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A MATHEMATICAL APPROACH TO FIND THE RELATIONSHIP BETWEEN THE WIENER NUMBERS OF ISOMERS OF PENTANE (C_5H_{12}) AND HEXANE (C_6H_{14}) AND ITS PHYSICAL PROPERTIES

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Abstract:
In molecular graph theory, the Wiener index or Wiener number is a topological invariant of a molecule which depends on its structure and it is defined as the sum of the lengths of the shortest paths between every pairs of vertices in the molecular graph representing the non-hydrogen atoms of the molecule. The term isomer is used for molecules having same molecular formula but different structural arrangement of the hydrocarbon main chain and the respective functional groups. In this paper, we prove that there is a high positive correlation between the topological invariants and the physical properties of isomers of Pentane (C5H12) and Hexane (C6H14).

Keywords: Molecular graph, Wiener number, isomers, Pentane, Hexane.

2010 Mathematics Subject Classification: 92E10, 11CXX, 05CXX, 05C07, 05C10, 05C12.

1. INTRODUCTION

The applications of graph theory are not restricted only to mathematics. Graph theory and mathematical modelling can be combined to study various chemical phenomena like characterization and identification of chemical compounds. Alkanes are organic chemical compounds that consist only of the elements carbon (C) and hydrogen (H) in proportions according to the general formula: $\mathbf{C_nH_{2n+2}}$ where the letter *n* represents the number of carbon atoms in each molecule. The atoms that form alkanes are linked exclusively by single bonds, hence alkanes are saturated hydrocarbons.

In general, there are three basic types of alkanes: linear Alkanes, branched alkanes and cyclic alkanes. Of these linear alkanes are the simplest to draw and explain. And therefore this research is restricted to these types of alkanes.

One example of an alkane is hexane, shown in Figure 1. Each carbon atom has four chemical bonds and each hydrogen atom has one chemical bond. Therefore, the hydrogen atoms can be removed without losing information about the molecule. This carbon tree can be represented as a graph by replacing the carbon atoms with vertices. Chemical bonds are then represented as an edge in the graph. Figure 2 shows the graphical representation of hexane composed of six vertices connected by a single edge.

Representation of an object giving information only about the number of elements composing it and their connectivity is named as topological representation of an object. A topological representation of a molecule is called molecular graph.

A molecular graph is a collection of points representing the atoms in the molecule and set of lines representing the covalent bonds.

C——C——C——C— C——C

Figure 1: Carbon tree of hexane

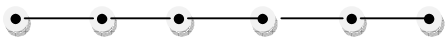


Figure 2: Carbon tree of hexane as a graph

The structure of alkanes determines its physical properties. The well-known and oldest graph matrices are the adjacency matrix, introduced by Poincare for Characterizing of labyrinths [1]. In more Recent time, with the growth of chemical graph theory, additional graph matrices have been introduced like: the wiener matrix [2-7]; the path –Wiener matrix [8]; the Szeged matrix and the revised Szeged matrix [9];the distance matrix [10]. Chemists make use of many quantities associated with molecular graph to estimate various physical properties like melting point, boiling point, etc. The Wiener Index also known as the "sum of distances", is one of the oldest method associated with the process of determining these physical properties. In general, the Wiener Index measures how compact a molecule is for its given weight. It therefore has predictive value and chemists and physicists have found many such uses for the Wiener Index.

2. PRELIMINARIES

2.1 Wiener Number of a Graph *G*

For a connected graph *G* with *n* vertices, denoted by 1, 2,..., *n*, let $W_k = \sum_{i<j,dij=k} d_{ij}, k = 1,2,....$ The vector (W_1, W_2, ...) is called the Wiener Vector of *G*, denoted by *WV* (*G*).Clearly; the sum of all components of the Wiener vector of *G* is just equal to the Wiener number of *G*.

2.2 Procedure for finding the D_M – matrix of a graph

Step 1:

Calculate D_S –Matrix for the graphs of Hexane isomers where D_S is the distance matrix and R_p is the greatest element in the p^{th} row of D_S , C_q is the greatest element in the q^{th} column of D_S.

Step 2:

Find D_M – Matrix for the molecular graphs considered by using the conditions below

$$(D_M)_{pq} = (D_S)_{pq} \quad \text{if} \quad (D_S)_{pq} \geq \min\{R_p, C_q\}$$

$(D_M)_{pq} = 0$ if $(D_S)_{pq} < \min\{R_p, C_q\}$

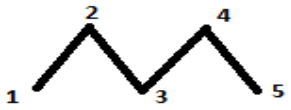
2.3 Notations

The number of non-zero entries above the main diagonal in D_M of smaller alkanes (N_E); the sum of non-zero entries above the main diagonal ($\sum PD_M$); the quotient $\sum PD_M / N_E$ giving the average matrix element (Q_w); partition of $\sum PD_M$ coming from distances of decreasing length (π_P);Ordered row sums(P) ; Wiener number (W), P = $\sum 2PD_M$; Boiling point B_p; Melting point M_p; Density D.

3. MAIN RESULTS

3.1 Evaluation of D_S – Matrices and D_M –Matrices

Pentane



D_S-Matrix

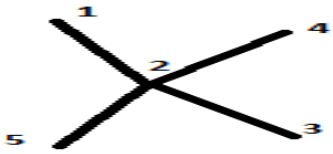
$$\begin{pmatrix} 0 & 1 & 2 & 3 & 4 \\ 1 & 0 & 1 & 2 & 3 \\ 2 & 1 & 0 & 1 & 2 \\ 3 & 2 & 1 & 0 & 1 \\ 4 & 3 & 2 & 1 & 0 \end{pmatrix} \begin{matrix} 10 \\ 6 \\ 3 \\ 1 \\ 0 \end{matrix}$$

D_M - Matrix

$$\begin{pmatrix} 0 & 0 & 2 & 3 & 4 \\ 0 & 0 & 0 & 0 & 3 \\ 2 & 0 & 0 & 0 & 2 \\ 3 & 0 & 0 & 0 & 0 \\ 4 & 3 & 2 & 0 & 0 \end{pmatrix} \begin{matrix} 9 \\ 3 \\ 4 \\ 3 \\ 9 \end{matrix}$$

N_E=5, $\sum PD_M$ =14, Q_W=2.8 , π_P= 1,2,2 , $P = \sum 2PD_M = 28$, $W = 20$

2,2 Dimethyl propane (Neopentane)



D_S-Matrix

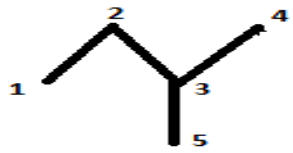
$$\begin{pmatrix} 0 & 1 & 2 & 2 & 2 \\ 1 & 0 & 1 & 1 & 1 \\ 2 & 1 & 0 & 2 & 2 \\ 2 & 1 & 2 & 0 & 2 \\ 2 & 1 & 2 & 2 & 0 \end{pmatrix} \begin{matrix} 7 \\ 3 \\ 4 \\ 2 \\ 0 \end{matrix}$$

D_M - Matrix

$$\begin{pmatrix} 0 & 1 & 2 & 2 & 2 \\ 1 & 0 & 1 & 1 & 1 \\ 2 & 1 & 0 & 2 & 2 \\ 2 & 1 & 2 & 0 & 2 \\ 2 & 1 & 2 & 2 & 0 \end{pmatrix} \begin{matrix} 7 \\ 3 \\ 4 \\ 2 \\ 0 \end{matrix}$$

N_E= 10, $\sum PD_M$ =16, Q_W=1.6, π_P= 6,4, $P = \sum 2PD_M = 32$ $W = 16$

2-Methylbutane



D_S**-Matrix**

$$\begin{pmatrix} 0 & 1 & 2 & 3 & 3 \\ 1 & 0 & 1 & 2 & 2 \\ 2 & 1 & 0 & 1 & 1 \\ 3 & 2 & 1 & 0 & 2 \\ 3 & 2 & 1 & 2 & 0 \end{pmatrix} \begin{matrix} 9 \\ 5 \\ 2 \\ 2 \\ 0 \end{matrix}$$

D_M **- Matrix**

$$\begin{pmatrix} 0 & 0 & 2 & 3 & 3 \\ 0 & 0 & 0 & 2 & 2 \\ 2 & 0 & 0 & 0 & 0 \\ 3 & 2 & 0 & 0 & 0 \\ 3 & 2 & 0 & 0 & 0 \end{pmatrix} \begin{matrix} 8 \\ 4 \\ 2 \\ 5 \\ 5 \end{matrix}$$

N_E=5, $\sum PD_M$ =12, Q_W=2.6 , π_P= 2,3, $P = \sum 2PD_M = 24$, $W = 18$

Table 1:

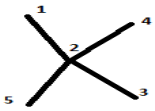
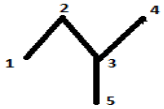
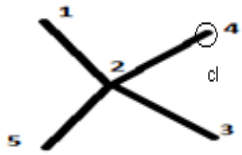
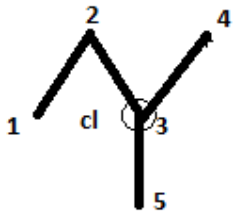
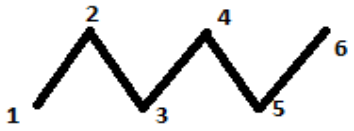
Alkanes	Diagram	W	P	Boiling point	Melting point	Density
Pentane		20	28	309.25K	143.3K	626Kg/m^3
2,2 -Dimethyl propane		16	32	282.65K	256.6K	601.17Kg/m^3
2-Methyl butane		18	24	300.95K	112.1K	616Kg/m^3

Table 2:

Chloroalkane	Diagram	W	P	Boiling point	Melting point	Density
1ChloroPentane		20	28	380.35K	174.15K	0.9g/cm^3
1Chloro 2,2 -Dimethyl Propane		16	32	357.15K	253.15K	0.85 g/cm^3
2 Chloro 2-Methyl butane		18	24	358.15K	200.15K	0.87 g/cm^3

3.2 Evaluation of D_S – Matrices and D_M –Matrices of Hexane Isomers

Hexane



D_S-Matrix

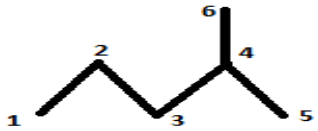
$$\begin{pmatrix} 0 & 1 & 2 & 3 & 4 & 5 & 15 \\ 1 & 0 & 1 & 2 & 3 & 4 & 10 \\ 2 & 1 & 0 & 1 & 2 & 3 & 6 \\ 3 & 2 & 1 & 0 & 1 & 2 & 3 \\ 4 & 3 & 2 & 1 & 0 & 1 & 1 \\ 5 & 4 & 3 & 2 & 1 & 0 & 0 \end{pmatrix}$$

D_M - Matrix

$$\begin{pmatrix} 0 & 0 & 0 & 3 & 4 & 5 & 12 \\ 0 & 0 & 0 & 0 & 0 & 4 & 4 \\ 0 & 0 & 0 & 0 & 0 & 3 & 3 \\ 3 & 0 & 0 & 0 & 0 & 0 & 3 \\ 4 & 0 & 0 & 0 & 0 & 0 & 4 \\ 5 & 4 & 3 & 0 & 0 & 0 & 12 \end{pmatrix}$$

N_E=5, $\sum PD_M$ =19, Q_W=3.8, π_P= 1,2,2, P= $\sum 2PD_M = 38$ $W = 35$

2-Methylpentane



D_S- Matrix

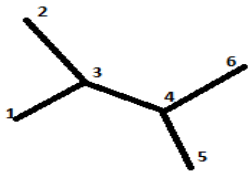
$$\begin{pmatrix} 0 & 1 & 2 & 3 & 4 & 4 & 14 \\ 1 & 0 & 1 & 2 & 3 & 3 & 9 \\ 2 & 1 & 0 & 1 & 2 & 2 & 5 \\ 3 & 2 & 1 & 0 & 1 & 1 & 2 \\ 4 & 3 & 2 & 1 & 0 & 2 & 2 \\ 4 & 3 & 2 & 1 & 2 & 0 & 0 \end{pmatrix}$$

D_M - Matrix

$$\begin{pmatrix} 0 & 0 & 2 & 3 & 4 & 4 & 13 \\ 0 & 0 & 0 & 0 & 3 & 3 & 6 \\ 2 & 0 & 0 & 0 & 2 & 2 & 6 \\ 3 & 0 & 0 & 0 & 0 & 0 & 3 \\ 4 & 3 & 2 & 0 & 0 & 0 & 9 \\ 4 & 3 & 2 & 0 & 0 & 0 & 9 \end{pmatrix}$$

N_E=8, $\sum PD_M$ =23, Q_W = 2.875, π_P= 2,3,3, $P = \sum 2PD_M = 46$ $W = 32$

2, 3-Dimethylbutane



D_S-Matrix

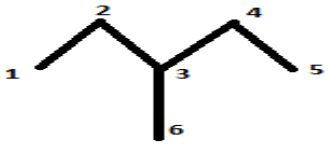
$$\begin{pmatrix} 0 & 2 & 1 & 2 & 3 & 3 & 11 \\ 2 & 0 & 1 & 2 & 3 & 3 & 9 \\ 1 & 1 & 0 & 1 & 2 & 2 & 5 \\ 2 & 2 & 1 & 0 & 1 & 1 & 2 \\ 3 & 3 & 2 & 1 & 0 & 2 & 2 \\ 3 & 3 & 2 & 1 & 2 & 0 & 0 \end{pmatrix}$$

D_M - Matrix

$$\begin{pmatrix} 0 & 0 & 0 & 2 & 3 & 3 & 8 \\ 0 & 0 & 0 & 2 & 3 & 3 & 8 \\ 0 & 0 & 0 & 0 & 2 & 2 & 4 \\ 2 & 2 & 0 & 0 & 0 & 0 & 4 \\ 3 & 3 & 2 & 0 & 0 & 0 & 8 \\ 3 & 3 & 2 & 0 & 0 & 0 & 8 \end{pmatrix}$$

N_E=8, $\sum PD_M$ =20, Q_W = 2.5, π_P= 4,4, $P = \sum 2PD_M = 40$, $W = 29$

3-Methylpentane

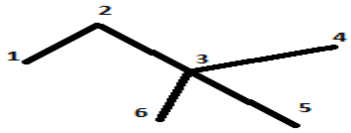


***D_S*-Matrix** ***D_M* - Matrix**

$$\begin{pmatrix} 0 & 1 & 2 & 3 & 4 & 3 \\ 1 & 0 & 1 & 2 & 3 & 2 \\ 2 & 1 & 0 & 1 & 2 & 1 \\ 3 & 2 & 1 & 0 & 1 & 2 \\ 4 & 3 & 2 & 1 & 0 & 3 \\ 3 & 2 & 1 & 2 & 3 & 0 \end{pmatrix} \begin{matrix} 13 \\ 8 \\ 4 \\ 3 \\ 3 \\ 0 \end{matrix} \qquad \begin{pmatrix} 0 & 0 & 2 & 3 & 4 & 3 \\ 0 & 0 & 0 & 0 & 3 & 0 \\ 2 & 0 & 0 & 0 & 2 & 0 \\ 3 & 0 & 0 & 0 & 0 & 0 \\ 4 & 3 & 2 & 0 & 0 & 3 \\ 3 & 0 & 0 & 0 & 3 & 0 \end{pmatrix} \begin{matrix} 12 \\ 3 \\ 4 \\ 3 \\ 12 \\ 6 \end{matrix}$$

N_E=7, $\sum PD_M$ =20, Q_W =2.8571, π_P= 1,4,2, $P = \sum 2PD_M = 40$ $W = 31$

2,2-Dimethylbutane



***D_S*-Matrix** ***D_M* - Matrix**

$$\begin{pmatrix} 0 & 1 & 2 & 3 & 3 & 3 \\ 1 & 0 & 1 & 2 & 2 & 2 \\ 2 & 1 & 0 & 1 & 1 & 1 \\ 3 & 2 & 1 & 0 & 2 & 2 \\ 3 & 2 & 1 & 2 & 0 & 2 \\ 3 & 2 & 1 & 2 & 2 & 0 \end{pmatrix} \begin{matrix} 12 \\ 7 \\ 3 \\ 4 \\ 2 \\ 0 \end{matrix} \qquad \begin{pmatrix} 0 & 0 & 2 & 3 & 3 & 3 \\ 0 & 0 & 0 & 2 & 2 & 2 \\ 2 & 0 & 0 & 0 & 0 & 0 \\ 3 & 2 & 0 & 0 & 0 & 0 \\ 3 & 2 & 0 & 0 & 0 & 0 \\ 3 & 2 & 0 & 0 & 0 & 0 \end{pmatrix} \begin{matrix} 11 \\ 6 \\ 2 \\ 5 \\ 5 \\ 5 \end{matrix}$$

N_E=7, $\sum PD_M$ =17, Q_W =2.4285, π_P= 3,4, $P = \sum 2PD_M = 34$ $W = 28$

Table 3:

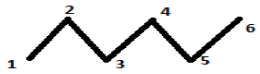
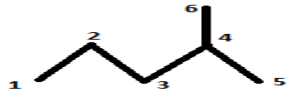
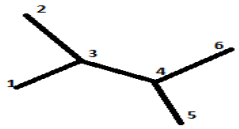
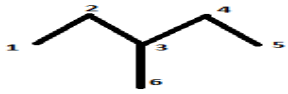
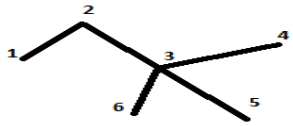
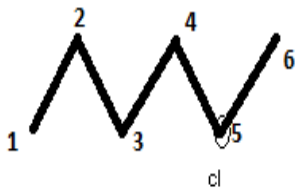
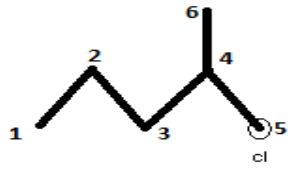
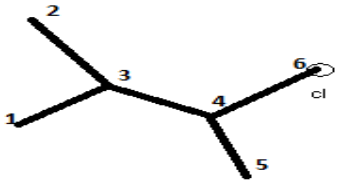
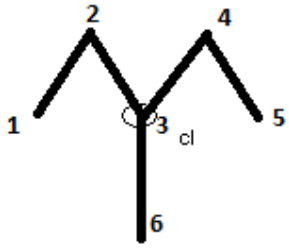
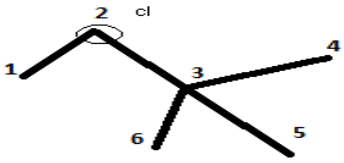
Alkanes	Structure	W	P	Boiling point(B_P)
Hexane		35	38	341.15K
2-Methyl pentane		32	46	333.15K
2,3-Dimethylbutane		29	40	331.05K
3-Methylpentane .		31	40	336.15K
. 2,2-Dimethylbutane		28	34	322.85K

Table 4:

Chloroalkanes	Structure	Boiling point (B_P)	W	P	M_P	D
2Chlorohexane		398.15K	35	38	238.05	0.87

1Chloro 2-Methyl Pentane		398.15K	32	46	238.05	0.88
1 Chloro 2,3-Dimethylbutane		390.85K	29	40	238.05	0.9
3 Chloro 3-Methylpentane		387.55K	31	40	238.05	0.9
3 chloro 2,2-Dimethylbutane		384.15K	28	34	272.15	0.9

4. CONCLUSION

The comparative study between the various physical properties and the topological invariants of pentane and hexane is performed. The Correlation coefficient '*r*' between Weiner Number *W* and Boiling Point B_P of alkanes of Pentane is 0.98; Correlation coefficient '*r*' between Weiner Number *W* and *D* of alkanes of Pentane is 1.0; Correlation coefficient '*r*' between Weiner Number *W* and Melting point M_P of alkanes of Pentane is 0.94; Correlation coefficient '*r*' between Weiner Number *W* and B_P of Chloroalkanes is 0.88; Correlation coefficient '*r*' between *P* and M_P of Chloroalkanes is 0.65; Correlation coefficient '*r*' between Weiner Number *W* and *D* of Chloroalkanes is 0.8; Correlation Between Weiner Number and Boiling Point of Hexa-alkanes is 0.9; Correlation Between Weiner Number and Boiling Point of Hexa-Chloroalkanes is 0.82. From the above process it can be seen that the topological invariants play a vital role in the study of the physical properties of compounds and their pharmaceutical inventions.

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