{22\times 2^{2n}-22}{3}}{\sqrt{13}} + \frac{\frac{4\times 2^{2n}-4}{3}}{3\sqrt{2}}\right]$$

$${}^{m}SO(TBD-G_n) = \left(\frac{6\times 2^{2n}}{3\sqrt{5}} + \frac{10\times 2^{2n}-4}{3\times 2\sqrt{2}} + \frac{22\times 2^{2n}-22}{3\sqrt{13}} + \frac{4\times 2^{2n}-4}{3\times 3\sqrt{2}}\right)$$

$${}^{m}SO(TBD-G_n) = \frac{2^{2n}}{9\sqrt{130}}\left(22\sqrt{10}+18\sqrt{26}+19\sqrt{65}\right) - \frac{2}{3}\left(33\sqrt{2}+3\sqrt{13}\right)$$

Corollary 3: By using table 1 and definition 1.13. We have

$$RSO[TBD-G_n] = \left[\frac{6\times 2^{2n}}{3}\sqrt{1^2} + \left(\frac{10\times 2^{2n}-4}{3}\right)\sqrt{2} + \left(\frac{22\times 2^{2n}-22}{3}\right)\sqrt{5} + \frac{4\times 2^{2n}-4}{3}\sqrt{8}\right]$$

$$RSO[PDL-G_n] = \left[\frac{6\times 2^{2n}}{3}\sqrt{1^2} + \left(\frac{10\times 2^{2n}}{3}\right)\sqrt{2} - \frac{4}{3}\sqrt{2} + \left(\frac{22\times 2^{2n}}{3}\right)\sqrt{5} - \frac{22}{3}\sqrt{5} + \frac{4\times 2^{2n}}{3}\sqrt{8} - \frac{4}{3}\sqrt{8}\right]$$

$$RSO[TBD-G_n] = \left[\frac{2^{2n}}{3}\left[6+18\sqrt{2}+22\sqrt{5}\right] - \frac{2}{3}\left[6\sqrt{2}+22\sqrt{5}\right]\right]$$

Corollary 4: By using table 1 and definition 1.14. We have

$${}^{m}RSO[TBD-G_n] = \left[\frac{\frac{6\times 2^{2n}}{3}}{\sqrt{1}} + \frac{\frac{10\times 2^{2n}-4}{3}}{\sqrt{2}} + \frac{\frac{22\times 2^{2n}-22}{3}}{\sqrt{5}} + \frac{\frac{4\times 2^{2n}-4}{3}}{2\sqrt{2}}\right]$$

$${}^{m}RSO[TBD-G_n] = \left[\left[\frac{6\times 2^{2n}}{3} + \frac{10\times 2^{2n}-4}{3\sqrt{2}} + \frac{22\times 2^{2n}-22}{3\sqrt{5}} + \frac{4\times 2^{2n}-4}{6\sqrt{2}}\right]\right]$$

$${}^{m}RSO[TBD-G_n] = \left[\frac{2^{2n}}{3\sqrt{10}}\left[6\sqrt{10}+12\sqrt{5}+22\sqrt{2}\right] - \frac{2}{3}\left[\sqrt{5}+11\sqrt{2}\right]\right]$$

Theorem 2: The First Reduced (a,b)−K.A. index of TBD−G_n is

$$RKA^1(a,b)[TBD-G_n]=\begin{bmatrix}\frac{2^{2n}}{3}\left[6+5(2^{b+1})+22(1+2^a)^b+2^{ab+b+2}\right]- \\ \frac{2}{3}\left[2^{b+1}+11(1+2^a)^b+2^{ab+b+2}\right]\end{bmatrix}$$

Proof: By using table 1 and definition 1.15. We have

$RKA^1(a,b)[PDL-G_n]$

$$=\begin{bmatrix}\frac{6\times 2^{2n}}{3}[(1-1)^a+(2-1)^a]^b+[(2-1)^a+(2-1)^a]^b\left[\frac{10\times 2^{2n}-4}{3}\right]+ \\ \frac{22\times 2^{2n}-22}{3}[(2-1)^a+(3-1)^a]^b+\frac{4\times 2^{2n}-4}{3}[(3-1)^a+(3-1)^a]^b\end{bmatrix}$$

$$RKA^1(a,b)[TBD-G_n]=\begin{bmatrix}\frac{6\times 2^{2n}}{3}+[2]^b\left[\frac{10\times 2^{2n}-4}{3}\right]+\frac{22\times 2^{2n}-22}{3}[1+(2)^a]^b \\ +\frac{4\times 2^{2n}-4}{3}[(2)^{a+1}]^b\end{bmatrix}$$

$$RKA^1(a,b)[TBD-G_n]=\begin{bmatrix}\frac{2^{2n}}{3}\left[6+5(2^{b+1})+22(1+2^a)^b+2^{ab+b+2}\right]- \\ \frac{2}{3}\left[2^{b+1}+11(1+2^a)^b+2^{ab+b+2}\right]\end{bmatrix}$$

Theorem 3: The Second Reduced (a,b)−K.A. index of TBD −G_n is

$$RKA^2(a,b)[TBD-G_n]=\left[\frac{2^{2n}}{3}[10+22(2^a)^b+(2)^{ab+b+2}]-\frac{2}{3}[2+11\times 2^{ab}+(2)^{ab+b+1}\right]$$

Proof. By using table 1 and definition 1.16. We have

$RKA^2(a,b)[TBD-G_n]$

$$=\begin{bmatrix}\frac{6\times 2^{2n}}{3}[(1-1)^a(2-1)^a]^b+[(2-1)^a(2-1)^a]^b\left[\frac{10\times 2^{2n}-4}{3}\right] \\ +\frac{22\times 2^{2n}-22}{3}[(2-1)^a(3-1)^a]^b+\left[\frac{4\times 2^{2n}-4}{3}\right][(3-1)^a(3-1)^a]^b\end{bmatrix}$$

$RKA^2(a,b)[TBD-G_n]$

$$=\left[\left[\frac{10\times 2^{2n}-4}{3}+\frac{22\times 2^{2n}-22}{3}+[(2)^a]^b+\left[\frac{4\times 2^{2n}-4}{3}\right][(2)^{a+1}]^b\right]\right]$$

$$RKA^2(a,b)[TBD-G_n]=\left[\frac{2^{2n}}{3}[10+22(2^a)^b+(2)^{ab+b+2}]-\frac{2}{3}[2+11\times 2^{ab}+(2)^{ab+b+1}\right]$$

Theorem 4: The weighted entropy of $TBD-G_n$ with the first Zagreb Index is

$$I(TBD-G_n,M_1)=\log\left[64.2^{2n}-50\right]-\frac{1}{\left[64.2^{2n}-50\right]}\begin{bmatrix}(42.74430424141)2^{2n}- \\ 35.0650967824\end{bmatrix}$$

Proof. By definition 1.1, We have

$$M_1(TBD-G_n)=64.2^{2n}-50$$

by definition 1.9,

$$I(TBD-G_n, M_1) = \log[64.2^{2n}-50] - \frac{1}{[64.2^{2n}-50]}\begin{bmatrix}(1+2)|E_1|\log(1+2)+\\(2+2)|E_2|\log(2+2)+\\(2\ +\ 3)|E_3|\log(2+3)+\\(3+\ 3)|E_4|\log(3+3)\end{bmatrix}$$

$$I(TBD-G_n, M_1) = \log[64.2^{2n}-50] - \frac{1}{[64.2^{2n}-50]}\begin{bmatrix}(3)|E_1|\log(3)+\\(8)|E_2|\log(2)+(5)|E_3|\log(5)+\\(6)|E_4|\log(2)+(6)|E_4|\log(3)\end{bmatrix}$$

$$I(TBD-G_n, M_1) = \log[64.2^{2n}-50] - \frac{1}{[64.2^{2n}-50]}\begin{bmatrix}2^{2n}\left(\frac{104}{3}log2+14log3+\frac{110}{3}log5\right)-\\\left(\frac{56}{3}log2+8log3+\frac{110}{3}log5\right)\end{bmatrix}$$

$$I(TBD-G_n, M_1) = \log[64.2^{2n}-50] - \frac{1}{[64.2^{2n}-50]}\begin{bmatrix}(42.74430424141)2^{2n}-\\35.0650967824\end{bmatrix}$$

Theorem 5: The weighted entropy of $TBD-G_n$ with the second Zagreb Index is

$$I(TBD-G_n, M_2) = \log\left[\frac{220.2^{2n}-184}{3}\right] - \frac{3}{[220.2^{2n}-184]}\begin{bmatrix}(48.55953493425)2^{2n}-\\42.53893502097\end{bmatrix}$$

Proof. By definition 1.2. We have,

$$M_2(TBD-G_n) = \frac{220.2^{2n}-184}{3}$$

by definition 1.9,

$$I(TBD-G_n, M_2) = \log\left[\frac{220.2^{2n}-184}{3}\right] - \frac{3}{[220.2^{2n}-184]}\begin{bmatrix}(1.2)|E_1|\log(1.2)+\\(2.2)|E_2|\log(2.2)+\\(2.3)|E_3|\log(2.3)+\\(3.3)|E_4|\log(3.3)\end{bmatrix}$$

$$I(TBD-G_n, M_2) = \log\left[\frac{220.2^{2n}-184}{3}\right] - \frac{3}{[220.2^{2n}-184]}\begin{bmatrix}2|E_1|\log(2)+8|E_2|\log 2+\\6|E_3|\log 2+6|E_3|log3\\18|E_4|\log 3\end{bmatrix}$$

$$I(TBD-G_n, M_2) = \log\left[\frac{220.2^{2n}-184}{3}\right] - \frac{3}{[220.2^{2n}-184]}\begin{bmatrix}2^{2n}\left(\frac{224}{3}log2+\frac{164}{3}log3\right)-\\\left(\frac{164}{3}log2+\frac{164}{3}log3\right)\end{bmatrix}$$

$$I(TBD-G_n, M_2) = \log\left[\frac{220.2^{2n}-184}{3}\right] - \frac{3}{[220.2^{2n}-184]}\begin{bmatrix}(48.55953493425)2^{2n}-\\42.53893502097\end{bmatrix}$$

Theorem 6: The entropy of $TBD-G_n$ with modified 2nd Zagreb weight is

$$I(TBD-G_n, {}^{m}M_2) = log\left[\frac{36.2^{2n}-36}{3}\right] - \frac{3}{[36.2^{2n}-36]}\begin{bmatrix}46.49231178526\\-2^{2n}(48.90055175057)\end{bmatrix}$$

Proof. By definition 1.3. We have,

$${}^{m}M_2(TBD-G_n) = \frac{36.2^{2n}-36}{3}$$

by definition 1.9,

$$I\,(TBD-G_n,{}^{m}M_2) = log\left[\frac{36.2^{2n}-36}{3}\right] - \frac{3}{[36.2^{2n}-36]}\begin{bmatrix}\frac{1}{1.2}|E_1|log\frac{1}{1.2}+\frac{1}{2.2}|E_2|log\frac{1}{2.2}\\+\frac{1}{2.3}|E_3|log\frac{1}{2.3}+\frac{1}{3.3}|E_4|log\frac{1}{3.3}\end{bmatrix}$$

$$I\,(TBD-G_n,{}^{m}M_2) = log\left[\frac{36.2^{2n}-36}{3}\right] - \frac{3}{[36.2^{2n}-36]}\begin{bmatrix}-\frac{1}{2}|E_1|log2-\frac{1}{2}|E_2|log2\\-\frac{1}{6}|E_3|log2-\frac{1}{6}|E_3|log3-\frac{2}{9}|E_4|log3\end{bmatrix}$$

$$I\,(TBD-G_n,{}^{m}M_2) = log\left[\frac{36.2^{2n}-36}{3}\right] - \frac{3}{[36.2^{2n}-36]}\left[\begin{pmatrix}\frac{140}{3}log2+\frac{204}{3}log3\\-2^{2n}\left(\frac{164}{3}log2+\frac{204}{3}log3\right)\end{pmatrix}\right]$$

$$I\,(TBD-G_n,{}^{m}M_2) = log\left[\frac{36.2^{2n}-36}{3}\right] - \frac{3}{[36.2^{2n}-36]}\begin{bmatrix}46.49231178526\\-2^{2n}(48.90055175057)\end{bmatrix}$$

Theorem 7: The entropy of $\mathrm{TBD}-\mathrm{G_n}$ with Augmented Zagreb weight is

$$I(TBD-G_n,AZI) = \log\left(\frac{5593.\,2^{2n}-4057}{48}\right) - \frac{48}{5593.\,2^{2n}-4057}\begin{bmatrix}(162.42215137306)2^{2n}-\\133.52327178932\end{bmatrix}$$

Proof: By definition 1.4. We have,

$$AZI(TBD-G_n) = \frac{5593.\,2^{2n}-4057}{48}$$

by definition 1.9,

$$I(TBD-G_n,AZI) = \log\left(\frac{5593.\,2^{2n}-4057}{48}\right) - \frac{48}{5593.\,2^{2n}-4057}\begin{bmatrix}\left(\frac{1.2}{1+2-2}\right)^3|E_1|log\left(\frac{1.2}{1+2-2}\right)^3+\\\left(\frac{2.2}{2+2-2}\right)^3|E_2|log\left(\frac{2.2}{2+2-2}\right)^3\\+\left(\frac{2.3}{2+3-2}\right)^3|E_3|log\left(\frac{2.3}{2+3-2}\right)^3+\\\left(\frac{3.3}{3+3-2}\right)^3|E_4|log\left(\frac{3.3}{3+3-2}\right)^3\end{bmatrix}$$

$$I(TBD-G_n,AZI) = \log\left(\frac{5593.\,2^{2n}-4057}{48}\right) - \frac{48}{5593.\,2^{2n}-4057}\begin{bmatrix}24|E_1|log2+24|E_2|log2+\\24|E_3|log2+\frac{4374}{64}|E_4|log3-\\\frac{4374}{64}|E_4|log2\end{bmatrix}$$

$$I(TBD-G_n,AZI) = \log\left(\frac{5593.2^{2n}-4057}{48}\right) - \frac{48}{5593.2^{2n}-4057}\left[\begin{array}{c}\left(\frac{3161}{8}log2+\frac{4374}{48}log3\right)2^{2n}- \\ \left(\frac{2393}{8}log2+\frac{4374}{48}log3\right)\end{array}\right]$$

$$I(TBD-G_n,AZI) = \log\left(\frac{5593.2^{2n}-4057}{48}\right) - \frac{48}{5593.2^{2n}-4057}\left[\begin{array}{c}(162.42215137306)2^{2n}- \\ 133.52327178932\end{array}\right]$$

Theorem 8: The entropy of $\mathrm{TBD}-\mathrm{G_n}$ with hyper, Zagreb's second weight is

$$I(TBD-G_n,H_2) = \log\left(\frac{1300.2^{2n}-1800}{3}\right) - \frac{3}{1300.2^{2n}-1800}\left[\begin{array}{c}(686.0164546)2^{2n}- \\ 642.6681352\end{array}\right]$$

Proof: By definition 1.5. We have,

$$H_2(TBD-G_n) = \left[\frac{1300.2^{2n}-1800}{3}\right]$$

by definition 1.9,

$$I(TBD-G_n,H_2) = \log\left(\frac{1300.2^{2n}-1800}{3}\right) - \frac{3}{1300.2^{2n}-1800}\left[\begin{array}{c}(1.2)^2|E_1|log(1.2)^2+ \\ (2.2)^2|E_2|log(2.2)^2+ \\ (2.3)^2|E_3|log(2.3)^2+ \\ (3.3)^2|E_4|log(3.3)^2\end{array}\right]$$

$$I(TBD-G_n,H_2) = \log\left(\frac{1300.2^{2n}-1800}{3}\right) - \frac{3}{1300.2^{2n}-1800}\left[\begin{array}{c}8|E_1|log2+64|E_2|log2+ \\ 72|E_3|log2+72|E_3|log3 \\ 324|E_4|log3\end{array}\right]$$

$$I(TBD-G_n,H_2) = \log\left(\frac{1300.2^{2n}-1800}{3}\right) - \frac{3}{1300.2^{2n}-1800}\left[\begin{array}{c}log2(8|E_1|+64|E_2|+72|E_3|)+ \\ log3(72|E_3|+324|E_4|)\end{array}\right]$$

$$I(TBD-G_n,H_2) = \log\left(\frac{1300.2^{2n}-1800}{3}\right) - \frac{3}{1300.2^{2n}-1800}\left[\begin{array}{c}log2\left(\frac{2272.2^{2n}}{3}-\frac{1840}{3}\right)+ \\ log3\left(\frac{2880.2^{2n}}{3}-\frac{2880}{3}\right)\end{array}\right]$$

$$I(TBD-G_n,H_2) = \log\left(\frac{1300.2^{2n}-1800}{3}\right) - \frac{3}{1300.2^{2n}-1800}\left[\begin{array}{c}(686.0164546)2^{2n}- \\ 642.6681352\end{array}\right]$$

Theorem 9: The entropy of $\mathrm{TBD}-\mathrm{G_n}$ with redefined first Zagreb weight is

$$I(TBD-G_n, ReZ(G_1)) = \log\left[\left(\frac{40.2^{2n}-25}{3}\right)\right] - \frac{3}{\left[40.2^{2n}-25\right]}\begin{bmatrix}5.191071046+\\(0.112137179)2^{2n}\end{bmatrix}$$

Proof: By definition, 1.6. We have,

$$ReZG_1(TBD-G_n) = \left[\frac{40.2^{2n}-25}{3}\right]$$

by definition 1.9,

$$I(TBD-G_n, ReZ(G_1)) = \log\left[\left(\frac{40.2^{2n}-25}{3}\right)\right] - \frac{3}{[40.2^{2n}-25]}\begin{bmatrix}\frac{1+2}{1.2}|E_1|log\frac{1+2}{1.2}+\frac{2+2}{2.2}|E_2|log\frac{2+2}{2.2}+\\ \frac{2+3}{2.3}|E_3|log\frac{2+3}{2.3}+\frac{3+3}{3.3}|E_4|log\frac{3+3}{3.3}\end{bmatrix}$$

$$I(TBD-G_n, ReZ(G_1))$$

$$= \log\left[\left(\frac{40.2^{2n}-25}{3}\right)\right] - \frac{3}{[40.2^{2n}-25]}\begin{bmatrix}\frac{3}{2}|E_1|log3-\frac{3}{2}|E_1|log2+\\ \frac{5}{6}|E_3|log5-\frac{5}{6}|E_3|log2-\\ \frac{5}{6}|E_3|log3+\frac{2}{3}|E_4|log2-\frac{2}{3}|E_4|log3\end{bmatrix}$$

$$I(TBD-G_n, ReZ(G_1))$$

$$= \log\left[\left(\frac{40.2^{2n}-25}{3}\right)\right] - \frac{3}{[40.2^{2n}-25]}\begin{bmatrix}log2\left(-\frac{3}{2}|E_1|-\frac{5}{6}|E_3|+\frac{2}{3}|E_4|\right)+\\ log3\left(\frac{3}{2}|E_1|-\frac{5}{6}|E_3|-\frac{2}{3}|E_4|\right)+\\ log5\left(\frac{5}{6}|E_3|\right)\end{bmatrix}$$

$$I(TBD-G_n, ReZ(G_1)) = \log\left[\left(\frac{40.2^{2n}-25}{3}\right)\right] - \frac{3}{[40.2^{2n}-25]}\begin{bmatrix}log2\left(\frac{-74.2^{2n}}{9}-\frac{47}{9}\right)+\\ log3\left(-4.2^{2n}-\frac{47}{9}\right)+\\ log5\left(\frac{110.2^{2n}}{18}-\frac{110}{18}\right)\end{bmatrix}$$

$$I(TBD-G_n, ReZ(G_1)) = \log\left[\left(\frac{40.2^{2n}-25}{3}\right)\right] + \frac{3}{[40.2^{2n}-25]}\begin{bmatrix}5.191071046+\\(0.112137179)2^{2n}\end{bmatrix}$$

Theorem 10: The entropy of $TBD-G_n$ with redefined second Zagreb weight is

$$I(TBD-G_n, ReZ(G_2)) = \log\left[\left(\frac{232.2^{2n}-182}{15}\right)\right] + \frac{15}{\left[232.2^{2n}-182\right]}\begin{bmatrix}(4.91481316336)2^{2n}\\-5.14960150877\end{bmatrix}$$

Proof: By definition 1.7. We have,

$$ReZG_2(TBD-G_n) = \frac{232.2^{2n}-182}{15}$$

by definition 1.9,

$$I(TBD-G_n, ReZ(G_2))$$

$$= \log\left[\left(\frac{232.2^{2n}-182}{15}\right)\right] + \frac{15}{\left[232.2^{2n}-182\right]}\begin{bmatrix}\frac{1.2}{1+2}|E_1|log\frac{1.2}{1+2}+\frac{2.2}{2+2}|E_2|log\frac{2.2}{2+2}+\\ \frac{2.3}{2+3}|E_3|log\frac{2.3}{2+3}+\frac{3.3}{3+3}|E_3|log\frac{3.3}{3+3}\end{bmatrix}$$

$$I(TBD-G_n, ReZ(G_2)) = \log\left[\left(\frac{232.2^{2n}-182}{15}\right)\right] + \frac{15}{[232.2^{2n}-182]}\begin{bmatrix} \frac{2}{3}|E_1|log2 - \frac{2}{3}|E_1|log3 + \\ \frac{6}{5}|E_3|log2 + \frac{6}{5}|E_3|log3 \\ -\frac{6}{5}|E_3|log5 + \frac{2}{3}|E_4|log2 - \frac{2}{3}|E_4|log3 \end{bmatrix}$$

$$I(TBD-G_n, ReZ(G_2)) = \log\left[\left(\frac{232.2^{2n}-182}{15}\right)\right] + \frac{15}{[232.2^{2n}-182]}\begin{bmatrix} log2\left(\frac{2}{3}|E_1| + \frac{6}{5}|E_3| + \frac{2}{3}|E_4|\right) + \\ log3\left(-\frac{2}{3}|E_1| + \frac{6}{5}|E_3| - \frac{2}{3}|E_4|\right) + \\ log5\left(-\frac{6}{5}|E_3|\right) \end{bmatrix}$$

$$I(TBD-G_n, ReZ(G_2)) = \log\left[\left(\frac{232.2^{2n}-182}{15}\right)\right] + \frac{15}{[232.2^{2n}-182]}\begin{bmatrix} log2\left(\frac{122.2^{2n}}{15} - \frac{102}{15}\right) + \\ log3\left(\frac{142.2^{2n}}{15} - \frac{162}{15}\right) + \\ log5\left(\frac{-44.2^{2n}}{15} + \frac{44}{15}\right) \end{bmatrix}$$

$$I(TBD-G_n, ReZ(G_2)) = \log\left[\left(\frac{232.2^{2n}-182}{15}\right)\right] + \frac{15}{[232.2^{2n}-182]}\begin{bmatrix} (4.91481316336)2^{2n} \\ -5.14960150877 \end{bmatrix}$$

Theorem 11: The entropy of $\mathrm{TBD}-\mathrm{G_n}$ with redefined third Zagreb weight is

$$I(TBD-G_n, ReZ(G_3)) = \log\left[\left(\frac{1072.2^{2n}-940}{3}\right)\right] + \frac{3}{[1072.2^{2n}-940]}\begin{bmatrix} (513.62361429725)2^{2n} \\ -465.75395984766 \end{bmatrix}$$

Proof. By definition, 1.8. We have,

$$ReZG_3(TBD-G_n) = \frac{1072.2^{2n}-940}{3}$$

by definition 1.9,

$$I(TBD-G_n, ReZ(G_3)) = \log\left[\left(\frac{1072.2^{2n}-940}{3}\right)\right] + \frac{3}{[1072.2^{2n}-940]}\begin{bmatrix} (1.2)(1+2)|E_1|\log(1.2)(1+2) + \\ (2.2)(2+2)|E_2|\log(2.2)(2+2) + \\ (2.3)(2+3)|E_3|\log(2.3)(2+3) + \\ (3.3)(3+3)|E_4|\log(3.3)(3+3) \end{bmatrix}$$

$$I(TBD-G_n, ReZ(G_3)) = \log\left[\left(\frac{1072.2^{2n}-940}{3}\right)\right] + \frac{3}{[1072.2^{2n}-940]}\begin{bmatrix} 6|E_1|\log 6 + 16|E_2|\log 16 + \\ 30|E_3|\log 30 + 54|E_3|\log 54 \end{bmatrix}$$

$$I(TBD-G_n, ReZ(G_2)) = \log\left[\left(\frac{232.2^{2n}-182}{15}\right)\right] + \frac{15}{[232.2^{2n}-182]}\begin{bmatrix} log2(6|E_1| + 64|E_2| + 30|E_3| + 54|E_4|) + \\ log3(6|E_1| + 30|E_3| + 162|E_4|) + \\ log5(30|E_3|) \end{bmatrix}$$

$$I(TBD-G_n, ReZ(G_2)) = \log\left[\left(\frac{232.2^{2n}-182}{15}\right)\right] + \frac{15}{[232.2^{2n}-182]}\begin{bmatrix} log2\left(\frac{1456.2^{2n}}{3}-\frac{1036}{3}\right)+ \\ log3\left(\frac{1344.2^{2n}}{3}-\frac{1308}{3}\right)+ \\ log5\left(\frac{660.2^{2n}}{3}-\frac{660}{3}\right) \end{bmatrix}$$

$$I(TBD-G_n, ReZ(G_3)) = \log\left[\left(\frac{1072.2^{2n}-940}{3}\right)\right] + \frac{3}{[1072.2^{2n}-940]}\begin{bmatrix}(513.62361429725)2^{2n} \\ -465.75395984766\end{bmatrix}$$

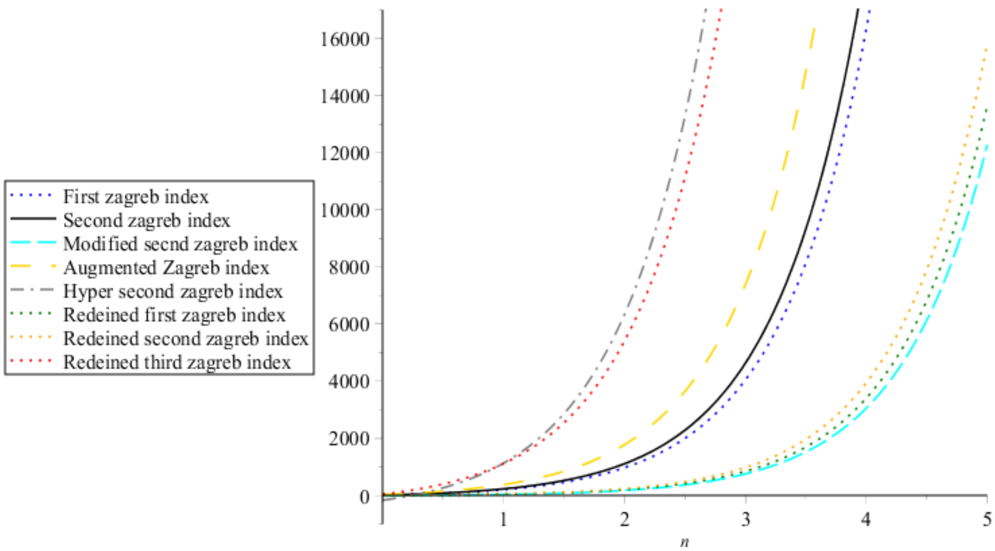


Figure 4: *Comparison of Topological indices for TBD−G_n*

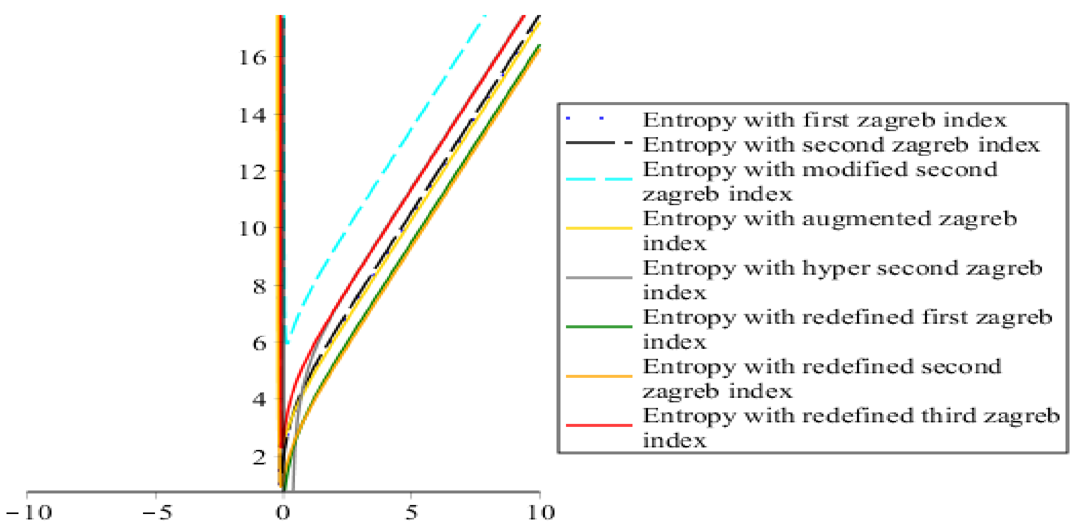


Figure 5: *Comparison of Entropies for TBD− Gn*

Conclusions and Further work:

In this paper, we dealt with Triazine Based Dendrimers and studied topological indices such as the First (*a*, *b*) *K.A.* Index, Sombor Index, Modified Sombor Index, Reduced Sombor Index, Reduced modified Sombor Index, Reduced 1^{st} (a, b) *K.A.* Index, Reduced 2nd -(a, b) *K.A.* Index for $TBD- G_n$. We used some topological properties such as the First Zagreb index, Second Zagreb index, modified second Zagreb index, Augmented Zagreb Index, Hyper Zagreb 2nd Index, Redefined 1st Zagreb Index, Redefined 2nd Zagreb Index and Redefined 3rd Zagreb Index to compute weighted entropies of $TBD - G_n$ Which will be helpful in computational chemistry. Dendrimers have an underlying structure that can be explored and understood by people working in network science with the help of analytical closed formulas developed for $TBD - G_n$ in this article. Our future research interests will be designing new architectures/networks and studying their topological indices to understand their underlying topologies and entropies

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Declaration:

- **Availability of data and materials:** The data is provided at the request of the authors.
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