DEGREE FACTORIAL ENERGY OF HYDROCARBON GRAPHS AND BENZENOID SYSTEM

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Abstract

In this paper, we explore the degree factorial characteristic polynomial and the degree factorial energy of three types of hydrocarbons—Alkanes, Alkenes, and Alkynes. We investigate the relationship between the molar mass of these hydrocarbons and the degree factorial energy of their corresponding molecular graphs. Additionally, we examine the relationship between the degree factorial energy of Alkanes, Alkenes, and Alkynes.

We further study the degree factorial characteristic polynomial and energy of polycyclic aromatic hydrocarbons (PAHs), including hydrogen-depleted PAHs, and analyze the correlation between them. The degree factorial energy of Fullerene graphs and their variants is discussed by introducing degree factorial energy for r-regular graphs. We also derive upper and lower bounds for the degree factorial energy of simple graphs with n vertices, and the degree factorial energy for various Benzenoid systems such as Jagged Rectangular Benzenoids, Triangular Benzenoid systems, Zigzag Benzenoids, and Concealed non-Kekulean Benzenoids.

We introduce Degree Factorial Energy (DFE) as a novel molecular descriptor, demonstrating a linear correlation with Log P, thereby offering insights into the prediction of molecular lipophilicity. Additionally, the degree factorial energy of standard graph families such as path graphs, cycle graphs, complete graphs, grid graphs, wheel graphs, star graphs, and triangular snake graphs were obtained in [5]

Keywords: Degree factorial matrix of molecular graph, Degree factorial polynomial and Degree factorial energy of molecular graph, Polycyclic Aromatic hydrocarbons (PAHn), hydrogen depleted polycyclic aromatic hydrocarbon HDPAHn, Fullerene graph, Benzenoid system, Log P.

Introduction

Let G (V, E) be a simple graph. Let $V = \{v_1, v_2, ..., v_n\}$. The degree factorial matrix of the graph G is denoted by DFM(G) = $[a_{ij}]$ and is defined as follows: DFM(G) = $d(v_i)!$ $if\ i = j$ and 0! $otherwise$. The characteristic polynomial of DFM(G) is $P_{DFM(G)}(\lambda) = det\ (DFM(G) - \lambda I)$ is known as degree factorial polynomial of G where I is the identity matrix. The roots of the equation $DFM(G)(\lambda) = 0$ are called as the degree factorial eigen values of G (or) degree factorial characteristic values of G. The set of all eigen values $\lambda_1, \lambda_2, ..., \lambda_n$ of this polynomial $DFM(G)(\lambda)$ is known as the degree factorial spectrum of G. The sum of the absolute values of the degree factorial eigen values of G is known as the degree factorial energy of G and is denoted by $DF\text{E}(G)$. $i.e.$, $DF\text{E}(G) = \sum |\lambda i|$, i=1to n [5]. A molecular graph is a simple graph in which atoms are considered as vertices and the edges to the bonds. Chemical graph theory is a branch of mathematical chemistry which applies graph theory to mathematical modelling of chemical phenomena. This theory had an important effect on the development of the chemical sciences. In this paper, we studied the topological index that is degree factorial energy of the molecular graphs [2,4,7,11].

2. Main Results

HYDROCARBONS

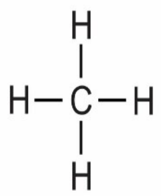
Degree factorial energy of Alkane, Alkene, Alkyne are given below.

Theorem 2.1. *The degree factorial energy of the Alkane C_nH_{2n+2} is 2(13n+1) where n ≥ 1.*

Proof. Let C_nH_{2n+2} be a molecular graph with $3n + 2$ vertices and $3n+1$ edges. The degree factorial matrix of C_nH_{2n+2} where n=1 is,

$$DFM(C_nH_{2n+2}) = \begin{bmatrix} 4! & 1 & 1 & 1 & 1 \\ 1 & 1! & 1 & 1 & 1 \\ 1 & 1 & 1! & 1 & 1 \\ 1 & 1 & 1 & 1! & 1 \\ 1 & 1 & 1 & 1 & 1! \end{bmatrix}$$

and it is obtained from the molecular structure of CH_4.



The characteristic equation of above matrix is $\lambda^3(\lambda^2 - 28\lambda + 92) = 0$.

The degree factorial energy is 28.

For n>1, The degree factorial matrix of C_nH_{2n+2} is

$$DFM\big((\mathrm{C}_n\mathrm{H}_{2n+2}\,)\,\big) = \begin{bmatrix} 4!\,I_{n\times n} + J_{n\times n} - I_{n\times n} & J_{n\times 2n+2} \\ J_{2n+2\times n} & J_{2n+2\times 2n+2} \end{bmatrix}$$

The degree factorial Characteristic polynomial is $(\lambda - 23)^{n-1}\lambda^{2n+1}(\lambda^2 - (3n+25)\lambda + (2n+25))$.

The degree factorial energy is $2(13n + 1)$.

Theorem 2.2. *The degree factorial energy of the Alkene C_nH_{2n} is* $2(13n\text{-}18)$ *where $n \geq 2$.*

Proof. The molecular graph of Alkene contains 3n vertices and 3n-1 edges.

The characteristic matrix for C_2H_4 is

$$DFM\big((\mathrm{C}_2\mathrm{H}_4\,)\big) = \begin{bmatrix} 3! & 1 & 1 & 1 & 1 & 1 \\ 1 & 3! & 1 & 1 & 1 & 1 \\ 1 & 1 & 1! & 1 & 1 & 1 \\ 1 & 1 & 1 & 1! & 1 & 1 \\ 1 & 1 & 1 & 1 & 1! & 1 \\ 1 & 1 & 1 & 1 & 1 & 1! \end{bmatrix}$$

The degree factorial Characteristic polynomial is $(\lambda\text{-}5)\lambda^3(\lambda^2 - 11\lambda + 20)$.
The degree factorial energy is 16.
For n>2, The degree factorial matrix for $\mathrm{C}_n\mathrm{H}_{2n}$ is

$$DFM\big((\mathrm{C}_n\mathrm{H}_{2n}\,)\,\big) = \begin{pmatrix} \begin{matrix} 3! & 1 \\ 1 & 3! \end{matrix} & J_{2\times n-2} & J_{2\times 2n} \\ J_{n-2\times 2} & 4!\,I_{n-2\times n-2} + J_{n-2\times n-2} - I_{n-2\times n-2} & J_{n-2\times 2n} \\ J_{2n\times 2} & J_{2n\times n-2} & J_{2n\times 2n} \end{pmatrix}$$

The degree factorial Characteristic polynomial is

$$(\lambda - 23)^{n-3}\lambda^{2n-1}(\lambda^3 - (3n+28)\lambda^2 + (61n+151)\lambda - 230n)).$$

The degree factorial energy is $2(13n\text{-}18)$.

Theorem 2.3. *The degree factorial energy of the Alkyne C_nH_{2n-2} is* $2(13n-23)$ *where* $n \geq 2$.

Proof. The molecular graph of Alkyne contains 3n-2 vertices and 3n-3 edges.

The degree factorial matrix for C_2H_2 is

$$DFM(C_2H_2) = \begin{bmatrix} 2! & 1 & 1 & 1 \\ 1 & 2! & 1 & 1 \\ 1 & 1 & 1! & 1 \\ 1 & 1 & 1 & 1! \end{bmatrix}$$

The degree factorial Characteristic polynomial is $(\lambda-1)\lambda(\lambda^2 - 5\lambda + 2)$.
The degree factorial energy is 6.
For n > 2, The degree factorial matrix for C_nH_{2n-2} is

$$DFM(C_nH_{2n-2}) = \begin{pmatrix} \begin{matrix} 2! & 1 \\ 1 & 2! \end{matrix} & J_{2\times n-2} & J_{2\times 2n-2} \\ J_{n-2\times 2} & 4!\, I_{n-2\times n-2} + J_{n-2\times n-2} - I_{n-2\times n-2} & J_{n-2\times 2n} \\ J_{2n\times 2} & J_{2n\times n-2} & J_{2n\times 2n} \end{pmatrix}$$

The degree factorial Characteristic polynomial is

$(\lambda - 23)^{n-3}\lambda^{2n-3}(\lambda - 1)(\lambda^3 - (3n + 22)\lambda^2 + (49n + 19)\lambda - 46(n - 1))$.
The degree factorial energy is $2(13n-23)$.

Relation between Degree factorial energy of Alkane, Alkene and Alkyne

DFE (C_nH_{2n+2}) = DFE (C_nH_{2n}) - 38 =DFE (C_nH_{2n-2}) - 48.

POLYCYCLIC AROMATIC HYDROCARBONS

Polycyclic Aromatic hydrocarbons considered here is a family of hydrocarbons which contains several copies of benzene C_6 and play an important role in graphitization of organic materials [3, 9,10,12].

The first famous members of this hydrocarbon family (PAH family) are denoted and shown as follow PAH_n is structured as:

For n=1 we obtain the Benzene with six carbon (C) and six hydrogen (H) atoms,

For n=2, Coronene with 24 carbon and twelve hydrogen atoms,

For n=3 Circumcoronene with 54 carbon and eighteen hydrogen atoms.

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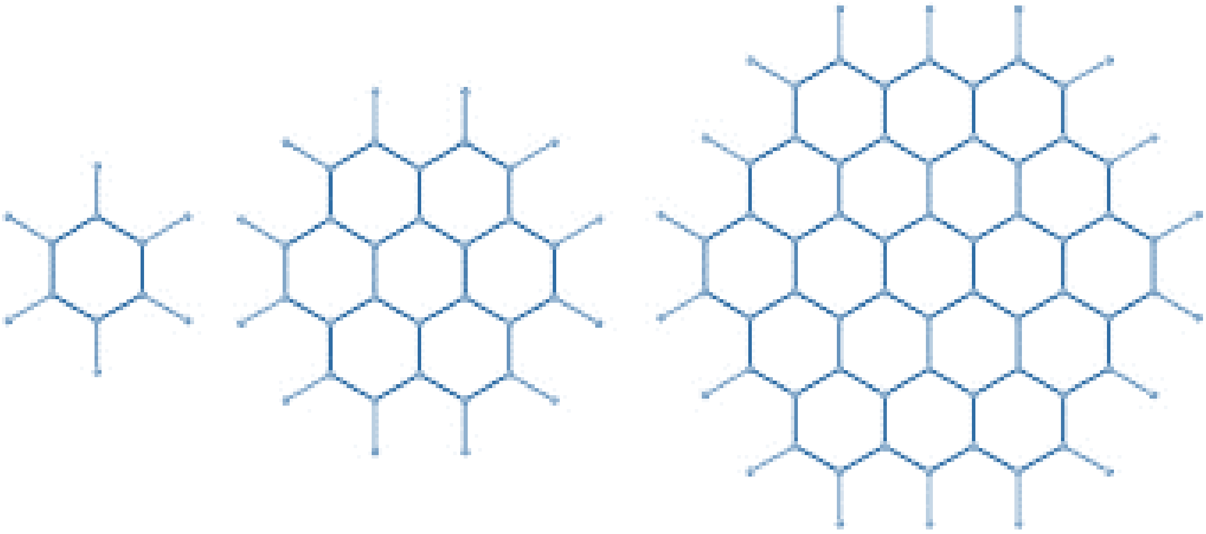

FIGURE.1: POLYCYCLIC AROMATIC HYDROCARBANS PAH_1, PAH_2, PAH_3.

The first few members of *hydrogen depleted polycyclic aromatic hydrocarbon* $HDPAH_n$ are as follow

$HDPAH_n$ is structured as:

For n=1 we have $HDPAH_1$ with six carbon atoms,

For n=2, $HDPAH_2$ with 24 carbon atoms,

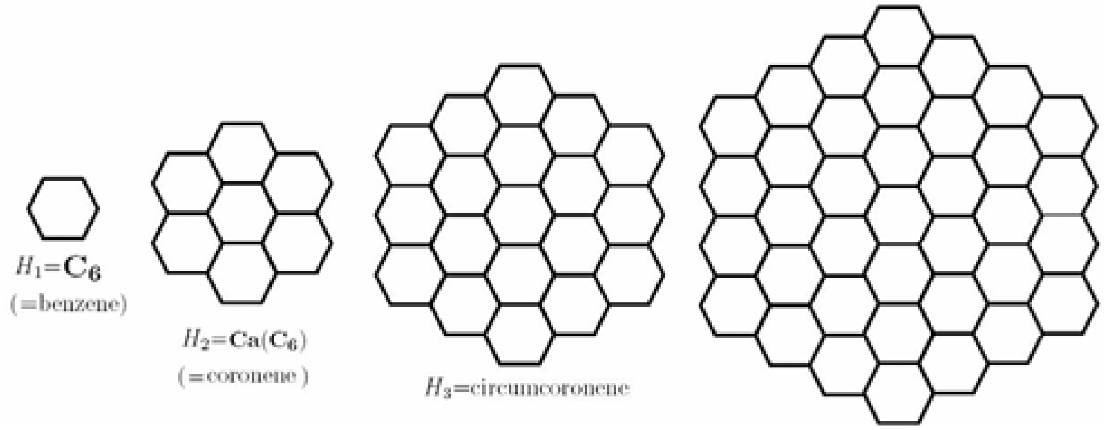

FIGURE.2: HYDROGEN DEPLETED POLYCYCLIC AROMATIC HYDROCARBANS $HDPAH_1$, $HDPAH_2$, $HDPAH_3$, $HDPAH_4$.

And the nth growth given as below:

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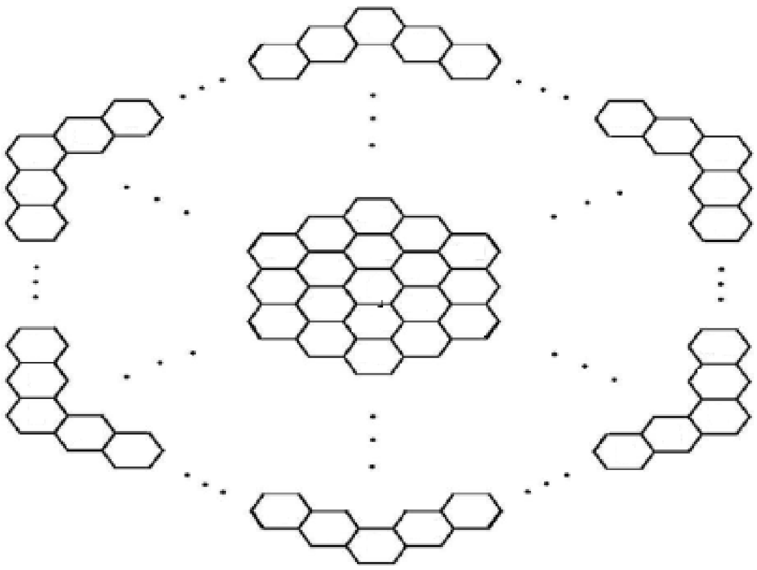

FIGURE3:HYDROGEN DEPLETED POLYCYCLIC AROMATIC HYDROCARBANS HDPAH$_n$

Theorem 2.4. *The degree factorial energy of polycyclic aromatic hydrocarbon PAH_n is 6n(6n+1).*

Proof. Let PAH_n be a molecular graph with $6n^2 + 6n$ vertices and $9n^2+3n$ edges. The degree of poly aromatic hydrocarbons graph has $6n^2$ three degree vertices and 6n one degree vertices. The degree factorial matrix of PAH_n where n=1 is,

$$DFM(PAH_1) = \begin{bmatrix} 3! & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & 3! & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & 3! & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 3! & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 & 3! & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 & 1 & 3! & 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \end{bmatrix}$$

The degree factorial characteristic equation of above matrix is $(\lambda - 15)(\lambda - 2)\lambda^5(\lambda - 5)^5$.

The degree factorial energy is 42.

For n>1, The degree factorial matrix of PAH$_n$ is

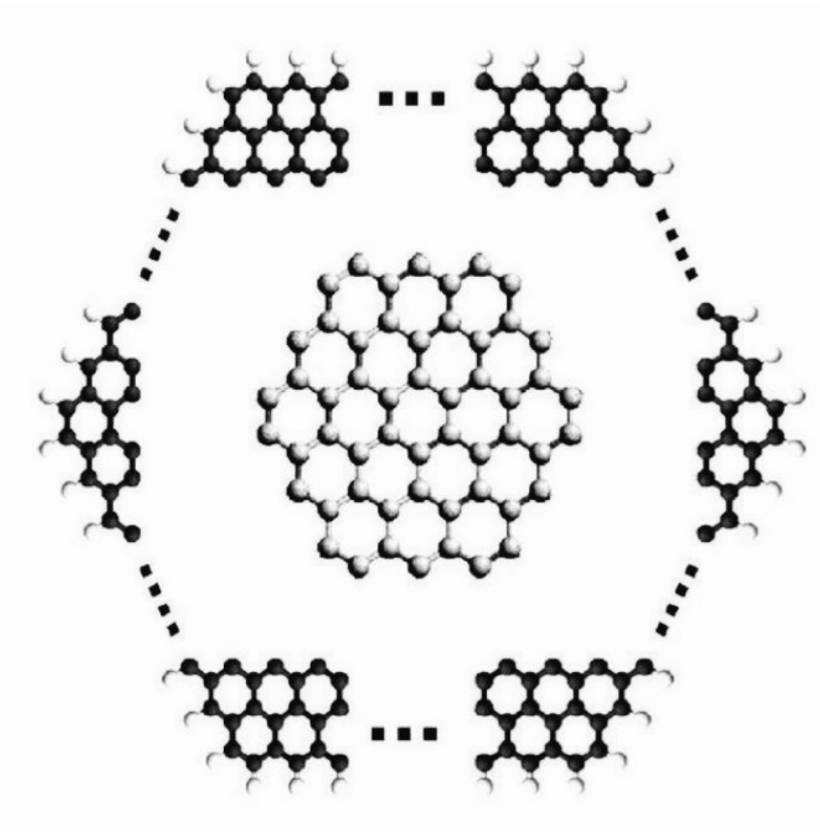

FIGURE.4: POLYCYCLIC AROMATIC HYDROCARBANS PAH_n

$$DFM(\text{PAHn}) = \begin{bmatrix} 3!\, I_{6n^2\times 6n^2} + J_{6n^2\times 6n^2} - I_{6n^2\times 6n^2} & J_{6n^2\times 6n} \\ J_{6n\times 6n^2} & J_{6n\times 6n} \end{bmatrix}$$

The degree factorial Characteristic polynomial is

$$(\lambda-5)^{6n^2-1}\lambda^{6n-1}(\lambda^2-(6n^2+6n+5)\lambda+30n))$$

The degree factorial eigen values are
$5(6n^2-1\ times), 0\ (6n-1\ times)$,

$$(\,(6n^2+6n+5) \pm \sqrt{(36n^4+72n^3+96n^2-60n+25)}\,)\,/\,2$$

The degree factorial energy is *6n(3n-2).*

Theorem 2.5. *The degree factorial energy of hydrogen depleted polyromantic hydrocarbon $HDPAH_n$ is 12n(6n+1).*

Proof. Let $HDPAH_n$ be a molecular graph with $6n^2$ + 6n vertices and $9n^2+3n$ edges. The degree of poly aromatic hydrocarbons graph has $6n^2$ three degree vertices and 6n one degree vertices.

The degree factorial matrix of $HDPAH_n$ where n=1 is,

$$DFM(HDPAH_1) = \begin{bmatrix} 2! & 1 & 1 & 1 & 1 & 1 \\ 1 & 2! & 1 & 1 & 1 & 1 \\ 1 & 1 & 2! & 1 & 1 & 1 \\ 1 & 1 & 1 & 2! & 1 & 1 \\ 1 & 1 & 1 & 1 & 2! & 1 \\ 1 & 1 & 1 & 1 & 1 & 2! \end{bmatrix}$$

The degree factorial characteristic equation of above matrix is

$$(\lambda - 7)(\lambda - 1)^5.$$

The degree factorial energy is 12.

For n>1, The degree factorial matrix of $HDPAH_n$ is

$$DFM(\mathrm{HDPAH}_n) = \begin{bmatrix} 2!\,I_{6n\times 6n} + J_{6n\times 6n} - I_{6n\times 6n} & J_{6n\times 6n^2-6n} \\ J_{6n^2-6n\times 6n} & 3!\,I_{6n^2-6n\times 6n^2-6n} + J_{6n^2-6n\times 6n^2-6n} - I_{6n^2-6n\times 6n^2-6n} \end{bmatrix}$$

The degree factorial Characteristic polynomial is

$$(\lambda - 5)^{6n^2-6n-1}(\lambda - 1)^{6n-1}\left(\lambda^2 - (6n^2 + 6n)\lambda + (6n^2 + 24n + 5)\right).$$

The degree factorial eigen values are 5 $(6n^2 - 6n - 1\ times)$, 1 $(6n - 1)\ times$,
$3n^2 + 3n \pm \sqrt{(9n^4 + 18n^3 + 3n^2 - 24n - 5)}$

The degree factorial energy is $12n(3n - 2)$.

Relation between degree factorial energy of polycyclic aromatic hydrocarbons and Hydrogen depleted Poly aromatic hydrocarbons:

1.DFE (polycyclic aromatic hydrocarbons) = DFE (Hydrogen depleted Polycyclic aromatic hydrocarbons)-30n.

2.DFE($HDPAH_n$) is always less than (DFE(PAH_n)).

FULLERENE

Fullerene graphs by introducing the degree factorial energy of r regular graphs. Fullerene graph is 3-connected and 3-regular graph with only pentagonal and hexagonal faces. Fullerene graph with n vertices exist for all even numbers n greater than or equal to 24 and for n=20. It is a pure form of carbon. It is used in skin care products and drug deliveries and many more places. Fullerenes is a carbon allotrope. Fullerenes are carbon molecules with spherical (Bucky ball), Regular fullerenes exist with two different geometries, depending on the orientation of the graphene sheet on the faces of the polyhedron. The icosahedral fullerenes contain $60k^2$atoms and the triacontahedral fullerenes contain $20k^2$atoms, with k a non-zero positive integer. Extensive research has been carried out to investigate the biomedical applications of Fullerene since its discovery. In particular, studies from 2003 onwards have explored the potential use of Fullerene in medicine. These investigations have demonstrated its remarkable ability to bind specific antibiotics, effectively targeting drug-resistant bacteria. Additionally, Fullerene has shown promising selectivity towards certain cancer cells, including melanoma. A notable publication in Chemistry & Biology. It has extensive potential applications across multiple industries including electronics, energy, and others [8].

Theorem 2.6: The degree factorial energy of r-regular graph with n vertices is n(r!).

Proof: Let G be a graph with n vertices and each vertex has degree r**.**
The degree factorial matrix is,

$$DFM(G) = \begin{pmatrix} r! & 1 & \dots & 1 \\ 1 & r! & \cdots & 1 \\ \vdots & \vdots & \ddots & \vdots \\ 1 & 1 & \cdots & r! \end{pmatrix}$$

That is DFM(G) = $(r! - 1)I_{nxn} + J_{nxn}$.
Since all the eigen values of identity matrix are 1 and the eigen values of J are n one time and zero for (n-1) times, the r regular graph has eigen values as $(r! - 1 + n)$ one time and $r! - 1$ for $(n - 1)$ times (by the properties of eigen values).
Hence the degree factorial characteristic polynomial of r - regular graph is

$$(\lambda - (r! - 1))^{n-1}(\lambda - (r! - 1 + n))$$

And the degree factorial energy of regular graph is $\text{r}! - 1 + \text{n} + (\text{n} - 1)(\text{r}! - 1) = \text{nr}!$.

Upper and Lower bound for degree factorial energy of simple graphs with n vertices.

Theorem 2.7: For any simple graph with n vertices, n ≤ DFE(G) ≤ n!

Proof: Let G be a simple graph with n vertices. Then the possibilities of degree of each vertex is $0 \leq d(v_i) \leq n$. To find the lower bound let us assume the graph in which no vertex is adjacent with each other, That is totally disconnected graph. Then the degree factorial matrix for totally disconnected graph is all one matrix.
And the eigen values of rank one matrix is n (one time), remaining are zero.
Hence the degree factorial energy of totally disconnected graph is n which is a lower bound for degree factorial energy.
Now, to find the upper bound consider the simple graph with maximum possible degree. That is every vertex having adjacency with every other vertices.
In this case every vertex has degree $n - 1$.
So the degree factorial matrix is $(((n-1)! - 1) I_{nxn} + J_{nxn}.)$
By the properties of eigen values the above matrix has eigen values as $n! - 1 + n$ one time and $(n! - 1)$ $(n - 1)$ times.
Therefore degree factorial energy is $(n - 1)! - 1 + n + (n - 1)((n - 1)! - 1) = n!$.

Or by using previous theorem we can obtain the upper bound.

Degree factorial energy of fullerene (3 – regular graphs)

Degree factorial energy for r-regular graph is $n(r!)$. Since Fullerene is a 3- regular graph, the degree factorial energy of fullerene graph is $n(3!)$, where n is number of carbon atoms. Some types of fullerene graphs given below. We obtain the degree factorial energy of these types of fullerene [8].

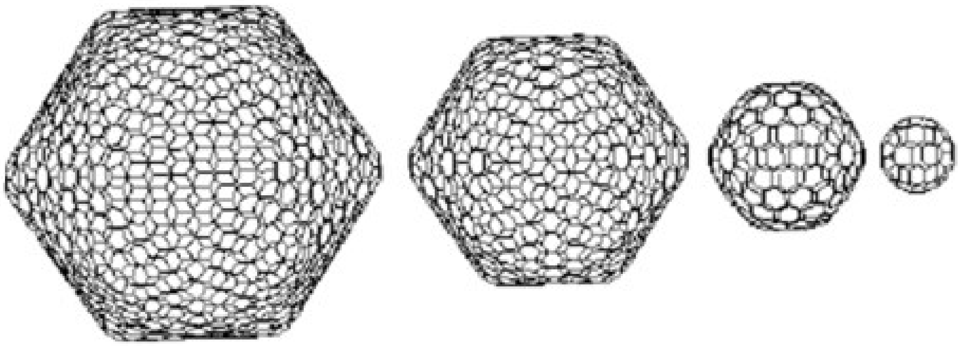

FIGURE 5. ICOSAHEDRAL FULLERENES C_{1280}, C_{720}, C_{240} AND C_{60}.

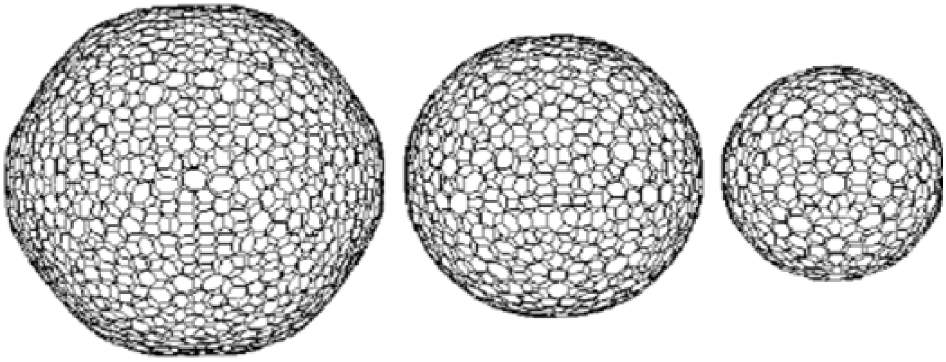

FIGURE 6. STONE–WALES ROUNDED FULLERENES C_{2000}, C_{1280} AND C_{720}.

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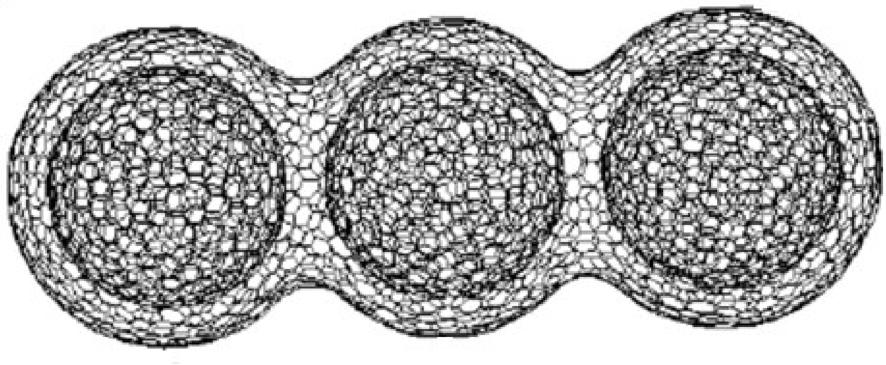

FIGURE 7. POD-OF-PEAS FULLERENE C_{5540} CONTAINING 3 'PEAS' SPHERICAL C_{720}, WITH AN EXTERNAL LAYER MADE BY PART OF SPHERICAL C_{1280}.

FULLERENE	MOLECULAR FORMULA	DFE
Icosahedral fullerenes	C_{60} (Bucky ball)	360
	C_{240}	1440
	C_{720}	4320
	C_{1280}	7680
Stone–Wales rounded fullerenes.	C_{2000}	12000
	C_{1280}	7680
	C_{720}	4320
Pod-of-peas fullerene C_{5540} containing 3 'peas' spherical C_{720},with an external layer made by part of spherical C_{1280}	C_{5540}	33240

BENZENOID SYSTEMS

Benzenoid systems have significant importance in theoretical chemistry due to their natural graph representation of benzenoid hydrocarbons. In a hexagonal system, there exists a vertex that belongs to three hexagons, which is known as the internal vertex of the hexagonal system. Benzenoid hydrocarbons are commonly found in our surroundings, minerals, and food and are also produced as byproducts in certain reactions, with a wide range of applications in chemical synthesis. However, despite their widespread use, benzenoid hydrocarbons are known to be pollutants and carcinogenic. Benzenoid systems are essentially hydrogen-deprived benzenoid system [1,12].

Jagged Rectangular Benzenoid System

Let JB[m, n] denotes a jagged-rectangle benzenoid system for all m ∈N−{1} and n ∈ N. A Benzenoid jagged-rectangle forms a rectangle and the number of benzenoids called in each chain m-1 and m alternatively [1,12].

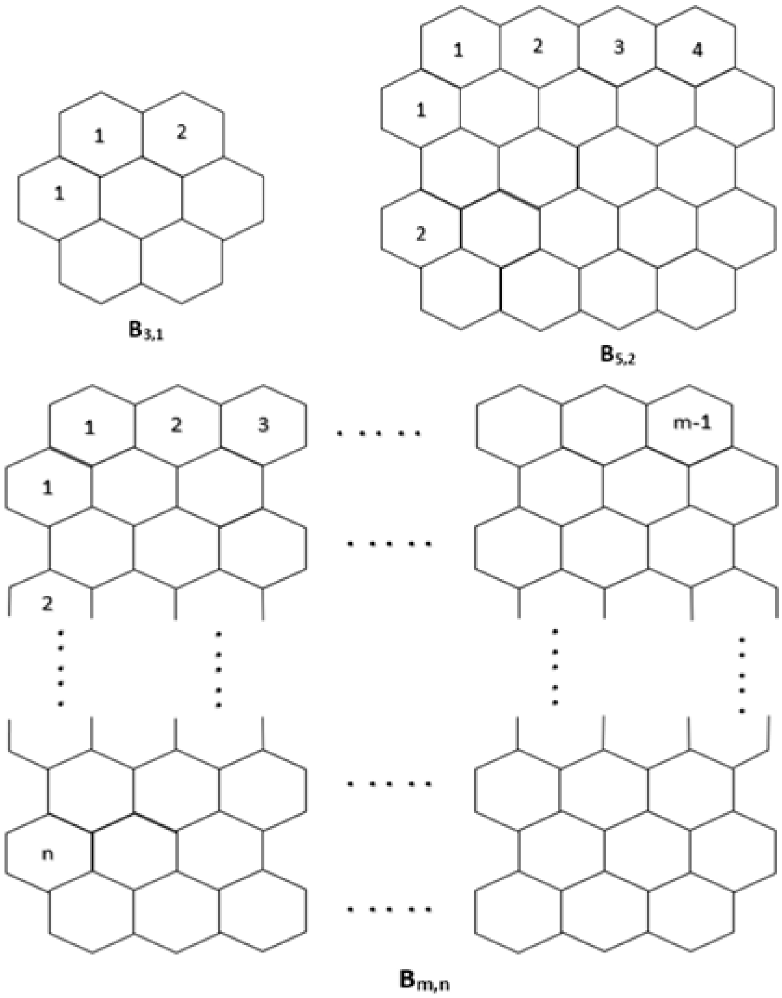

FIGURE 8. JAGGED RECTANGULAR BENZENOID SYSTEM

Theorem 2.8: The degree factorial energy of Jagged Rectangular Benzenoid System is $4(6mn + 4m - n - 5)$.

Proof. Let JB[m,n] be the Jagged Rectangular Benzenoid system with $4mn + 4m + 2n - 2$ vertices and $6mn + 5m + n - 4$ edges. Among the vertices $2m + 2 + 4n$ has degree 2 and $4mn + 2m - 2n - 4$ has degree 3.

So the degree factorial characteristic matrix is

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$$DFM(\mathrm{JB}[\mathrm{m},\mathrm{n}]) = \begin{bmatrix} 2!\,I_{2m+2+4n} + J_{2m+2+4n} - I_{2m+2+4n} & J_{2m+2+4n\times 4mn+2m-2n-4} \\ J_{4mn+2m-2n-4\times 2m+2+4n} & 3!\,I_{4mn+2m-2n-4} + J_{4mn+2m-2n-4} - I_{4mn+2m-2n-4} \end{bmatrix}$$

The degree factorial characteristic polynomial is

$$(\lambda-1)^{2m+4n+1}(\lambda-5)^{4mn+2m-2n-5}(\lambda^2-(4mn+4m+2n+4)\lambda+(4mn+12m+18n+12))$$

The degree factorial eigen values are,

$$1\ (2m+4n+1\ times), 5\ (4mn+2m-2n-5\ times),$$

$$\frac{4mn+4m+2n+4 \pm \sqrt{(6n-4mn+10)^2+4(2m+4n+2)(4mn+2m-2n-4)}}{2}$$

The degree factorial energy is $2m+4n+1+5(4mn+4m-2n-3)+4mn+4m+2n+4 = 4(6mn+4m-n-5)$.

Zig zag Benzenoid system

The graph ZB_n, which consists of prows, witheach row consisting of two hexagonal units sharing one common edge. Continuing inthe same pattern, we can deduce that ZB_n has $10n+1$ edges and $8n+2$ vertices[1,12].

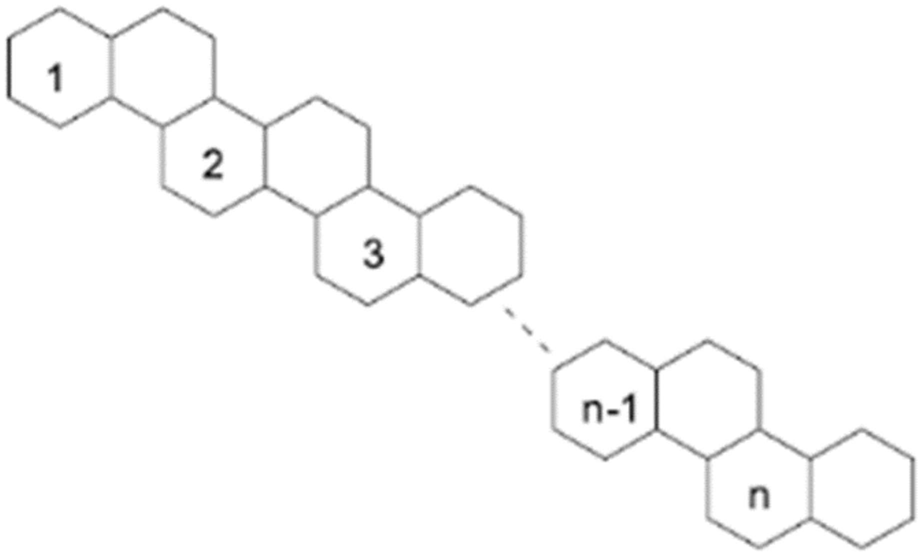

FIGURE. 9: ZIG ZAG BENZENOID SYSTEM

Theorem 2.9: The degree factorial energy of Zig zag Benzenoid System is $4(8n-1)$.

Proof. Let ZB_n be the Jagged Rectangular Benzenoid system with $8n+2$ vertices and

$10n + 1$ edges. Among the vertices $4n + 4$ has degree 2 and $4n - 2$ has degree 3.
So the degree factorial characteristic matrix is

$$DFM(\text{ZBn}) = \begin{bmatrix} 2!\,I_{4n+4} + J_{4n+4} - I_{4n+4} & J_{4n+4\times 4n-2} \\ J_{4n-2\times 4n+4} & 3!\,I_{4n-2} + J_{4n-2} - I_{4n-2} \end{bmatrix}$$

The degree factorial characteristic polynomial is
$(\lambda - 1)^{4n+3}(\lambda - 5)^{4n-3}(\lambda^2 - (8n + 8)\lambda + (24n + 23))$.

The degree factorial eigen values are 1 (4n+3 times), 5 (4n-3 times),

$$4n + 4 \pm \sqrt{(16n)^2 + 8n - 7}$$

The degree factorial energy is $4(8n - 1)$.

Concealed non kekulean Benzenoid system

Concealed non-kekulean benzenoid graphs, each of which has $12r +\ 14$ vertices and 17r−14edges. An initial count places the number of structures in this cluster at eight. Graphs can be split in half by severing the cut of the edge [,5,12]**.**

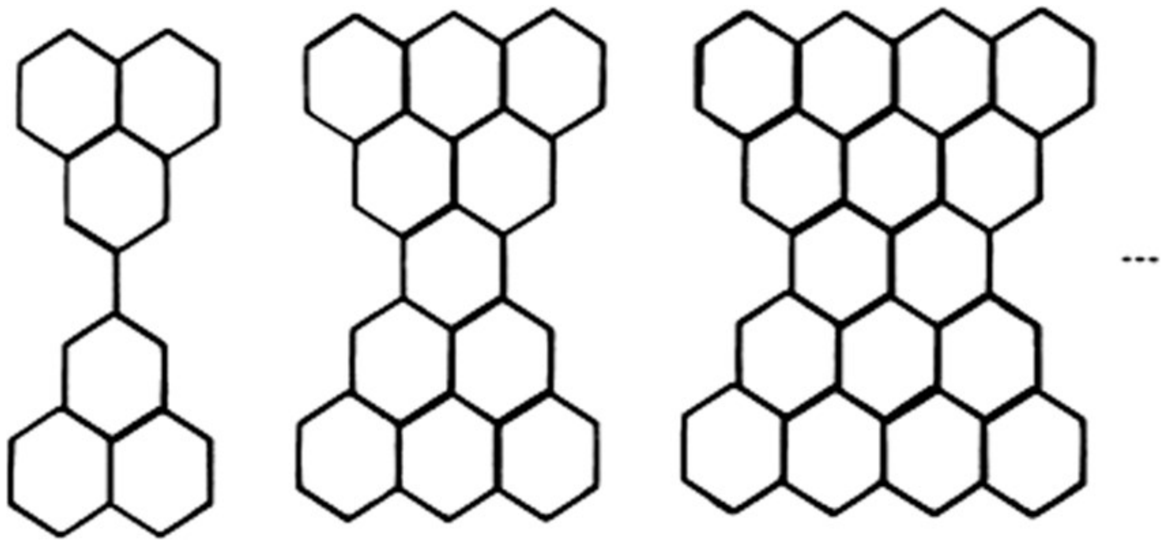

FIGURE. 10: CONCEALED NON KEKULEAN BENZENOID

Theorem 2.10: The degree factorial energy of Concealed non-kekulean benzenoid System is $4(16r + 7)$.

Proof. Let NKB_r be the Concealed non-kekulean benzenoid system with $12r +\ 14$ vertices and $10n + 1$ edges. Among the vertices $2r + 14$ has degree 2 and $10r$ has degree 3.
So the degree factorial characteristic matrix is

$$DFM(\text{NKBr}) = \begin{bmatrix} 2!\,I_{2r+14} + J_{2r+14} - I_{2r+14} & J_{2r+14\times 10r} \\ J_{10r\times 2r+14} & 3!\,I_{10r} + J_{10r} - I_{10r} \end{bmatrix}$$

The degree factorial characteristic polynomial is
$(\lambda-1)^{2r+13}(\lambda-5)^{10r-1}(\lambda^2-(12r+20)\lambda+(20r+75))$.

The degree factorial eigen values are 1 $(2r+13\ times)$, 5 $(10r-1\ times)$,

$$6r+10 \pm \sqrt{(6r)^2+100r+25}$$

The degree factorial energy is $4(16r+7)$.

Triangular Benzenoid System

The benzenoid Triangular system are the special arrangement of hexagons, which is obtained by decreasing the number of hexagon rings from bottom to top**.** The molecular graph of the triangular Benzenoid system has n^2+4n+1 and the number of edges is $(3/2)\ n(n+3)$. There are $3(n+1)$ vertices with degree two and n^2+n-2 vertices with degree three [1,12].

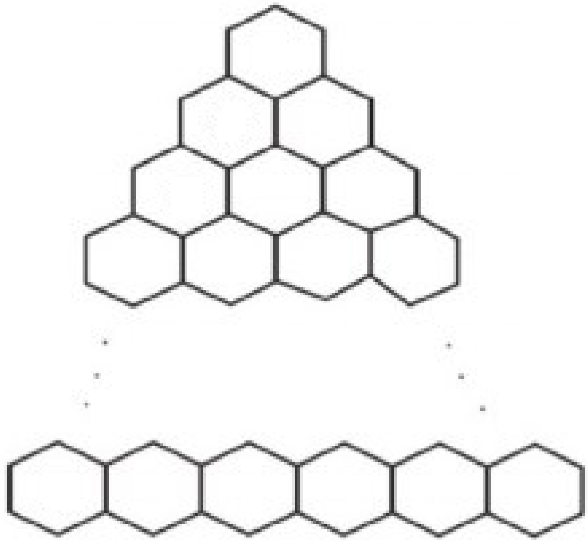

FIGURE. 11: TRIANGULAR BENZENOID SYSTEM

Theorem 2.11: The degree factorial energy of Triangular Benzenoid System is $6(n^2+2n-1)$.

Proof. Let TB_n be The molecular graph of the triangular Benzenoid system has n^2+4n+1 and the number of edges is $(3/2)\ n(n+3)$. There are $3(n+1)$ vertices with degree two and n^2+n-2 vertices with degree three.

So the degree factorial characteristic matrix is

$$DFM(\text{TBn}) = \begin{bmatrix} 2!\,I_{3n+3} + J_{3n+3} - I_{3n+3} & J_{3n+3\times n^2+n-2} \\ J_{n^2+n-2\times 3n+3} & 3!\,I_{n^2+n-2} + J_{n^2+n-2} - I_{n^2+n-2} \end{bmatrix}$$

The degree factorial characteristic polynomial is
$(\lambda-1)^{3n+2}(\lambda-5)^{n^2+n-3}(\lambda^2-(n^2+4n+7)\lambda+(n^2+16n+18))$.

The degree factorial eigen values are 1 (3n+2 times), 5 (n^2+n-3 times),
$$\frac{n^2+4n+7\pm\sqrt{(2n-n^2+5)^2+4(3n+3)(n^2+n-2)}}{2}$$
The degree factorial energy is $6(n^2+2n-1\ )$.

Rhombic Benzenoid System:
Consider a benzenoid system in which hexagons are arranged to form a rhombic shape Rp, where p -denotes the number of hexagons along each rhombic boundary is shown in FIGURE.12.There are $2n\ (n+\ 2)$ vertices and $3n^2+\ 4n-1$ edges in this benzenoid system [1,12].

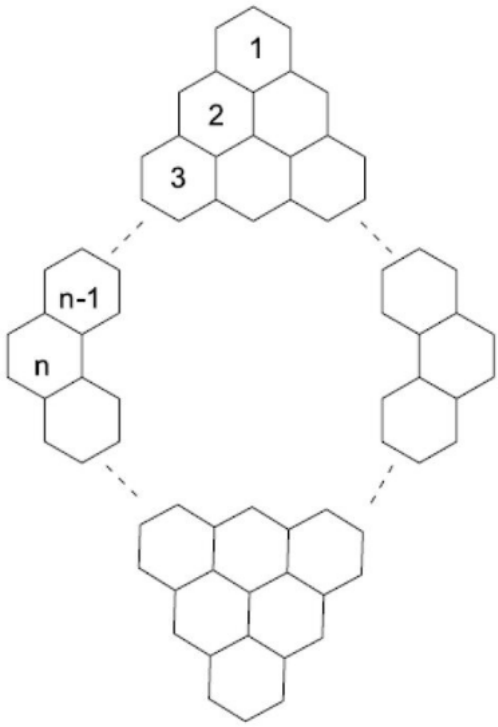

FIGURE 12: RHOMBIC BENZENOID SYSTEM

Theorem 2.12: The degree factorial energy of Triangular Benzenoid System is $4(3n^2+4n-4\ )$.

Proof. Let RB_n be The molecular graph of the triangular Benzenoid system has $2n^2+4n$ vertices among them there are $2n+4$ vertices with degree two and $2n^2+2n-4$ vertices with degree three.
So the degree factorial characteristic matrix is
$$DFM(\mathrm{RBn})=\begin{bmatrix}2!\,I_{2n+4}+J_{2n+4}-I_{2n+4} & J_{2n+4\times 2n^2+2n-4}\\ J_{2n^2+2n-4\times 2n+4} & 3!\,I_{2n^2+2n-4}+J_{2n^2+2n-4}-I_{2n^2+2n-4}\end{bmatrix}$$

The degree factorial characteristic polynomial is
$(\lambda-1)^{2n+3}(\lambda-5)^{2n^2+2n-5}(\lambda^2-(2n^2+4n+6)\lambda+(2n^2+12n+21))$.

The degree factorial eigen values are 1 (2n+3 times), 5 ($2n^2+2n-5$ times),

$$n^2+2n+3\pm\sqrt{n^4+4n^3+8n^2-12}$$

The degree factorial energy is $4(3n^2+4n-4)$.

LOG P: THE PARTITION COEFFICIENT

Log P is the logarithm of the partition coefficient (P), which measures the distribution of a compound between a hydrophobic (usually 1-octanol) and a hydrophilic (water) phase.

$$LogP=\mathrm{Log}_{10}\left(\frac{[compound]_{octanol}}{[compound]_{water}}\right)$$

A positive log P indicates lipophilicity (compound favors the lipid phase). A negative log P indicates hydrophilicity (compound favors the aqueous phase).

LIPOPHILICITY HYDROPHOBICITY

Lipophilicity is commonly measured using the partition coefficient (P), which is the ratio of a compound's concentration in a hydrophobic solvent to its concentration in water. Hydrophobicity broadly describes the tendency to repel water. Usually, a molecule that is highly lipophilic is also hydrophobic, meaning it prefers lipid environments and avoids water. Hydrophilicity, on the other hand, means a molecule prefers water (polar environment) and is usually less lipophilic.

In drug design, balancing lipophilicity and hydrophilicity is crucial to ensure good absorption and distribution in the body.

MEASURING AND PREDICTING LOG P

Experimental Methods: Shake-flask method (gold standard), reversed-phase HPLC.

DFE AS PREDICTOR AND LIPOPHILICITY INTERPRETER IN HYDROCARBONS

In this study, the topological descriptor Degree Factorial Energy (DFE) is evaluated not only as a predictive variable for Log P but also as a structural interpretation scale for lipophilicity across hydrocarbon classes — alkanes, alkenes, and alkynes.

A linear model was developed from experimental Log P data of n-alkanes:

$$Log\ P = 0.02091 \times DFE + 0.588$$

This model was then extended to alkenes and alkynes using their respective DFE definitions:

$$Alkanes: \quad DFE = 26n + 2$$
$$Alkenes: \quad DFE = 26n - 36$$
$$Alkynes: \quad DFE = 26n - 46$$

DFE AS LOG P INTERPRETATION SCALE

Since DFE is linearly related to Log P, it can be used to interpret hydrophobicity in the same way Log P is traditionally used[6].

$$DFE = \frac{(Log\ P - 0.588)}{0.02091}$$

we obtain DFE thresholds that align with standard lipophilicity categories.

Log P Range	DFE Range	Lipophilicity Category
< 1.5	DFE < 43.65	Hydrophilic (water-preferring)
1.5 – 2.5	43.65 – 91.70	Slightly hydrophobic
2.5 – 3.5	91.70 – 139.75	Moderately hydrophobic
3.5 – 4.5	139.75 – 187.80	Hydrophobic
4.5 – 5.5	187.80 – 235.85	Strongly hydrophobic
5.5 – 6.5	235.85 – 283.90	Very lipophilic (oily)
> 6.5	DFE > 283.90	Extremely lipophilic (bio accumulative)

CONCLUSION

In this study, Degree Factorial Energy of various molecular graphs like hydrocarbons and Benzenoid system are obtained and DFE was proposed as a computational descriptor for predicting log P, an important parameter for assessing molecular hydrophobicity. The Degree Factorial Energy (DFE) serves a dual role in quantitative structure–property relationships(QSPR). It predicts Log P through linear model across linear hydrocarbons. It provides a topology-based lipophilicity scale, allowing chemists to interpret DFE directly as an indicator of hydrophobic behaviour.

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