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ON CORRELATION OF PHYSICOCHEMICAL PROPERTIES AND THE HYPER ZAGREB INDEX FOR SOME MOLECULAR STRUCTURES

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Abstract: In this article, the physico-chemical properties of octane isomers such as entropy, acentric factor, enthalpy of vaporization (HVAP) and Heat of fusion (DHVAP) are tested by using hyper Zagreb index $HM(G)$. Here we show that the hyper Zagreb index has a great correlation with these chemical properties and observe that the index $HM(G)$ highly correlates with acentric factor. Further, we also establish the results on bounds for $HM(G)$ interms of order and size of a graph G. Also, we compute the results of $HM(G)$ for Fractal and Cayley tree type dendrimers.

Keywords and Phrases: First Zagreb index, hyper Zagreb index.

2020 Mathematics Subject Classification: 05C05, 05C07.

1. Introduction

Let $G = (n, m)$ be a simple(molecular) graph with vertex set $|V(G)| = n$ and edge set $|E(G)| = m$. The degree of vertex v is denoted as $d_G(v)$, where $d_G(v)$ is the number of edges incident to vertex v. The maximum degree and minimum degree of a graph G is denoted by $\Delta(G)$ and $\delta(G)$ respectively. For a real number x, $\lfloor x \rfloor$ denotes the floor, which is the greatest integer less than or equal to x. Similarly, $\lceil x \rceil$ denotes the ceil, which is least integer greater than or equal to x. For undefined terminologies we refer [10].

Molecules and molecular compounds are often modeled by molecular graphs. A molecular graph is a structural representation formula of a chemical compound, whose vertices corresponds to the atoms of the compound and edges corresponds to bonds.

We are living in an era where every day sees better innovation than the previous, with the same trend in the enhancement and innovation in the production of different types of medicines, chemical compounds and drugs for the improved health of humans and other living species on the planet. A great amount of time and money is required to test these drugs and chemical compounds to determine their pharmacological, chemical and biological characteristics using expensive equipment, which in truth makes the task more cumbersome. In countries with economic imbalance the task of evaluating the biological behavior and existence of side effects of chemical compounds becomes more difficult. In this respect, computing different types of topological indices have provided the indicators of such medicinal behaviour of several compounds and drugs. The computation method of topological indices has proven its worth by yielding medical information of drugs with less use of chemical related equipment.

Chemical graph theory is a branch of mathematics which combines graph theory and chemistry. Graph theory is used to mathematically model the molecules in order to gain the insight into the physical properties of these chemical compounds. The basic idea of chemical graph theory is that physico-chemical properties of molecules can be studied by using the information encoded in their corresponding chemical graphs.

In recent days chemical graph theory is rapidly growing because of its application in quantitative structure property relationships (QSPR) and quantitative structure activity relationships (QSAR). A graph associated to a chemical molecule is easier to study in terms of graph invariants. Topological indices are such graph invariants. Due to this special property, topological indices are extensively used in chemistry. Numerous applications of topological indices can be found in [8, 11, 12, 14, 15, 21]. There are numerous indices defined so far. One of the oldest and most thoroughly studied topological indices in graph theory is **Wiener index** denoted as $W(G)$, which is related to molecular branching [22], introduced by Wiener in the year 1947 and is defined as,

$$W(G) = \sum_{u,v \in V(G)} d(u,v). \tag{1}$$

The first Zagreb index is the first degree based topological index conceived in 1972 [9].

$$M_1 = M_1(G) = \sum_{uv \in E(G)} [d_G(u) + d_G(v)]. \tag{2}$$

In 2013, Shirdel et al. [19] defined the hyper Zagreb index as,

$$HM(G) = \sum_{uv \in E(G)} [d_G(u) + d_G(v)]^2. \tag{3}$$

The present paper is organized as follows: In Section 2, we study the chemical applicability of the hyper Zagreb index. In Section 3.1, we obtain the upper and lower bounds for hyper Zagreb index. In section 3.2, we establish the results on Fractal and Cayley tree type dendrimers by using hyper Zagreb index.

2. On the Chemical Applicability of Hyper Zagreb Index

In this section, we discuss the linear regression analysis of hyper Zagreb index $HM(G)$ with entropy, acentic factor, DHVAP and HVAP of an octane isomers taken as molecular graph. The topological indices with the high correlation factor are of foremost important in quantitative structure-property relationships (QSPR) and quantitative structure-activity relationships (QSAR) analysis. The hyper Zagreb index was tested using a dataset of octane isomers found in **http://www.moleculardiscriptors.eu/dataset.htm**. We have noticed that this index is highly correlated with acentric factor ($|r| = 0.982914$). The dataset of octane isomers (coloumns 1-5 of Table 1) are taken from above web link whereas the last coloumn of Table 1 is calculated by using the definition of $HM(G)$ i.e., from equation (2).

Table 1: Experimental values of the entropy, AcentFac, HVAP, DHVAP and corresponding value of $HM(G)$ of octane isomers.

Alkane	**Entropy**	**AcentFac**	**DHVAP**	**HVAP**	**HM(G)**
n-octane	111.67	0.397898	9.915	73.19	98
2-methyl-heptane	109.84	0.377916	9.484	70.3	114
3-methyl-heptane	111.26	0.371002	9.521	71.3	116
4-methyl-heptane	109.32	0.371504	9.483	70.91	116
3-ethyl-hexane	109.43	0.362472	9.476	71.1	118
2,2-dimethyl-hexane	103.42	0.339426	8.915	67.7	152
2,3-dimethyl-hexane	108.02	0.348247	9.272	70.2	134
2,4-dimethyl-hexane	106.98	0.344223	9.029	68.5	132
2,5-dimethyl-hexane	105.72	0.35683	9.051	68.6	130
3,3-dimethyl-hexane	104.74	0.322596	8.973	68.5	156
3,4-dimethyl-hexane	106.59	0.340345	9.316	70.2	136
2-methyl-3-ethyl-pentane	106.06	0.332433	9.209	69.7	136
3-methyl-3-ethyl-pentane	101.48	0.306899	9.081	69.3	160
2,2,3-trimethyl-pentane	101.31	0.300816	8.826	67.3	174
2,2,3-trimethyl-pentane	104.09	0.30537	8.402	64.87	168
2,2,3-trimethyl-pentane	102.06	0.293177	8.897	68.1	176
2,2,3-trimethyl-pentane	102.39	0.317422	9.014	68.37	152
2,2,3,3-tetramethylbutane	93.06	0.255294	8.41	66.2	214

The linear regression models for the entropy, acentric factor, DHVAP and HVAP using the data of Table 1 are obtained by using the least squares fitting procedure as implemented in R software [18] The fitted models are,

$$Entropy = 127.3197(\pm 1.5956) - 0.15272(\pm 0.0109)HM(G) \quad (4)$$
$$AcentFac = 0.5115(\pm 0.008379) - 0.00123(\pm 0.0000573)HM(G) \quad (5)$$
$$DHVAP = 10.87453(\pm 0.210176) - 0.01219(\pm 0.001439)HM(G) \quad (6)$$
$$HVAP = 77.77334(\pm 1.401771) - 0.06002(\pm 0.009596)HM(G) \quad (7)$$

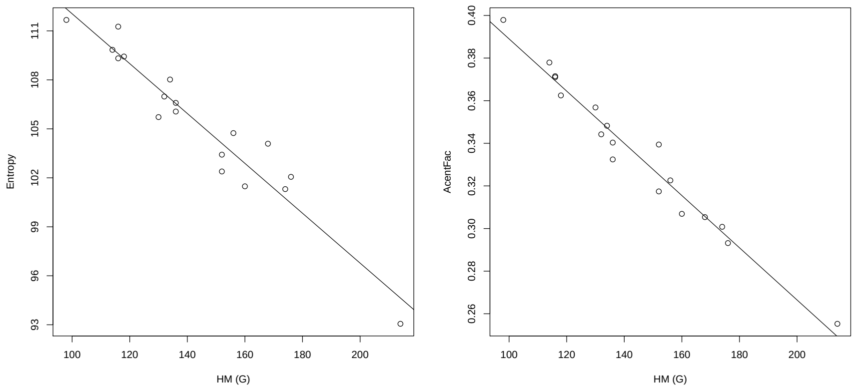

Figure 1

Figure 1: Scatter Diagram *Entropy* on $HM(G)$ and $AcentFac$ on $HM(G)$ superimposed by the fitted regression line.

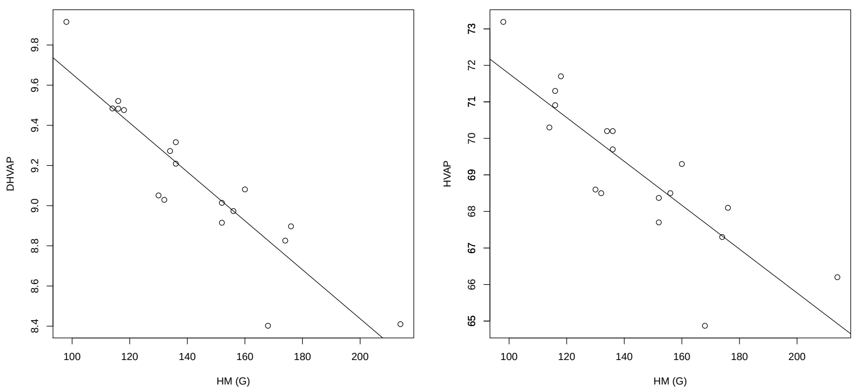

Figure 2

Figure 2: Scatter Diagram $DHVAP$ on $HM(G)$ and $HVAP$ on $HM(G)$ superimposed by the fitted regression line.

In Figure 1 and Figure 2, the direction of the dots on the scatterplot displays a strong negative correlation of $HM(G)$ to Entropy, AcentFac, $DHVAP$ and $HVAP$. The dots much closer to the fitted line in all the scatterplot diagram indicates that model is good fit.

Note: The values in the brackets of equations (4) to (7) are the corresponding standard errors of the regression coefficients.

Table 2: Correlation coefficient and residual standard error of regression models

Physical Property	**Absolute value of the correlation coefficient** ($\|r\|$)	**Residual Standard error**
Enthalpy	0.961428	1.28083
Acentric Factor	**0.982914**	**0.006726**
DHVAP	0.904252	0.168711
HVAP	0.842475	1.125216

From Table 2, we observe that $HM(G)$ highly correlates with acentric factor which is better than first Zagreb index($|r| = 0.973087869$ and residual standard error is 0.008424), F-index ($|r| = 0.965038859$ and residual error is 0.009577) [3] and (β, α)-connectivity index ($|r| = 0.95802$ and residual error is 0.01047) [2]. Further the remaining physical properties of hyper Zagreb index correlates more in comparison with the first neighbourhood Zagreb index such as Enthalpy ($|r| = 0.9526144$ and residual error is 1.416), DHVAP($|r| = 0.8935526$ and residual error is 0.1774) and HVAP ($|r| = 0.8260472$ and residual error is 0.8260472), which was said to be the better correlation [1]. Closer $|r|$ to 1, better is the index.

3. Results

3.1. Mathematical Properties of the Hyper Zagreb Index

Some important theorems which are used through out this section are mentioned below.

Theorem 3.1. [17] *Suppose a_i and b_i, $1 \le i \le n$ are positive real numbers, then*

$$\sum_{i=1}^{n} a_i^2 \sum_{i=1}^{n} b_i^2 \le \frac{1}{4}\left(\sqrt{\frac{M_1M_2}{m_1m_2}} + \sqrt{\frac{m_1m_2}{M_1M_2}}\right)^2 \left(\sum_{i=1}^{n} a_ib_i\right)^2$$

where $M_1 = max_{1\le i\le n}(a_i)$; $M_2 = max_{1\le i\le n}(b_i)$; $m_1 = min_{1\le i\le n}(a_i)$; $m_2 = min_{1\le i\le n}(b_i)$.

Theorem 3.2. [16] *Let a_i and b_i, $1 \le i \le n$ are nonnegative real numbers, then*

$$\sum_{i=1}^{n} a_i^2 \sum_{i=1}^{n} b_i^2 - \left(\sum_{i=1}^{n} a_ib_i\right)^2 \le \frac{n^2}{4}\left(M_1M_2 - m_1m_2\right)^2$$

where M_1M_2 and m_1m_2 are defined similarly to Theorem 3.1.

Theorem 3.3. [5] *Suppose a_i and b_i, $1 \leq i \leq n$ are positive real numbers, then*

$$\left| n\sum_{i=1}^{n} a_i b_i - \sum_{i=1}^{n} a_i \sum_{i=1}^{n} b_i \right| \leq \mu(n)(A-a)(B-b)$$

where a, b, A and B are real constants, that for each i, $1 \leq i \leq n$, $a \leq a_i \leq A$ and $b \leq b_i \leq B$. Further, $\mu(n) = n\lfloor \frac{n}{2} \rfloor \left(1 - \frac{1}{n}\lfloor \frac{n}{2} \rfloor\right)$.

Theorem 3.4. [7] *Let a_i and b_i, $1 \leq i \leq n$ are nonnegative real numbers, then*

$$\sum_{i=1}^{n} b_i^2 + rR\sum_{i=1}^{n} a_i^2 \leq (r+R)\left(\sum_{i=1}^{n} a_i b_i\right)$$

where r and R are real constants. So that for each i, $1 \leq i \leq n$ holds $ra_i \leq b_i \leq Ra_i$.

Remark A. *Let $G = (V, E)$ be a graph with $|V| = n$ and $|E| = m$. Then*

$$M_1(G) \leq 2m(n-1). \tag{8}$$

Remark A holds, from the fact that maximum degree of a vertex in any graph G of order n is $(n-1)$ and the remaining vertices may have degree less than or equal to $(n-1)$.
If the graph G is complete graph then all of its vertices have the degree $(n-1)$ and the first Zagreb index is equal to $2m(n-1)$. This is possible only if G is a complete graph. Hence

$$M_1(G) = 2m(n-1). \tag{9}$$

Theorem 3.5. *Let $G = (V, E)$ be a graph with $|V| = n$ and $|E| = m$. Then,*

$$HM(G) \leq 4m(n-1)^2$$

Further, the equality of this equation holds for the graph $G = K_n$.

Proof. Let $a_1, a_2, a_3, ..., a_m$ and $b_1, b_2, b_3, ..., b_m$ be any two sequence of real numbers. Now we consider the Cauchy-Schwarz inequality [4] i.e.,

$$\left(\sum_{i=1}^{n} a_i b_i\right)^2 \leq \left(\sum_{i=1}^{n} a_i^2\right)\left(\sum_{i=1}^{n} b_i^2\right)$$

By applying $a_i = 1$ and $b_i = (d_i + d_j)$, $i, j = 1, 2, 3, ..., m$ then the inequality becomes,

$$\begin{aligned}\left(\sum_{i,j=1}^{m}(1)(d_i+d_j)\right)^2 &\leq \left(\sum_{i=1}^{m}1^2\right)\left(\sum_{i,j=1}^{m}(d_i+d_j)^2\right)\\ \left(\sum_{i,j=1}^{m}(d_i+d_j)\right)^2 &\leq mHM(G)\\ [M_1(G)]^2 &\leq mHM(G)\\ M_1(G) &\leq \sqrt{mHM(G)}\end{aligned}$$

From equation (8), we have

$$\begin{aligned}1 &\leq \frac{2m(n-1)}{\sqrt{mHM(G)}}\\ \sqrt{mHM(G)} &\leq 2m(n-1)\\ mHM(G) &\leq 4m^2(n-1)^2\\ HM(G) &\leq 4m(n-1)^2\end{aligned}$$

Corollary 3.6. *Let $G = (V, E)$ be a graph with $|V| = n$ and $|E| = m$. Then,*

$$HM(G) \leq 2(n-1)M_1(G).$$

Further, the equality of this equation holds for the graph $G = K_n$.

Proof. Proof follows from Remark A and Theorem 3.5.

Theorem 3.7. *Let G be (n, m) graph and $\delta(G)$ and $\Delta(G)$ are minimum and maximum degree of a graph G respectively, then the following inequality holds.*

$$HM(G) \ \leq \ m(n-1)^2\left(\frac{\Delta(G)}{\delta(G)}+\frac{\delta(G)}{\Delta(G)}\right)^2.$$

Proof. Let G be (n, m) graph with $\delta(G)$ and $\Delta(G)$ as minimum and maximum degree of a graph G respectively.
We have the inequality from the Theorem 3.1.

$$\sum_{i=1}^{n}a_i^2\sum_{i=1}^{n}b_i^2 \leq \frac{1}{4}\left(\sqrt{\frac{M_1M_2}{m_1m_2}}+\sqrt{\frac{m_1m_2}{M_1M_2}}\right)^2\left(\sum_{i=1}^{n}a_ib_i\right)^2.$$

Assume $a_i = 1$, $b_i = (d_i + d_j)$, $M_1 = M_2 = \Delta(G)$ and $m_1 = m_2 = \delta(G)$ then,

$$\begin{aligned}
\sum_{i=1}^{m} 1^2 \sum_{i,j=1}^{m} (d_i + d_j)^2 &\leq \frac{1}{4}\left(\sqrt{\frac{\Delta(G)^2}{\delta(G)^2}} + \sqrt{\frac{\delta(G)^2}{\Delta(G)^2}}\right)^2 \left(\sum_{i,j=1}^{m} (1)(d_i + d_j)\right)^2 \\
mHM(G) &\leq \frac{1}{4}\left(\frac{\Delta(G)}{\delta(G)} + \frac{\delta(G)}{\Delta(G)}\right)^2 (M_1(G))^2 \\
HM(G) &\leq \frac{1}{4m}\left(\frac{\Delta(G)}{\delta(G)} + \frac{\delta(G)}{\Delta(G)}\right)^2 (4m^2(n-1)^2) \\
HM(G) &\leq m(n-1)^2 \left(\frac{\Delta(G)}{\delta(G)} + \frac{\delta(G)}{\Delta(G)}\right)^2 .
\end{aligned}$$

Theorem 3.8. *Let G be (n, m) graph and $\delta(G)$ and $\Delta(G)$ are minimum and maximum degree of a graph G respectively, then the following inequality holds.*

$$HM(G) \leq \frac{1}{m}\left[\frac{n^2}{4}(\Delta(G)^2 - \delta(G)^2)^2 + 4m^2(n-1)^2\right].$$

Proof. Let G be (n, m) graph with $\delta(G)$ and $\Delta(G)$ as minimum and maximum degree of a graph G respectively.
From Theorem 3.2 we have the inequality,

$$\sum_{i=1}^{n} a_i^2 \sum_{i=1}^{n} b_i^2 - \left(\sum_{i=1}^{n} a_i b_i\right)^2 \leq \frac{n^2}{4}\left(M_1 M_2 - m_1 m_2\right)^2$$

Assume $a_i = 1$, $b_i = (d_i + d_j)$, $M_1 = M_2 = \Delta(G)$ and $m_1 = m_2 = \delta(G)$ then,

$$\begin{aligned}
\sum_{i=1}^{m} 1^2 \sum_{i,j=1}^{m} (d_i + d_j)^2 - \left(\sum_{i,j=1}^{m} 1(d_i + d_j)\right)^2 &\leq \frac{n^2}{4}\left(\Delta(G)^2 - \delta(G)^2\right)^2 \\
mHM(G) - (M_1(G))^2 &\leq \frac{n^2}{4}\left(\Delta(G)^2 - \delta(G)^2\right)^2 \\
mHM(G) - \left(4m^2(n-1)^2\right) &\leq \frac{n^2}{4}\left(\Delta(G)^2 - \delta(G)^2\right)^2 \\
HM(G) &\leq \frac{1}{m}\left[\frac{n^2}{4}\left(\Delta(G)^2 - \delta(G)^2\right)^2 + 4m^2(n-1)^2\right].
\end{aligned}$$

Theorem 3.9. *Let G be (n, m) graph and $\delta(G)$ and $\Delta(G)$ are minimum and maximum degree of a graph G respectively, then the following inequality holds.*

$$HM(G) \leq \frac{\mu(n)(\Delta(G) - \delta(G))^2 + 4m^2(n-1)^2}{m}.$$

Proof. Let G be (n,m) graph with $\delta(G)$ and $\Delta(G)$ as minimum and maximum degree of a graph G respectively.
From Theorem 3.3 we have the inequality,

$$\left| n\sum_{i=1}^{n} a_i b_i - \sum_{i=1}^{n} a_i \sum_{i=1}^{n} b_i \right| \leq \mu(n)(A-a)(B-b)$$

Let $a_1, a_2, ..., a_m$ and $b_1, b_2, ..., b_m$ are the real numbers for which there exist real constants a, b, A and B, so that for each i, $i = 1, 2, ..., m$, $a \leq a_i \leq A$ and $b \leq b_i \leq B$.

We choose $a_i = (d_i + d_j) = b_i$, $A = \Delta(G) = B$ and $a = \delta(G) = b$ for the terms in Theorem 3.3, then the inequality reduces to,

$$\begin{aligned} \left| n\sum_{i,j=1}^{m} (d_i + d_j)^2 - \left(\sum_{i,j=1}^{m} (d_i + d_j) \right)^2 \right| &\leq \mu(n)(\Delta(G) - \delta(G))(\Delta(G) - \delta(G)) \\ \left| nHM(G) - (M_1)^2 \right| &\leq \mu(n)(\Delta(G) - \delta(G))^2. \end{aligned}$$

Theorem 3.10. *Let G be (n,m) graph and suppose $\delta(G)$ and $\Delta(G)$ are minimum and maximum degree of a graph G respectively, then the following inequality holds.*

$$HM(G) \leq (\delta(G) + \Delta(G))(2m(n-1)) - m\delta(G)\Delta(G).$$

Proof. Let G be (n,m) graph with $\delta(G)$ and $\Delta(G)$ as minimum and maximum degree of a graph G respectively.
Let $a_1, a_2, ..., a_m$ and $b_1, b_2, ..., b_m$ are the real numbers for which there exist real constants r and R, so that for each i, $i = 1, 2, ..., m$ holds $ra_i \leq b_i \leq Ra_i$. Then inequality from Theorem 3.4 is,

$$\sum_{i=1}^{n} b_i^2 + rR\sum_{i=1}^{n} a_i^2 \leq (r+R)\left(\sum_{i=1}^{n} a_i b_i \right)$$

We choose $b_i = (d_i + d_j)$, $a_i = 1$, $R = \Delta(G)$ and $r = \delta(G)$,

$$\begin{aligned} \sum_{i,j=1}^{m} (d_i + d_j)^2 + \delta(G)\Delta(G)\sum_{i=1}^{m} 1^2 &\leq (\delta(G) + \Delta(G)) \left(\sum_{i,j=1}^{m} (d_i + d_j) \right) \\ HM((G) + \delta(G)\Delta(G)m &\leq (\delta(G) + \Delta(G))M_1(G) \\ HM(G) &\leq (\delta(G) + \Delta(G))M_1(G) - m\delta(G)\Delta(G). \end{aligned}$$

3.2. Hyper Zagreb Index of Fractal and Cayley Tree Type Dendrimers

Dendrimers consist of highly branched organic macromolecules with successive generations/iterations of branch units surrounding a central core. There are different types of dendrimers that are discovered so far. These have a wide range of applications in the field of chemistry, nanoscience, biology, etc. The topological indices of some dendrimers are recently investigated in [6, 20]. Here we consider two types of dendrimers namely, Fractal tree dendrimer and Cayley Tree dendrimer.

Fractal Tree Dendrimer: [19] The word fractal comes from the Latin word meaning "to break". Fractals are geometric patterns in which every smaller part of the structure is similar to the whole. The fractal tree dendrimers are generally denoted by F_p, where $p \geq 0$ is the iterations. If $p = 0$, then F_0 is an edge connecting two vertices. F_p is obtained from F_{p-1} by using two steps on each existing edge in F_{p-1}. The first step is to create a path of three links with the two same end points. The second step is to create k new vertices for each of the two middle vertices in the path. After that, attach them to the middle vertices.

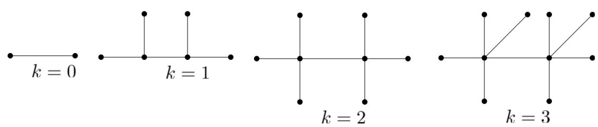

Figure 3: Some construction model for next generations of the Fractal trees [13].

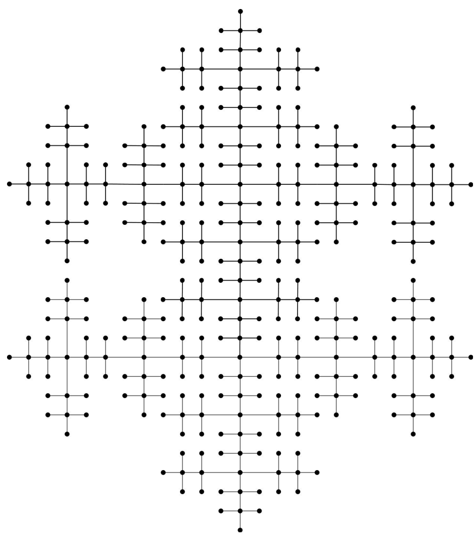

Figure 4: Fractal tree F_3 for $k = 2$ [13].

Table 3: Edge partition of F_p based on degree of end vertices of each edge [13]

d_u, d_v	Frequency
$(1, k+2)$	$42pk - 28k + 14p - 8$
$(4, k+2)$	$28p - 20$
$(k+2, K+2)$	$21p - 14$

Theorem 3.11. *Let F_p with p and $k \geq 2$ be a fractal tree dendrimer for p iterations. Then the hyper Zagreb index of F_p is*

$$HM(F_p) = 14k^3(3p-2) + 126k^2(p-2) + 18k(77p+30) + 2(735p-508).$$

Proof. The hyper Zagreb index of F_p is computed by using Table 3 in the following formula.

$$\begin{aligned} HM(G) &= \sum_{uv \in E(G)} (d_u + d_v)^2 = 42pk - 28k + 14p - 8(1+k+2)^2 \\ &+ 28p - 20(4+k+2)^2 + (21p-14)(k+2+k+2)^2 \end{aligned}$$

After Simplification, we get

$$HM(F_p) = 14k^3(3p-2) + 126k^2(p-2) + 18k(77p+30) + 2(735p-508).$$

Cayley tree dendrimer:

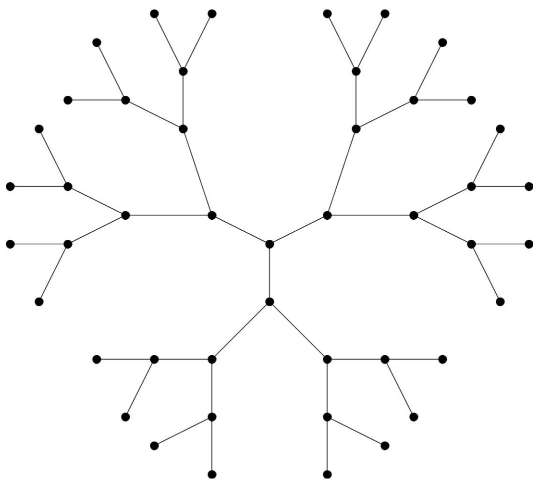

Figure 5: Cayley tree network $C_{3,2}$ [13].

The Cayley tree is one among the different types of dendrimers, also called Bethe lattice. The construction procedure of Cayley tree $C_{s,t}(s \geq 3, t \geq 0)$ consists of t iterations. s is the number of nodes at first iteration. $C_{s,0}$, for $t = 0$, consists of only a central vertex. For $t = 1$,$C_{s,1}$ is obtained by creating s nodes and attaching them to the central vertex by an edge. For $t > 1$, the Cayley tree $C_{s,t}$ is obtained from $C_{s,t-1}$ by creating $s - 1$ nodes and attaching them to each of the pendent vertices of $C_{s,t-1}$.

Table 4: Edge partition of F_p based on degree of end vertices of each edge [13]

d_u, d_v	**Frequency**
$(1, s)$	$s(s-1)^{t-1}$
(s, s)	$s\sum_{i=1}^{t}(s-1)^{i-1} - s(s-1)^{t-1}$

Theorem 3.12. *Let Cayley tree dendrimer $C_{s,t}$ with s and $t \geq 3$ be a tree graph for t iterations, then the hyper Zagreb index is*

$$HM(C_{s,t}) = s(s-1)^{t-1}\left((s+1)^2 - 4s\right) + 4s^3\sum_{i=1}^{t}(s-1)^{i-1}.$$

Proof. Let $C_{s,t}$ with s and $t \geq 3$ be a Cayley tree dendrimer. The hyper Zagreb index of $C_{s,t}$ is computed by using Table 4 in the following formula.

$$\begin{aligned} HM(G) &= \sum_{uv\in E(G)} (d_u + d_v)^2 \\ &= s(s-1)^{t-1}(1+s)^2 + \left[s\sum_{i=1}^{t}(s-1)^{i-1} - s(s-1)^{t-1}\right](s+s)^2 \\ &= s(s-1)^{t-1}\left((s+1)^2 - 4s\right) + 4s^3\sum_{i=1}^{t}(s-1)^{i-1}. \end{aligned}$$

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