INDEPENDENCE POLYNOMIAL AND CONNECTIVITY - ENERGY QUOTIENT OF ALKANES

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Abstract
In this paper, we attempted to understand the independence polynomial, independence energy, and stability of alkane. We demonstrated that the alkane is stable regardless of the stability measure used. The energy of alkane is more than the double of connectivity index.
Keywords: Independence polynomial; Independence energy; Alkane;Stability.

1.Introduction

Graph representations of molecular structures are extensively used in com- putational chemistry and theoretical chemical research. Chemical graphs were initially used to illustrate molecules by 18(-)19th century scientists such as Higgins, Kopp, and Crum Brown. Molecular structures are represented graphically as graphs, with vertices representing atoms and edges denoting chemical bonds [6].
The number of independent sets in the molecular graph, the graph whose vertices are the molecules' atoms, with two atoms coupled by an edge if they share a bond, has been empirically discovered to be related to the stability and boiling point of specific compounds.
The number of independent vertex sets and the boiling point of certain hy- drocarbons was found to be related by Merrifield and Simmons [7]. The independence number is a predictor of Fullerene stability, according to Fajtlowicz and Larson [3].

2 . Preliminaries

Definition 2.1. [6] The independence polynomial I(G, z) is introduced by I.Gutman and F.Harary in 1983. Let s_k denote the number of independent sets of size k, which are induced sub graphs of then $I(G, z)= \sum_{k=0}^{\alpha(G)} s_k z^k$ where α(G) is the independence number of G.

Definition 2.2. [2] [1, 8] The energy E(G) of G is defined as the sum of the absolute values of the eigenvalues of an adjacency matrix of a graph.$E(G) = \sum_{i=1}^{n} |\lambda i|$.

Definition 2.3. [4] A polynomial P (z) is stable if the zero set of P (z),$Z(P(z)) = \{z \in C/P(z) = 0\} \subseteq \{z \in C/Re(z) \leqslant 0\}$.
As the energy of a graph G is defined in definition 2.2, we define independence energy of a graph G, IE(G) as

Definition 2.4. $IE(G) = \sum_{i=1}^{n} |\lambda i|$ where $\lambda i \in Z(I(G, z))$ and deg(I(G, z)) =n.

The next result gives a recurrence relation which helps us to decompose the independence polynomial of a graph vertex by vertex.

Theorem 2.5. [5] Let G be a simple graph. Let $v \in V(G)$ and N [v] be the closed neighborhood of v. Then I(G; z)=I(G − v; z) + zI(G − N [v]; z).

3. Alkanes

A hydrocarbon, a chemical compound consisting of carbon and hydrogen is an important class of molecules in organic chemistry. There are several sub- classes of hydrocarbons, defined by the saturation and the structure of the carbon atoms. In this paper we will consider alkanes.

A normal alkane is saturated hydrocarobon in which the carbons form a chain. So every atom is bonded to the maximum number of other atoms, the vertices representing carbon atoms have degree four, and those representing hydrogen atoms have degree one. The chemical formula for an alkane is of the form $C_n H_{2n+2}$.

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Number of Carbons	Alkane	Chemical formula
1	Methane	C_1H_4
2	Ethane	C_2H_6
3	Propane	C_3H_8
4	Butane	C_4H_{10}
5	Pentane	C_5H_{12}

Table 1: A table of Alkanes, $n \leq 5$

4. Measures of stability for Alkanes

Stability of hydrocarbon atoms are measured in various ways.We have considered the measures of stability as value of the independence polynomial at −1 and zero set of the polynomial is contained in left half plane.

Value of the independence polynomial at $z = -1$ is also known as alternating number in the literature [1]. The enumeration of independent sets of regular graphs is of interest in Molecular graph theory and statistical mechanics as it corresponds to the solution of hard particle models [14].

Let us tabulate $I(C_nH_{2n+2}, -1)$, whether $I(C_nH_{2n+2}, z)$ is stable or not,energy of C_nH_{2n+2}, independence energy of C_nH_{2n+2}; for $n = 1, 2, 3, 4, 5$.

n	Alkane	$I(C_nH_{2n+2}, -1)$	$I(C_nH_{2n+2}, z)$ is Stable Yes/No	$E(C_nH_{2n+2})$	$IE(C_nH_{2n+2})$
1	Methane	2	yes	4	5.0532
2	Ethane	13.25	yes	7.21	7.4079
3	Propane	4.5	yes	10.362	10.3865
4	Butane	5.75	yes	12.342	12.8662
5	Pentane	7	yes	14.456	16.1384

Based on the alkanes of order $n \leq 5$, we have the following results.

Result 4.1.

1. $I(C_nH_{2n+2}, -1) = 0, \forall n > 1.$
2. $I(C_nH_{2n+2}, z)$ is stable .
3. $IE(C_nH_{2n+2}) > E(C_nH_{2n+2})$.

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We will discuss one more measure of stability known as Randic Index. Randic Index (connectivity index) is a degree based topological index invented in 1976 by M.Randic [9]. Among the graph-based molecular structure descriptors[12, 13] the Randic index is the most widely applied in Chemistry and Pharmocology. Randic index used designing quantitative structure properly and structure activity relations as a measure of stability [11, 4, 5, 10].

Result 4.2. $R\left(C_n H_{2n+2}\right) = \frac{5n+3}{4}$.

Proof. Total number of vertices in $C_n H_{2n+2} = 2n + 2 + n = 3n + 2$. There are only two type of vertices as far as degree is concerned. All the carbon atoms have degree 4 and the hydrogen atomes have degree 1.

Number of vertices with degree 4 = n.

Number of vertices with degree $1 = 3n + 2 - n = 2n + 2$.

Number of edges in $C_n H_{2n+2} = 3n + 1$.

Among these $(3n + 1)$ edges, $(n - 1)$ edges can not between carbons atoms.

Since there are no edges between hydrogens,

$$R\left(C_n H_{2n+2}\right) = \frac{1}{\sqrt{d(u)d(v)}} = \sum_{C_i C_j \in E} \frac{1}{\sqrt{d(C_i)d(C_j)}} + \sum_{C_i H_j \in E} \frac{1}{\sqrt{d(C_i)d(H_j)}}$$

But $\frac{1}{\sqrt{d(C_i)d(C_j)}} = \frac{1}{\sqrt{4.4}} = \frac{1}{4}$ and $\frac{1}{\sqrt{d(C_i)d(H_j)}} = \frac{1}{\sqrt{2.2}} = \frac{1}{2}$

So $R\left(C_n H_{2n+2}\right) = \frac{1}{4}(n - 1) + \frac{1}{2}[(3n + 1) - (n - 1)]$

$= \frac{5n+3}{4}$.

Result 4.3. $\frac{R(C_n H_{2n+2})}{E(C_n H_{2n+2})} \leq \frac{1}{2}$

Proof. We will prove that $E(C_n H_{2n+2}) \geq 2R(C_n H_{2n+2})$.

We prove that for any graph G, $E(G) \geq 2R(G)$.

Let $vivj \in Ej$ the edge set of G.

Define, $f(vivj) = \frac{E(vi)}{d(vi)} + \frac{E(vj)}{d(vj)}$

where $E(vi) = ([A(Gi)][A(Gj)]^*)^{\frac{1}{2}}$ where $E(G) = \sum_{v_i \in V} E\left(v_i\right)$ (where $A(Gi)$ is the adjacency matrix of G and $A(Gj)^*$ is the transpose of $A(Gi)$).

$$\sum_{v_i v_j \in E} f(v_i v_j) = \sum_{v_i v_j \in E} \left[\frac{E(v_i)}{d(v_i)} + \frac{E(v_j)}{d(v_j)}\right] = \sum_{v_i \in V} \sum_{v_j \text{ is adjacent to } v_i} \frac{E(v_i)}{d(v_i)} + \sum_{v_j \in V} \sum_{v_i \text{ is adjacent to } v_j} \frac{E(v_i)}{d(v_i)}$$

$$= \frac{1}{2} \sum_{v_i \in V} E\left(v_i\right) + \frac{1}{2} \sum_{v_j \in V} E\left(v_j\right) = E(G)$$

But $f\left(v_i v_j\right) = \frac{E\left(v_i\right)}{d\left(v_i\right)} + \frac{E(v_j)}{d\left(v_j\right)} \geq 2\sqrt{\frac{E\left(v_i\right)E(v_j)}{d\left(v_i\right)d\left(v_j\right)}} \geq 2\sqrt{\frac{1}{d\left(v_i\right)d\left(v_j\right)}}$ $(since\ E\left(v_i\right)E(v_j) \geq 1)$

$$E(G) = \sum_{v_i v_j \in E} f(v_i v_j) \geq 2 \sum_{v_i v_j \in E} \sqrt{\frac{1}{d\left(v_i\right)d\left(v_j\right)}} = 2\,R(G)$$

Hence $\frac{R(G)}{E(G)} \leq \frac{1}{2}$.

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Corollary 4.4. $E(C_nH_{2n+2}) \geq \frac{5n+3}{2}$ *with equality only when* $n = 1$.

Proof. $R(C_nH_{2n+2}) = \frac{5n+3}{2}$

$\therefore E(C_nH_{2n+2}) \geq \frac{5n+3}{2}$ (by the above result)

5. Conclusion

The independence polynomial of alkanes not only enriches our understand- ing of the combinatorial aspects of these molecules but also bridges the gap between chemistry and graph theory. The polynomial's unique properties, particularly the evaluation at $z = 1$ resulting in zero, emphasize the structural balance inherent in alkane molecules. This intersection of disciplines opens new avenues for research, facilitating advancements in molecular classification and enhancing our comprehension of complex chemical systems through a mathematical lens.
In this paper we tried to get a glimpse of the stability of Alkanes by various measures of stability. Whatever be the measure of stability, it is found that C_nH_{2n+2} is stable. We have also prove that energy of Alkanes(as structure is concerned)is more than the double of connectivity index.

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