Wiener Index of Degree Splitting Graph of some Hydrocarbons

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ABSTRACT
In quantum chemistry, the physico–chemical properties of chemical compounds are often modeled by means of molecular–graph–based structure–descriptors, which are also referred to as topological indices. One of the most widely known topological descriptors is Wiener index. It is named after chemist Harold Wiener who introduced in the year 1947. It is defined by the sum of the distances between all (ordered) pairs of vertices of G. In this paper, we find the Wiener index of degree splitting of some aliphatic and aromatic hydrocarbons and classify its characterization using MATLAB.

Keywords
Hydro Carbons, Wiener Index, MATLAB

2010 Mathematics subject classification: 05C12, 05C85

1. INTRODUCTION
The Wiener index **W(G)** is a distance-based topological invariant much used in the study of the structure-property and the structure-activity relationships of various classes of biochemically interesting compounds introduced by Harold Wiener in 1947 for predicting boiling points of alkanes based on the formula

$$b.p = \alpha W + \beta w(3) + \gamma$$

Where α, β, γ are empirical constants, and w(3) is called path number. [9]
It is defined as the half sum of the distances between all pairs of vertices of G.

$$W(G) = \frac{1}{2}\sum_{u,v\in G} d(u,v)$$

Where d(u,v) is the number of edges in a shortest path connecting the vertices u & v in G.[10]

Notation:

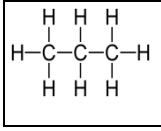
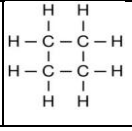
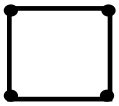
$$W(G) = \frac{1}{2}\sum_{u,v\in G} d(u,v) = \sum_{u<v} d(u,v) = \sum_{i<j} d(u_i,u_j)$$

Suppose chemical reaction is represented as the transformation of the chemical graph representing the The calculation of HMO total π-energy (that is, E) is not an easy task. The numerical work of this paper is based on [8]. The eigenvalues of the adjacency matrix of G are usually called to be the eigenvalues of G Let $\lambda_1, .., \lambda_n$ be the eigen values of G then **Energy** of the graph G is defined by

reaction's substrate into another chemical graph representing the degree splitting, the graph obtained in this manner may or may not exist in reality, but it is in the interest of the chemist to check the characterization of the so obtained new molecular structure. In this paper, we characterize the resultant degree splitting of some hydro carbons. The Wiener index W and the spectral radius λ_1 are popular topological indices. Finding the relation between W and λ_1 are very much used for modeling of properties of many types of chemical compounds. The vast majority of molecules of interest in chemistry are cyclic. Therefore finding relation between W and λ_1 is important not only in the case of alkanes, but also for other classes of organic compounds. The structural dependence of *W* and (separately) of λ_1 of benzenoid hydrocarbons was studied previously. In 2008, Slavko Radenković S and Ivan Gutman have discussed the relation between *W* and λ_1 for some alkanes and benzenoid molecules.[3], [7]

2. DEFINITIONS AND PRELIMINARIES
Our notation is standard and mainly taken from standard books of graph theory. We consider finite, nontrivial, simple and undirected graphs only. For a graph G, we denote by V(G) and E(G), its vertex and edge sets, respectively. Degree splitting graph DS(G) was introduced by R. Ponraj and S. Somasundaram. Let G = (V;E) be a graph with V = $S_1 \cup S_2 \cup \ldots\ldots\ldots \cup S_t \cup T$, where each S_i is a set of vertices having at least two vertices and having the same degree and T = V- $\cup S_i$. The degree splitting graph of G denoted by DS(G) is obtained from G by adding vertices $w_1, w_2, \ldots\ldots, w_t$ and joining w_i to each vertex of S_i $(1 \le i \le t)$. [4], [5], [6]

Fig.1

Molecular Structure of Propane	Molecular Graph (G)	Molecular Structure of Cyclo Butane	Degree splitting of G DS(G)
			

$E(G)=\sum_{i=1}^{n}|\lambda_i|$. A graph G on n vertices is said to be **hyper energetic** if E(G) > 2n – 2 and **hypo energetic** if E(G) < n.

The largest eigenvalue of G, referred to as the **spectral radius** of G, will be labeled by λ_1. Using λ_1 as a measure of branching was proposed by one of the present authors as early as in 1977. For decades this branching index has not attracted much attention of theoretical chemists. Recently, studies of the spectral radius as the measure of branching became attractive again. W depends on the size (number of carbon atoms) of the molecules examined, it is purposeful to restrict the consideration to classes of alkane isomers. Our investigation of the relation between W and λ_1 is being performed on certain class of degree splitting molecular graphs with the respective molecular graph.

In general, an Organic compound containing only carbon and hydrogen is called hydro carbons. Hydrocarbons without benzene rings and with benzene rings are called aliphatic and aromatic hydrocarbons respectively. Aliphatic hydrocarbons are classified into acyclic and cyclic hydrocarbons. In chemical graph theory, an acyclic hydrocarbon means that chemical tree. (ie) A chemical tree is tree in which no vertex has more than four neighbours.

3. WIENER INDICES OF G AND DS(G) FOR SOME ALIPHATIC HYDROCARBONS

3.1. Comparative study between Wiener indices of G and DS (G) for acyclic hydrocarbons

The results obtained for the Wiener index of G and Wiener index of degree splitting of G are given in Table 1. We have calculated and tabulated the Wiener indices, Spectral radius, Energy level (for both G and DS(G)) for acyclic hydro carbons.

The Wiener index of the molecular graph DS(G) of the 32 acyclic hydrocarbons with E, λ_1

Table 1

No. of carbon atoms	Hydro Carbon	W(G)	Energy Level of W(G)	Spectral Radius of (G)	W(DS(G))	Energy Level of W(DS(G))	Spectral Radius of DS(G)
1	Methane	-			-	-	-
2	Ethane	1	Non Hyper energetic Non Hypo energetic	1.0	3	Hyper energetic Non Hypo energetic	2.0
3	Propane	4	Non Hyper energetic Hypo energetic	1.40	8	Non Hyper energetic Non Hypo energetic	2.0
4	Butane	10	Non Hyper energetic Non Hypo energetic	1.61	24	Hyper energetic Non Hypo energetic	2.43
4	2-Methylpropane	9	Non Hyper energetic Hypo energetic	1.73	14	Non Hyper energetic Hypo energetic	2.44
5	Pentane	20	Non Hyper energetic Non Hypo energetic	1.73	37	Hyper energetic Non Hypo energetic	2.76
5	2-Methylbutane	18	Non Hyper energetic Non Hypo energetic	1.8	23	Non Hyper energetic Non Hypo energetic	2.39
5	2.2-Dimethylpropane	16	Hyper energetic Non Hypo energetic	2.00	22	Non Hyper energetic Hypo energetic	2.82
6	Hexane	35	Hyper energetic Non Hypo energetic	1.80	52	Hyper energetic Non Hypo energetic	3.04
6	2-Methylpentane	32	Non Hyper energetic Non Hypo energetic	1.90	53	Non Hyper energetic Non Hypo energetic	2.57
6	3-Methylpentane	31	Non Hyper energetic Non Hypo energetic	1.93	50	Non Hyper energetic Non Hypo energetic	2.56
6	2,2-Dimethylbutane	28	Non Hyper energetic Hypo energetic	2.07	33	Non Hyper energetic Non Hypo energetic	2.75
6	2,3-Dimethylbutane	29	Non Hyper energetic Non Hypo energetic	2.00	46	Non Hyper energetic Non Hypo energetic	2.80
7	Heptane	56	Non Hyper energetic Non Hypo energetic	1.87	70	Hyper energetic Non Hypo energetic	3.29
7	2-Methylhexane	52	Non Hyper energetic Non Hypo energetic	1.93	72	Non Hyper energetic Non Hypo energetic	2.80
7	3-Methylhexane	50	Non Hyper energetic Non Hypo energetic	1.96	54	Non Hyper energetic Non Hypo energetic	2.31
7	2,2-Dimethylpentane	46	Non Hyper energetic Hypo energetic	2.10	69	Non Hyper energetic Non Hypo energetic	2.81
7	2,3-Dimethylpentane	46	Non Hyper energetic Non Hypo energetic	2.05	65	Non Hyper energetic Non Hypo energetic	2.88
7	2,4-Dimethylpentane	48	Non Hyper energetic Hypo energetic	2.00	66	Non Hyper energetic Non Hypo energetic	2.82

7	3,3-Dimethylpentane	44	Non Hyper energetic Non Hypo energetic	2.13	65	Non Hyper energetic Non Hypo energetic	2.82
7	3 Ethylpentane	48	Non Hyper energetic Non Hypo energetic	2.00	72	Non Hyper energetic Non Hypo energetic	2.5
7	2,2,3-Trimethebutane	42	Non Hyper energetic Hypo energetic	2.17	45	Non Hyper energetic Non Hypo energetic	2.97
8	Octane	84	Non Hyper energetic Non Hypo energetic	1.87	90	Hyper energetic Non Hypo energetic	3.51
8	2,2,3,3-Trimethylbutane	58	Non Hyper energetic Hypo energetic	2.30	76	Non Hyper energetic Non Hypo energetic	3.40
8	3-Ethyl-2-methylpentane	67	Non Hyper energetic Non Hypo energetic	2.92	114	Non Hyper energetic Non Hypo energetic	2.92
8	3-Ethylhexane	72	Non Hyper energetic Non Hypo energetic	2.02	88	Non Hyper energetic Non Hypo energetic	2.98
8	3-Methylheptane	76	Non Hyper energetic Non Hypo energetic	1.99	89	Non Hyper energetic Non Hypo energetic	3.00
8	4-Methylheptane	75	Non Hyper energetic Non Hypo energetic	2.00	88	Non Hyper energetic Non Hypo energetic	2.99
8	2,2-Dimethylhexane	71	Non Hyper energetic Non Hypo energetic	2.92	91	Non Hyper energetic Non Hypo energetic	2.92
8	2,3-Dimethylhexane	70	Non Hyper energetic Non Hypo energetic	2.92	116	Non Hyper energetic Non Hypo energetic	2.92
8	2,4-Dimethylhexane	71	Non Hyper energetic Non Hypo energetic	2.04	111	Non Hyper energetic Non Hypo energetic	2.89
8	2,5-Dimethylhexane	74	Non Hyper energetic Non Hypo energetic	2.00	113	Non Hyper energetic Non Hypo energetic	2.87

We deem that these data will suffice for practically all imaginable considerations in chemical graph theory. The most remarkable feature seen in Table-1 is the fact that degree splitting of the acyclic Hydrocarbons will be cyclic and spectral radius of G & DS(G) variation increases maximum by one. The practical importance of this finding is that almost all degree splitting of acyclic molecules are Non Hypo energetic whatever G is Hypo energetic or not.

4. WIENER INDICES OF DEGREE SPLITTING OF SOME POLYCYCLIC AROMATIC HYDROCARBONS

In this section, we analyze the characterization between poly cyclic aromatic benzenoid hydrocarbons and degree splitting of some poly cyclic aromatic benzenoid hydrocarbons (both cata-condensed, not cata condensed). The Characteristic graph of a given benzenoid graph(cyclic graph) consists of vertices corresponding to hexagon(cycle) of the graph; two vertices are adjacent if the corresponding hexagons (cycle) share an edge. The benzenoid graph (cyclic) is called Cata-condensed if its Characteristic graph is a tree.[1], [2] To analyze the characterization between the molecules, we have taken the sample set of 12 poly cyclic benzenoid molecules (6 cata condensed, 6 not cata condensed).

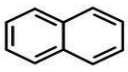
Molecular Structure of Naphthalene	Molecular Graph(G) (Cata-condensed)
	

Fig.2

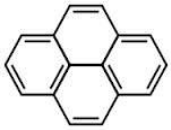
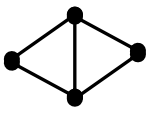
Molecular Structure of Pyrene	Molecular Graph(G) (Not Cata-condensed)
	

Fig.3

4.1. Wiener Indices of Degree Splitting of Some Poly Cyclic Aromatic Hydrocarbons (CATA- Condensed)

The results obtained for the Wiener index of G and Wiener index of degree splitting of G are given in Table 2. In additional, we tabulated the Spectral radius, Energy level (for both G and DS(G)) for polycyclic (cata condensed) aromatic hydrocarbons

The Wiener index of the DS(G) of the 6 polycyclic aromatic hydrocarbons (Cata-condensed) with E, λ_1

Table 2

No. of carbon atoms	Hydro Carbon	W(G)	Energy Level of W(G)	Spectral Radius of (G)	W(DS(G)	Energy Level of W(DS(G))	Spectral Radius of DS(G)
12	Biiphenylene	180	Non Hyper energetic Non Hypo energetic	2.5321	177	Hyper energetic Non Hypo energetic	4.0000
13	Fluorene	219	Non Hyper energetic Non Hypo energetic	2.4687	205	Hyper energetic Non Hypo energetic	4.1227
18	Napththacene	633	Non Hyper energetic Non Hypo energetic	2.3007	400	Non Hyper energetic Non Hypo energetic	4.4260
24	Tetraphenylene	1080	Non Hyper energetic Non Hypo energetic	2.5321	703	Non Hyper energetic Non Hypo energetic	5.0314
26	Hexacene	1637	Non Hyper energetic Non Hypo energetic	2.5129	820	Non Hyper energetic Non Hypo energetic	5.0817
30	Heptacene	2479	Non Hyper energetic Non Hypo energetic	2.5243	1095	Non Hyper energetic Non Hypo energetic	5.3288

4.2. Wiener Indices of Degree Splitting of Poly Cyclic Aromatic Hydrocarbons (Not CATA-Condensed)

Here, we have tabulated the Wiener index, Spectral radius, Energy level (for both G and DS(G)) for polycyclic (not cata condensed) aromatic hydrocarbons.

The Wiener index of the DS(G) of the 6 polycyclic aromatic hydrocarbons (Not Cata-condensed) with E, λ_1

Table3.

No. of carbon Atoms	Hydro Carbon	W(G)	Energy Level of W(G)	Spectral Radius of (G)	W(DS(G))	Energy Level of W(DS(G))	Spectral Radius of DS(G)
12	Acenaphthene	166	Non Hyper energetic Non Hypo energetic	2.4708	174	Hyper energetic Non Hypo energetic	4.0000
13	Phenalene	210	Non Hyper energetic Non Hypo energetic	2.4495	205	Hyper energetic Non Hypo energetic	4.1226
18	Pleiadene	519	Non Hyper energetic Non Hypo energetic	2.4815	395	Hyper energetic Non Hypo energetic	4.5443
24	Coronene	1002	Non Hyper energetic Non Hypo energetic	2.6751	721	Non Hyper energetic Non Hypo energetic	5.0000
26	Rubicene	1314	Non Hyper energetic Non Hypo energetic	2.6153	863	Non Hyper energetic Non Hypo energetic	5.0651
30	Pyranthrene	2043	Non Hyper energetic Non Hypo energetic	2.6608	1130	Non Hyper energetic Non Hypo energetic	5.3430

From 4.1 and 4.2., we see that there is no much difference of the topological index λ_1 of degree splitting of polycyclic aromatic hydrocarbons between Cata-condensed and not Cata-condensed. But topological index λ_1 of degree splitting of polycyclic aromatic hydrocarbons is twice as λ_1 of polycyclic aromatic hydrocarbons (Cata-condensed and not Cata-condensed). Energy level of polycyclic aromatic hydrocarbons (both Cata-condensed and not Cata-condensed) and degree splitting of polycyclic aromatic hydrocarbons (both Cata-condensed and not Cata-condensed) are non hypo energetic. But Energy level of some degree splitting of polycyclic aromatic hydrocarbons (both Cata-condensed and not Cata-condensed) becomes hyper energetic.

5. CONCLUSION

In this paper, we have examined the Wiener index of degree splitting of various hydro carbons and have classified its characterization like Energy, Spectral radius with hydro carbons using MATLAB.

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