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ORIGINAL ARTICLE

On physical analysis of synthesis strategies and entropy measures of dendrimers

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Abstract Dendrimers achieved great consideration in gene and drug delivery applications because of having highly administrable architecture. Unambiguous structure of dendrimers might reduce the unpredictability related to the molecule's shape and size, and also boost the accuracy of drug delivery. Dendrimers have exclusive physical and chemical properties due to which they have extensive range of potential applications like chemical sensors, light harvesting material, enhance the solubility, antitumer therapy, medical diagnostics, drug delivery system, catalysts, and many more. With the total π-electron energy, the degree-based topological indices have a lot of iterations.

In this paper, our desideration is to compute the topological aspects of degree based entropy for fractal and cayley tree type dendrimers. More preciously, we explore two tree type dendrimers denoted by F_r ant $C_{m,n}$. Moreover, entropies are estimated of these two structures by generating a correlation between degree based topological indices and their entropies.

1. Introduction

Dendrimers are a modern type of polymeric substances. They are fabricated three dimensional, maono-disperse structure having tree like branches (Sampathkumar and Yarema, 2007). Dendrimers are also called arborols and cascade. There are different kinds of dendrimers like radially layered poly dendrimers, chiral, liquid crytalline, tacto, hybride, peptide, and frechet type dendrimers (Singh et al., 2017). In 1985, Tomalia familiarized the term dendrimer for the first time. It is acquired from "dendrimer", that paraphrase to tree, and "meros(part)" (Gardikis et al., 2006).

Dendrimers rose up out of the ocean of polymer sciences in the mid 1980*s* as wonderful period. Stretched atoms in the shape of a star with an extraordinary formation and minimal polydispersity (Beer et al., 1999; Tomalia et al., 1986). In any case, the possibility of planning expanded particles was first imagined by Flory as ahead of schedule as (Flory, 1941). As

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on account of different revelations that were relatively revolutionary, the engineered and diagnostic techniques at that time were not adequately progressed to tentatively backing such a thought (Lin et al., 2010). In 1978, the principal paper that depicts the blend of purported course atoms, i.e., minimal sub-atomic mass dendritic polyamines, was distributed (Vogtle et al., 1978). Denkewalter, a long time later, used a different approach to protect the synthesis of poly(lysine) dendrimers until the ninth century (Denkewalter et al., 1982). Tomalia (Gardikis et al., 2006) published the combination of poly(amidoamine) (PAMAM) dendrimers up to the ninth century and characterised this type of polymers "dendrimers", that straightforwardly interpreted as "part of a tree". In the same year, Newkome initiated dispensing a poly(ether) dendrimer blend that was up to the third generation (Kono et al., 2008). Dendrimers are synthesised by two methods, divergent growth method and convergent growth method (Munir et al., 2016).

The synthesis of a dendrimer as indicated by the divergent technique continues step by step beginning from an activated core, $B_n (n \geqslant 2)$, to whose next dendrimer ages are developed by means of the consecutive connection of components termed as monomers (pattern 1). The monomers utilized are some type of $AB_n (n \geqslant 2)$, in which A and B_n mean 2 sorts of useful gatherings. The A-useful gathering of the AB_n monomer is a responsive gathering, whereas the B_n-useful gathering is disabled/secured, allowing for restrained development of the dendrimer. The monomers are joined to a substrate particle (a developing dendrimer) through a synthetic bond arrangement between the monomer's A-utilitarian gathering and one of the substrate's activated B-utilitarian gatherings.The linkage of the B-functionalities with a subsequent particle or the evacuation of assuring groupings can guide their actuation. Trifunctional monomers with anAB_2structure are the most commonly used monomers. Following the binding of these monomers to the centre, a unique dendrimer is formed. The two processes that follow, which are dependent on the activation of the B-functionalities on the original dendrimer and their coupling with another arrangement of monomers, result in a second age dendrimer (Sowinska and Urbanczyk-Lipkowska, 2014). The desired greater age dendrimer is attained due to the redundancy of these two steps, see Fig. 1.

Hawker and Frechet first described the convergent approach in 1989–1990, and it is an optional course for developing dendrimers. particular dendrimer wedges, known as dendrons, are orchestrated first and then connected to an activated core (Scheme 2). The regular AB_2 monomer, that has responsive B-functionalities and disabled/ensured A-usefulness, is used to direct the combination of dendrons. The monomer is subjected to a response with a molecule in the first phase, which will eventually establish the dendrimer's outskirts (outside). The presentation of secure bunches on monomer B-functionalities is frequently the most significant advancement. As a result, it is possible to make an original dendron (G1). The actuation of a dendron point of convergence and its coupling with the AB_2 monomers are the next two phases, resulting in a (G2) dendron. Every reiteration of these two steps results in an increase in the dendron age (Sowinska and Urbanczyk-Lipkowska, 2014), see Fig. 2.

Assume $Z(V_Z, E_Z)$ is a graph with V_Z for the vertex set and E_Z for the edge set. The order and size of the graph in Z are represented by p and q, correspondingly. Any chemical structure with vertices representing atoms and edges representing bonds forms a chemical graph. The number of edges associated with a vertex is called its degree, and it is symbolised by $\widetilde{\S}(x)$. A topological descriptor is an algorithmic measure accomplished via a projection. diverse sorts of topological indices exist. We shall explore degree-based topological descriptors in this work, which are defined by the degree of a graph's terminal vertices. (Siddiqui et al., 2016; Siddiqui et al., 2016 and Gao and Farahani, 2015; Gao et al., 2017; Imran et al., 2018) contain more information on topological indices formulas and their employment respectively.

Shannon (1948) was the first to introduce the concept of entropy. It is a measure of a system's information content's unpredictability. After this, it's been employed in chemical networks and graphs. Rashevsky entrenched the entropy of a graph (Rashevsky, 1955). Graph entropy is now employed in a variety of domains, see (Dehmer and Graber, 2013; Mehler et al., 2010; Ulanowicz, 2004).

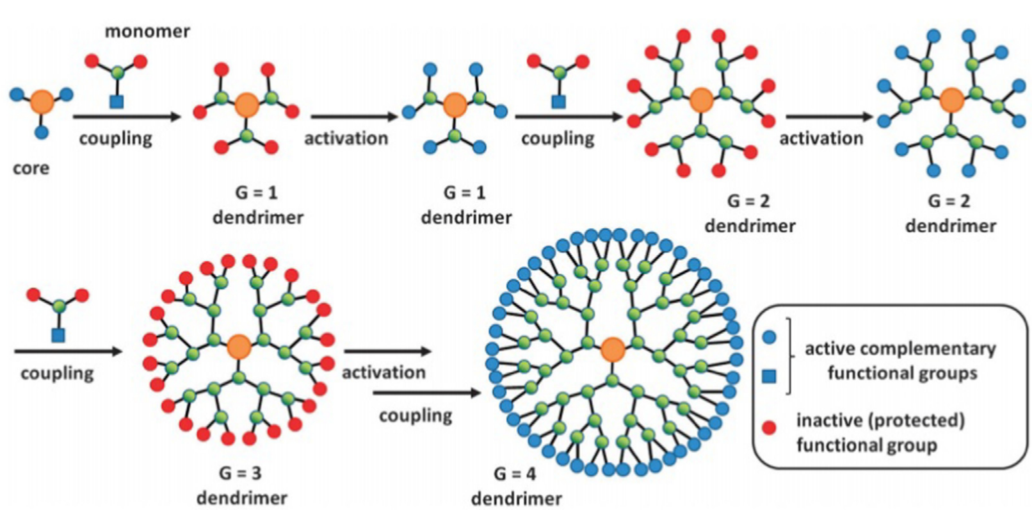


Fig. 1 The divergent growth method.

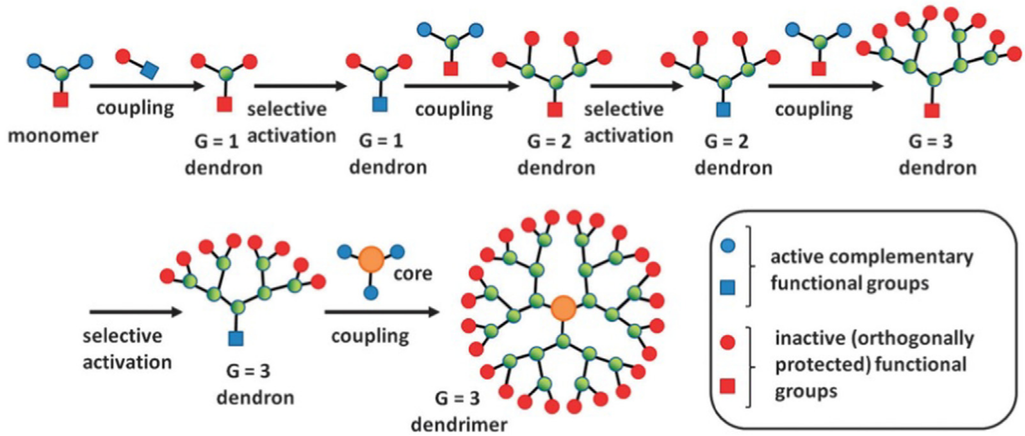


Fig. 2 The convergent growth method.

Intrinsic and extrinsic graph entropy measurements are used to correlate probability distributions with graph invariants (vertices, edges, and so on) (Mowshowitz and Dehmer, 2012). Dehmer (2008, 2012) researched the features of graph entropies, which are established on information functionals. See (Bonchev, 2003; Dehmer and Mowshowitz, 2011; Manzoor et al., 2020; Morowitz, 1953; Quastler, 1954; Rashevsky, 1955; Shannon, 2001; Sol and Valverde, 2004; Trucco, 1956; Tan and Wu, 2004) for more information.

The information entropy (Chen et al., 2014) based on Shannon's entropy (Shannon, 1948) is described as:

$$E_w(Z) = -\sum_{i=1}^{m} F_i \frac{w(x_i y_i)}{T_d} \log_2 \frac{w(x_i y_i)}{T_d} = \log(T_d) - \frac{1}{T_d}\sum_{i=1}^{m} F_i w(x_i y_i) \log_2 w(x_i y_i) \quad (1)$$

Where $T_d = \sum_{i=1}^{m} F_i w(x_i y_i)$ denotes the topological descriptor, m is the number of edge types, F_i is the frequency or number of repetition, and $w(xy)$ is the weight of the edge xy.

2. Structure of fractal tree dendrimer F_r

A geometrical figure that constitute a smaller curve or pattern that has rigorously the same shape is called Fractal. The way that the stem of a tree break down into shorter and shorter branches and limbs is an approximate fractal pattern. There are many other examples of fractals like Romanesco broccoli, lightning bolt, angelica flowerhead, and Von Koch snowflake, etc.

Dendrimers are macro-molecules with a ramification structure. These are also called fractal polymers. F_r where $r \geq 0$, stands for the anticipated fractal tree dendrimers in this work, and is the number of iterations. F_0 consists of an edge associating two vertices. F_r is made from F_{r-1} by taking two steps on each of the ongoing edges in F_{r-1}. In the first stage, a three-linked path with the same terminal points is built. In the second stage, each of the two intervening vertices in the path is used to construct l new vertices, join them to the neighboring vertices after that.

The Fig. 3 illustrates the structure for different values of l. In Fig. 4a) and Fig. 4(b), F_3 and F_4 are sketched. Firstly, we calculate above mentioned entropies by using degree-based

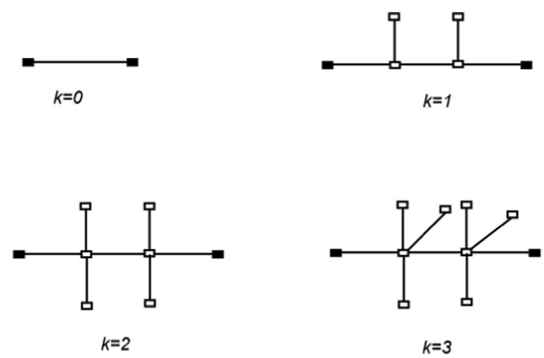


Fig. 3 Construction of the fractal trees for $k = 0, 1, 2, 3$.

topological indices for F_r. Edge partitioning and graph theoretical approaches are employed in this case. There are $42lr - 28l + 14r - 8$ pendent vertices in F_r. The vertices having degree 4 are $7r - 5$ and the vertices having degree $l + 2$ are $42r - 28$ in numbers. The edge set of F_r consists of three types of edges based on the degree of end vertices.

The edge partition of F_r is illustrated in Table 1.

2.1. Results for fractal tree dendrimer F_r

The entropies of the structure of the fractal tree dendrimer F_r are listed in this section.

The M_1 index is

$$M_1(Z) = 42l^2r + 210lr - 28l^2 - 140l + 294r - 200$$

Eq. (1) and Table 1 gives

$$E_{M_1}(F_r) = \log\left(42l^2r + 210lr - 28l^2 - 140l + 294r - 200\right) - \frac{(42lr - 28l + 14r - 8) \times (l+3)\log(l+3)}{(42l^2r + 210lr - 28l^2 - 140l + 294r - 200)} - \frac{(28r - 20) \times (l+6)\log(l+6)}{(42l^2r + 210lr - 28l^2 - 140l + 294r - 200)} - \frac{(21r - 14) \times (2l+4)\log(2l+4)}{(42l^2r + 210lr - 28l^2 - 140l + 294r - 200)}$$

The M_2 index is

$$M_2(Z) = 63l^2r - 42l^2 + 294lr - 200l + 336r - 232$$

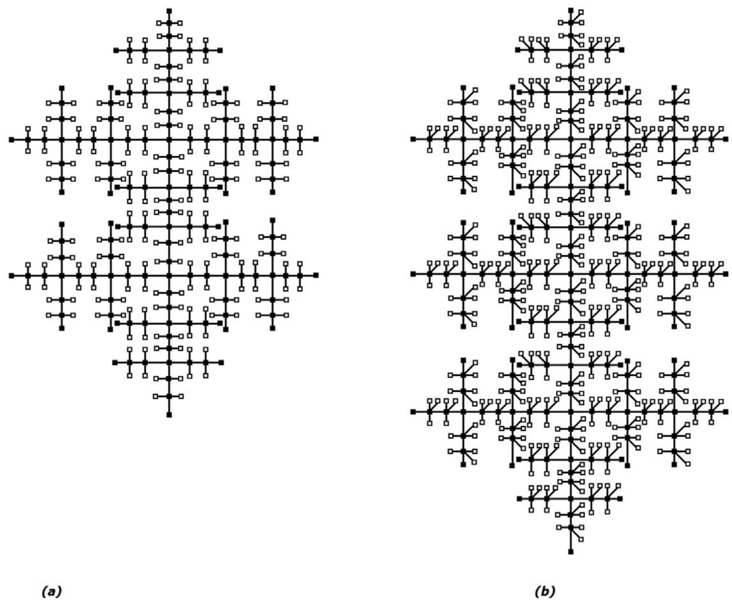


Fig. 4 (a) Fractal tree F_3 for $l = 2$, (b) Fractal tree F_4 for $l = 3$.

Table 1 Edge partition of F_r established on degrees of terminal vertices of every edge.

$\left(\widetilde{\S}(x),\ \widetilde{\S}(y)\right)$	Number of Repetition	Kind of Edges
$(1, 2+l)$	$42lr - 28l + 14r - 8$	E_{1Z}
$(4, 2+l)$	$28r - 20$	E_{2Z}
$(2+l, 2+l)$	$21l - 14$	E_{3Z}

Eq. (1) and Table 1 gives

$$E_{M_2}(F_r) = \log\left(63l^2r - 42l^2 + 294lr - 200l + 336r - 232\right) - \frac{(42lr - 28l + 14r - 8) \times (l+2)\log(l+2)}{(63l^2r - 42l^2 + 294lr - 200l + 336r - 232)} - \frac{(28r - 20) \times (4l + 8)\log(4l + 8)}{(63l^2r - 42l^2 + 294lr - 200l + 336r - 232)} - \frac{(21r - 14) \times (l^2 + 4l + 4)\log(l^2 + 4l + 4)}{(63l^2r - 42l^2 + 294lr - 200l + 336r - 232)}$$

The Hyper Zagreb index is

$$HM(Z) = 42l^3r - 28l^3 + 378l^2r - 252l^2 + 1134lr - 764l + 1470r - 1016$$

Eq. (1) with Table 1 gives

$$E_{HM}(F_r) = \log\left(42l^3r - 28l^3 + 378l^2r - 252l^2 + 1134lr - 764l + 1470r - 1016\right) - \frac{(42lr - 28l + 14r - 8) \times \left[(l+3)^2\right]\log\left[(l+3)^2\right]}{(42l^3r - 28l^3 + 378l^2r - 252l^2 + 1134lr - 764l + 1470r - 1016)} - \frac{(28r - 20) \times \left[(l+6)^2\right]\log\left[(l+3)^2\right]}{(42l^3r - 28l^3 + 378l^2r - 252l^2 + 1134lr - 764l + 1470r - 1016)} - \frac{(21r - 14) \times \left[(2l+4)^2\right]\log\left[(2l+4)^2\right]}{(42l^3r - 28l^3 + 378l^2r - 252l^2 + 1134lr - 764l + 1470r - 1016)}$$

The Forgotten index is

$$F(Z) = 42l^3r - 28l^3 + 252l^2r - 168l^2 + 546lr - 364l + 794r - 552$$

Eq. (1), with Table 1 gives

$$E_F(F_r) = \log\left(42l^3r - 28l^3 + 252l^2r - 168l^2 + 546lr - 364l + 794r - 552\right) - \frac{(42lr - 28l + 14r - 8) \times (l^2 + 4l + 5)\log[l^2 + 4l + 5]}{(42l^3r - 28l^3 + 252l^2r - 168l^2 + 546lr - 364l + 794r - 552)} - \frac{(28r - 20) \times (l^2 + 4l + 20)\log[l^2 + 4l + 20]}{(42l^3r - 28l^3 + 252l^2r - 168l^2 + 546lr - 364l + 794r - 552)} - \frac{(21r - 14) \times (2l^2 + 8l + 8)\log[2l^2 + 8l + 8]}{(42l^3r - 28l^3 + 252l^2r - 168l^2 + 546lr - 364l + 794r - 552)}$$

The Balaban index is

$$J(Z) = (42lr - 28l + 63r - 42)\left[\frac{42lr - 28l + 14r - 8}{\sqrt{l+2}} + \frac{28r - 20}{2\sqrt{l+2}} + \frac{21r - 14}{l+2}\right]$$

Eq. (1) with Table 1 gives

$$E_J(F_r) = \log(J(Z)) - \frac{(42lr - 28l + 14r - 8)}{(J(Z))} \times \left(\frac{42lr - 28l + 63r - 42}{\sqrt{l+2}}\right)\log\left[\frac{42lr - 28l + 63r - 42}{\sqrt{l+2}}\right] - \frac{(28r - 20)}{(J(Z))} \times \left(\frac{42lr - 28l + 63r - 42}{2\sqrt{l+2}}\right)\log\left[\frac{42lr - 28l + 63r - 42}{2\sqrt{l+2}}\right] - \frac{(21r - 14)}{(J(Z))} \times \left(\frac{42lr - 28l + 63r - 42}{l+2}\right)\log\left[\frac{42lr - 28l + 63r - 42}{l+2}\right]$$

The Redefined first Zagreb index is

$$ReZG_1(Z) = \frac{(42lr - 28l + 14r - 8)(l+3)}{(l+2)} + \frac{(28r - 20)(l+6)}{4(l+2)} + \frac{(21r - 14)(2l+4)}{(l+2)^2}$$

Eq. (1) with Table 1 gives

$$E_{ReZG_1}(F_r) = \log(ReZK_1(Z)) - \frac{(42lr - 28l + 14r - 8)}{(ReZK_1(Z))} \times \left(\frac{l+3}{l+2}\right)\log\left[\frac{l+3}{l+2}\right] - \frac{(28r - 20)}{(ReZK_1(Z))} \times \left(\frac{l+6}{4l+8}\right)\log\left[\frac{l+6}{4l+8}\right] - \frac{(21r - 14)}{(ReZK_1(Z))} \times \left(\frac{2l+4}{(l+2)^2}\right)\log\left[\frac{2l+4}{(l+2)^2}\right]$$

The Redefined second Zagreb index is

$$ReZG_2(Z) = \frac{(42lr - 28l + 14r - 8)(l+2)}{(l+3)} + \frac{(28r-20)(4l+8)}{l+6} + \frac{(21r-14)(l+2)^2}{2l+4}$$

Eq. (1) with Table 1 gives

$$E_{ReZG_2}(F_r) = \log(ReZK_2(Z)) - \frac{(42lr-28l+14r-8)}{(ReZK_2(Z))} \times \left(\frac{l+2}{l+3}\right) \log\left[\frac{l+2}{l+3}\right] - \frac{(28r-20)}{(ReZK_2(Z))} \times \left(\frac{4l+8}{l+6}\right) \log\left[\frac{4l+8}{l+6}\right] - \frac{(21r-14)}{(ReZK_2(Z))} \times \left(\frac{(l+2)^2}{2l+4}\right) \log\left[\frac{(l+2)^2}{2l+4}\right]$$

The Redefined third Zagreb index is

$$ReZG_3(Z) = 84l^3r - 56l^3 + 588l^2r - 396l^2 + 1722lr - 1184l + 1764r - 1232$$

Eq. (1) with Table 1 gives

$$E_{ReZG_3}(F_r) = \log(ReZK_3(Z)) - \frac{(42lr-28l+14r-8)}{(ReZK_3(Z))} \times (l^2+5l+6) \log[l^2+5l+6] - \frac{(28r-20)}{(ReZK_3(Z))} \times (4l^2+32l+48) \log[4l^2+32l+48] - \frac{(21r-14)}{(ReZK_3(Z))} \times 2(l+2)^3 \log\left[2(l+2)^3\right]$$

3. Structure of cayley tree type dendrimer $C_{m,n}$

A cayley tree is one in which each non-leaf graph vertex has a defined number of branches. The star graph is a one-of-a-kind m-cayley tree with $m+1$ nodes. The cayley tree, also known as Bathelallice, is a type od dendrimers. To construct the cayley tree $C_{m,n}$ where $m \geq 3, n \geq 0$, we use iterative method.Here m represents the nodes at first iteration. $C_{m,0}$ consists of only a central vertex. $C_{m,1}$ is achieved by creating m nodes and using an edge to connect them to the central vertex. $C_{m,n}$ is obtained from $C_{m,n-1}$ by generating $n-1$ nodes and join them to every pendent vertex of $C_{m,n}$. $C_{4,3}$ Is shown in Fig. 5. The number of pendent vertices is $m(m-1)^{n-1}$, while the number of vertices with degree m is

$$2\sum_{j=1}^{n}(m-1)^{j-1} - (m-1)^{n-1}$$

The $C_{m,n}$ edge set has two sorts of edges based on the degree of end vertices. Table 2 shows the edge partition of $C_{m,n}$.

$$2\sum_{j=1}^{n}(m-1)^{j-1} + (m-1)^{n}$$

and

$$m\sum_{j=1}^{n}(m-1)^{j-1}$$

are the total number of vertices and edges in $C_{m,n}$ respectively.

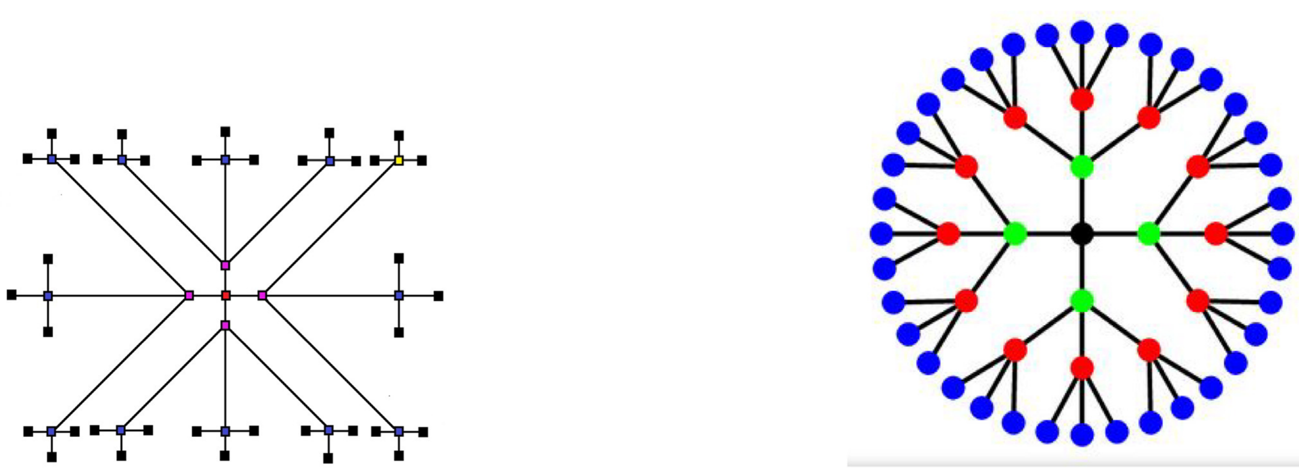
3.1. Results for Cayley tree type dendrimer $C_{m,n}$

The entropies of the structure of the Cayley tree dendrimer $C_{m,n}$ are listed in this section.

The first Zagreb index is

$$M_1(Z) = m\left(2m\sum_{j=1}^{n}(-1+m)^{j-1} - (-1+m)^{n}\right)$$

Eq. (1) with Table 2 gives



(a) (b)

Fig. 5 (a) The Molecular graph Cayley tree $C_{4,3}$, (b) The representation of Cayley tree $C_{4,3}$.

Table 2 $C_{m,n}$ edge partitioning established on degrees of terminal vertices.

$(\widetilde{\S}(x), \widetilde{\S}(y))$	Number of repetition	Different sorts of edge
$(1, m)$	$(m-1)^n \cdot \frac{m}{m-1}$	E_{1Z}
(m, m)	$m\left(\sum_{j=1}^{n}(-1+m)^{j-1} - (-1+m)^{n-1}\right)$	E_{2Z}

$$E_{M_1}(C_{m,n}) = \log\left(m\left(2m\sum_{j=1}^{n}(-1+m)^{j-1}-(-1+m)^{n}\right)\right) - \frac{(-1+m)^{n-1}\left(m+m^2\right)\log(m+1)}{\left(m\left(2m\sum_{j=1}^{n}(-1+m)^{j-1}-(-1+m)^{n}\right)\right)} - \frac{2m^2\left(\sum_{j=1}^{n}(-1+m)^{j-1}-(-1+m)^{n-1}\right)\log(2m)}{\left(m\left(2m\sum_{j=1}^{n}(-1+m)^{j-1}-(-1+m)^{n}\right)\right)}$$

The second Zagreb index is

$$M_2(Z) = m^2\left(m\sum_{j=1}^{n}(-1+m)^{j-1}-(-1+m)^{n}\right)$$

Eq. (1) with Table 2 gives

$$E_{M_2}(C_{m,n}) = \log\left(m^2\left(m\sum_{j=1}^{n}(-1+m)^{j-1}-(-1+m)^{n}\right)\right) - \frac{(-1+m)^{n}\cdot\frac{m^2\log(m)}{-1+m}}{\left(m^2\left(m\sum_{j=1}^{n}(-1+m)^{j-1}-(-1+m)^{n}\right)\right)} - \frac{2m^3\left(\sum_{j=1}^{n}(-1+m)^{j-1}-(-1+m)^{n-1}\right)\log\left(m^2\right)}{\left(m^2\left(m\sum_{j=1}^{n}(-1+m)^{j-1}-(-1+m)^{n}\right)\right)}$$

The Hyper Zagreb index is

$$F(Z) = m\left(2m^2\sum_{j=1}^{n}(-1+m)^{j-1}-(m+1)(-1+m)^{n}\right)$$

Eq. (1) with Table 2 gives

$$E_F(C_{m,n}) = \log\left(m\left(2m^2\sum_{j=1}^{n}(-1+m)^{j-1}-(m+1)(-1+m)^{n}\right)\right) - \frac{(-1+m)^{n}\cdot\frac{m\left(m^2+1\right)\log\left(1+m^2\right)}{-1+m}}{\left(m\left(2m^2\sum_{j=1}^{n}(-1+m)^{j-1}-(m+1)(-1+m)^{n}\right)\right)} - \frac{2m^3\left(\sum_{j=1}^{n}(-1+m)^{j-1}-(-1+m)^{n-1}\right)\log\left(2m^2\right)}{\left(m\left(2m^2\sum_{j=1}^{n}(-1+m)^{j-1}-(m+1)(-1+m)^{n}\right)\right)}$$

The hyper Zagreb index is

$$HM(Z) = m\left(4m^2\sum_{j=1}^{n}(-1+m)^{j-1}-\left(1-3m^2+2m\right)(-1+m)^{n-1}\right)$$

Eq. (1) with Table 2gives

$$E_{HM}(C_{m,n}) = \log\left(m\left(4m^2\sum_{j=1}^{n}(-1+m)^{j-1}-(1-3m^2+2m)(-1+m)^{n-1}\right)\right) - \frac{\left(m+m^3\right)(-1+m)^{n-1}\log\left(1+m^2\right)}{\left(m\left(4m^2\sum_{j=1}^{n}(-1+m)^{j-1}-(1-3m^2+2m)(-1+m)^{n-1}\right)\right)} - \frac{4m^3\left(\sum_{j=1}^{n}(-1+m)^{j-1}-(-1+m)^{n-1}\right)\log\left(4m^2\right)}{\left(m\left(4m^2\sum_{j=1}^{n}(-1+m)^{j-1}-(1-3m^2+2m)(-1+m)^{n-1}\right)\right)}$$

The Balaban index is

$$J(C_{m,n}) = \frac{m\sum_{j=1}^{n}(-1+m)^{j-1}}{(m-2)\sum_{j=1}^{n}(-1+m)^{j-1}-(-1+m)^{n}+2}\left[(\sqrt{m}-1)(-1+m)^{n-1}+\sum_{j=1}^{n}(-1+m)^{j-1}\right]$$

$$E_J(C_{m,n}) = \log(J(Z)) - \frac{\left[\frac{q\sqrt{m}(-1+m)^{n-1}}{q-p+2}\right]\log\left[\frac{q}{\sqrt{m}(q-p+2)}\right]}{(J(Z))} - \frac{\left[\frac{q\cdot m\left(\sum_{j=1}^{n}(-1+m)^{j-1}-(-1+m)^{n-1}\right)}{m(q-p+2)}\right]\log\left[\frac{q}{m(q-p+2)}\right]}{(J(Z))}$$

The Redefined first Zagreb index is

$$ReZG_1(Z) = -\frac{(-1+m)^{n}}{m}+2\sum_{j=1}^{n}(-1+m)^{j-1}$$

Eq. (1) with Table 2 gives

$$E_{ReZG_1}(C_{m,n}) = \log\left(-\frac{(-1+m)^{n}}{m}+2\sum_{j=1}^{n}(-1+m)^{j-1}\right) - \frac{\left(\frac{1+m}{m}\right)(-1+m)^{n-1}\log\left(\frac{1+m}{m^2}\right)}{\left(-\frac{(-1+m)^{n}}{m}+2\sum_{j=1}^{n}(-1+m)^{j-1}\right)} - \frac{2\left(\sum_{j=1}^{n}(-1+m)^{j-1}-(-1+m)^{n-1}\right)\log\left(\frac{2}{m}\right)}{\left(-\frac{(-1+m)^{n}}{m}+2\sum_{j=1}^{n}(-1+m)^{j-1}\right)}$$

The Redefined second Zagreb index is

$$ReZG_2(C_{m,n}) = -\frac{m^2}{2(1+m)(-1+m)^{2-n}}+\frac{m^2}{2}\sum_{j=1}^{n}(-1+m)^{j-1}$$

Eq. (1) with Table 2 gives

$$E_{ReZG_2}(C_{m,n}) = \log\left(-\frac{m^2}{2(1+m)(-1+m)^{2-n}}+\frac{m^2}{2}\sum_{j=1}^{n}(-1+m)^{j-1}\right) - \frac{\left(\frac{m^2}{1+m}\right)(-1+m)^{n-1}\log\left(\frac{m}{1+m}\right)}{\left(-\frac{m^2}{2(1+m)}(-1+m)^{n-2}+\frac{m^2}{2}\sum_{j=1}^{n}(-1+m)^{j-1}\right)} - \frac{\left(\frac{m^2}{2}\right)\left(\sum_{j=1}^{n}(-1+m)^{j-1}-(-1+m)^{n-1}\right)\log\left(\frac{m}{2}\right)}{\left(-\frac{m^2}{2(1+m)}(-1+m)^{n-2}+\frac{m^2}{2}\sum_{j=1}^{n}(-1+m)^{j-1}\right)}$$

Table 3 Comparison of first Zagreb entropy and second Zagreb entropy for F_r.

$[r, l]$	ENT_{M_1}	ENT_{M_2}
[1, 1]	1.5303	1.4622
[2, 2]	2.3808	2.1916
[3, 3]	2.7346	2.5261
[4, 4]	2.9778	2.7521
[5, 5]	3.1652	2.9239
[6, 6]	3.3183	3.0628
[7, 7]	3.4478	3.1793
[8, 8]	3.5603	3.2798
[9, 9]	3.6559	3.3680
[10, 10]	3.7488	3.4467

Table 4 Comparison of E_{HM}, E_F, and E_J Entropies for F_r.

$[r, l]$	E_{HM}	E_F	E_J
[1, 1]	1.4622	1.5085	1.5251
[2, 2]	2.0916	2.3711	2.2736
[3, 3]	2.4261	2.7293	2.6272
[4, 4]	2.6521	2.9743	2.8707
[5, 5]	2.8239	3.1626	3.0584
[6, 6]	2.9628	3.3161	3.2119
[7, 7]	3.0793	3.4358	3.3418
[8, 8]	3.2298	3.5585	3.4546
[9, 9]	3.4351	3.6583	3.5543
[10, 10]	3.5253	3.7476	3.6437

Table 5 Comparison of the Redefined Zagreb Entropies for F_r.

$[r, l]$	E_{ReZK_1}	E_{ReZK_2}	E_{ReZK_3}
[1, 1]	1.5169	1.4092	1.3998
[2, 2]	2.2621	2.1347	2.0240
[3, 3]	2.6151	2.4698	2.2471
[4, 4]	2.8588	2.6983	2.4602
[5, 5]	3.0470	2.8734	2.6193
[6, 6]	3.2060	3.0158	2.7461
[7, 7]	3.3316	3.1361	2.9015
[8, 8]	3.4450	3.2401	3.0115
[9, 9]	3.5451	3.3319	3.1201
[10, 10]	3.6350	3.4139	3.2201

The Redefined third Zagreb index is

$$ReZG_3(C_{m,n}) = -(-1+m)^{n-2} + 2m^4 \sum_{j=1}^{n} (-1+m)^{j-1}$$

Eq. 1 with Table 2 gives

$$E_{ReZG_3}(C_{m,n}) = \log\left(-(-1+m)^{n-2} + 2m^4 \sum_{j=1}^{n}(-1+m)^{j-1}\right) - \frac{(m^3+m^4)(-1+m)^{n-1}\log(m^2+m^3)}{\left(-(-1+m)^{n-2}+2m^4\sum_{j=1}^{n}(-1+m)^{j-1}\right)} - \frac{(2m^4)\left(\sum_{j=1}^{n}(-1+m)^{j-1}-(-1+m)^{n-1}\right)\log(2m^3)}{\left(-(-1+m)^{n-2}+2m^4\sum_{j=1}^{n}(-1+m)^{j-1}\right)}$$

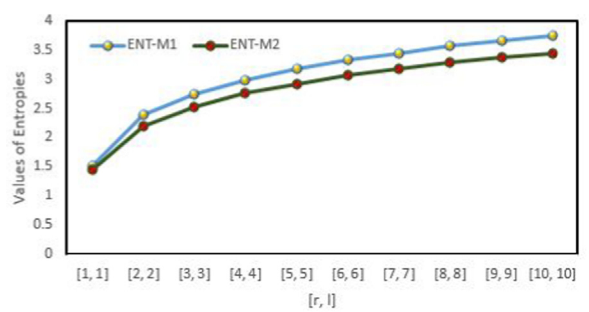


Fig. 6 The graphical comparison of the first Zagreb entropy and the second Zagreb entropy for F_r.

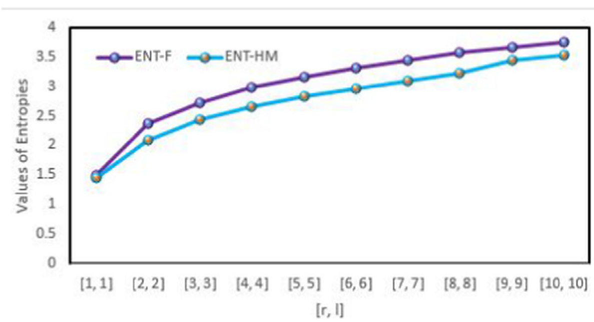


Fig. 7 Graphical comparison of the forgotten and the hyper Zagreb entropies for F_r.

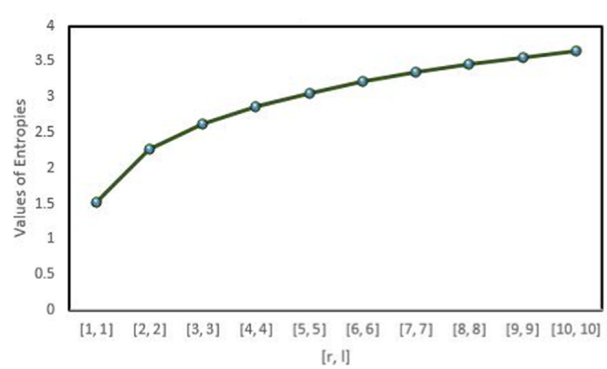


Fig. 8 Graphical representation of the Balaban entropy for F_r.

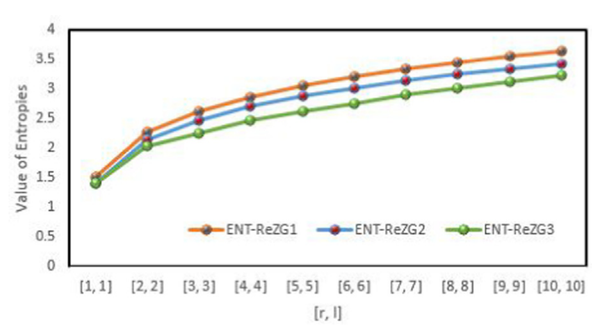


Fig. 9 Graphical comparison of redefined Zagreb entropies for F_r.

4. Comparisons and Discussion for Fractal tree type dendrimer F_r

Entropy is a structural descriptor that may be used to measure the complexity of chemical structures quickly. In research, degree-based entropy offers a wide range of uses characteristically in software engineering and pharmaceutical. Substantial properties of biological frameworks(strain energy, melting point etc) are confederated with the biological functions of the frameworks via topological indices. Degree-based indices can be used to carry out these assessments because they have a clear decision-making process and are quick. Because molecular structures are so complicated, several molecular descriptors and their entropy metrics are utilised to predict the most structural information. As a result, some degree-based entropies for diverse estimations of l, r for F_r have been calculated arithmetically in this articulation. For the assembly of F_r, we create Tables 3–5 for degree-based entropy to arithmetical correlation. For this, we utilized Maple software and MATLAB software. Diagrammatic illustrations are in Fig. 6, Fig. 7, Fig. 8 and Fig. 9 for distinct considerations of l, r. The entropy function of a fractal tree type dendrimer grew as the generation size increased. As a system's entropy rises, so does the uncertainty about its reaction. When the chemical structure F_r expands, the first Zagreb entropy develops more quickly than other entropy measurements of F_r, however the redefined third Zagreb entropy grows slowly.

5. Comparisons and Discussion for $C_{m,n}$

Computational techniques combined with different scientific fields provide a consistent strategy to better recognize a scientific subject. It is rare to be able to comprehend a problem based solely on one science discipline. As a result, incorporating some computational methodologies into the investigation may produce a clear image that aids in furthering our understanding of the underlying phenomenon. Creating a mathematical model to depict the dynamics of items in a research is a very practical way to approach and examine the problem. In this segment, for distinct considerations, we have quantitatively catalogued all degree-based entropies. This could be a quick technique to comprehend the molecular structure $C_{m,n}$ by looking at its chemical graph structure attributes. Numerically and visually results are shown in Tables 6–8 and Fig. 10–13. We can observe from these calculations that the entropy values grew as the number of unit cells increased. Furthermore, When the chemical structure $C_{m,n}$ expands, the redefined third Zagreb entropy develops more quickly than other entropy measurements of $C_{m,n}$, however the redefined second Zagreb entropy grows slowly.

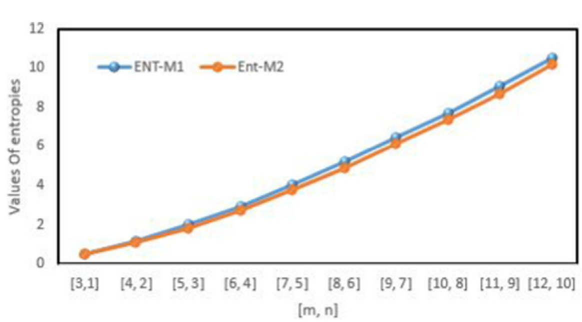


Fig. 10 The graphical comparison of first and second Zagreb entropies for $C_{m,n}$.

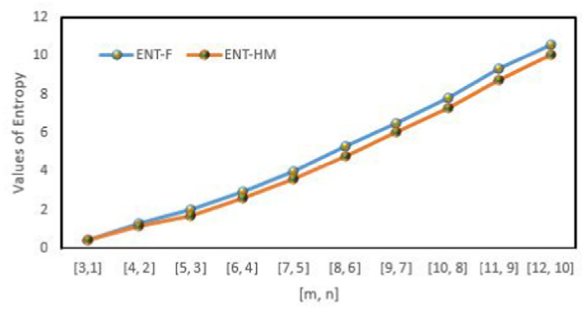


Fig. 11 Graphical comparison of the forgotten and the hyper Zagreb entropies for $C_{m,n}$.

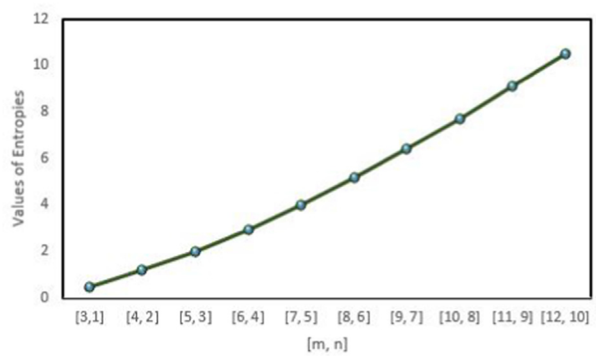


Fig. 12 Graphical representation of the Balaban entropy for $C_{m,n}$.

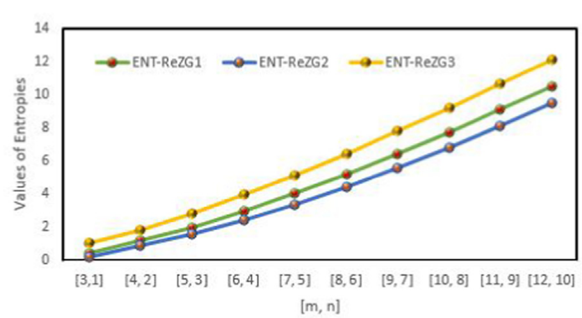


Fig. 13 Graphical comparison of redefined Zagreb entropies for $C_{m,n}$.

6. Conclusion

The physico-chemical features of dendrimer molecules and aggregates are based on chemical structures with regular branching. Theoretically and experimentally, regular dendrimers have been examined. The information entropy technique is used to examine regular dendrimer aggregates in this

Table 6 Comparison of First Zagreb Entropy and second Zagreb Entropy for $C_{m,n}$.

$[m,n]$	E_{M_1}	E_{M_2}
[3, 1]	0.4771	0.47712
[4, 2]	1.1938	1.1031
[5, 3]	2.0092	1.7856
[6, 4]	2.9591	2.7555
[7, 5]	4.0250	3.7959
[8, 6]	5.1842	4.8965
[9, 7]	6.4399	6.1058
[10, 8]	7.7206	7.3563
[11, 9]	9.0774	8.6554
[12, 10]	10.4838	10.1531

Table 7 Comparison of E_{HM}, E_F, and E_J Entropies for $C_{m,n}$.

$[m,n]$	ENT_F	ENT_{HM}	ENT_J
[3, 1]	0.47712	0.4771	0.4511
[4, 2]	1.2848	1.1592	1.1891
[5, 3]	2.0009	1.6683	2.0025
[6, 4]	2.9520	2.6154	2.9527
[7, 5]	4.0190	3.5805	4.0190
[8, 6]	5.2991	4.7901	5.1786
[9, 7]	6.5159	6.0164	6.4147
[10, 8]	7.8177	7.2781	7.7155
[11, 9]	9.2957	8.7511	9.0726
[12, 10]	10.5817	10.0437	10.4792

Table 8 Comparison of the Redefined Zagreb Entropies for $C_{m,n}$.

$[m,n]$	E_{ReZK_1}	E_{ReZK_2}	E_{ReZK_3}
[3, 1]	0.47712	0.2348	1.0399
[4, 2]	1.1938	0.8774	1.8329
[5, 3]	2.0092	1.5781	2.8147
[6, 4]	2.9591	2.4105	3.9325
[7, 5]	4.0250	3.3709	5.1442
[8, 6]	5.1842	4.4378	6.4280
[9, 7]	6.4199	5.5926	7.7715
[10, 8]	7.7206	6.8213	9.1668
[11, 9]	9.0774	8.1137	10.6080
[12, 10]	10.4838	9.4619	12.0905

paper. As demonstrated above, the information entropy of a regular fractal and Cayley tree type dendrimer grows with the number of generations. As a result, the system's information capacity must be temporarily increased to transfer it from one informational stable condition to another. Information storage with nano patterned materials (Rosen et al., 2009) is one of the potential applications of dendrimers and a material's information storage is determined by its information entropy (Chawla et al., 2020). The dendrimer's subsequent frameworks have a greater number of equivalent building blocks. It produces the dendrimer structure more homogeneous with each subsequent generation, and homogeneity is achieved faster with larger generation values, as entropy values indicate. Fascinatingly, in the class of dendrimers, increased information entropy corresponds to structures with minimal branching. The information entropy, of fractal and tree type dendrimer structures, represents the balance between order and disorder, and it may be used to measure this balance numerically in structural design. This could be advantageous if dendrimers are used as energy storage materials (Bar-Haim et al., 1997). In addition, the correlation between the entropy values and other branching parameters must be examined (Bonchev and Trinajstic, 1978). Configuration entropy of glass-forming liquids (Champion and Thurieau, 2020) or thermodynamic entropy of enzyme-substrate complexions (Graf et al., 2013; Putz et al., 2006) are examples of thermodynamic entropy used in molecular dynamics investigations on complex chemical systems. Analogously, a new step in this direction could be to use information entropy as a critical structural criterion.

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Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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