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STATISTCAL STUDY OF TOPOLOGICAL INDICES OF ISOMERS OF OCTANE

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ABSTRACT

A topological index is a numerical parameter, mathematically derived from the graph structure. Graph is a set V of elements (v_i) called vertices and set E of elements (e_i) called edges, that couple two distinct vertices. Correlation and regression of physico-chemical properties of isomers of octane are investigated.

Keywords: Reciprocal distance matrix, molecular graph, isomers of octane, correlation.

1. INTRODUCTION

A molecular graph can be represented by a number, sequence of numbers, matrix or polynomial [1].The importance of graph theory for chemistry stems from the existence of phenomenon of isomerism, which is rationalized by chemical structure theory [2].The distance between two distinct vertices of graph, u and v, written as d (u, v) is the smallest length of path between them in graph [3]. The reciprocal distance matrix of a graph G with N-vertices R D (G) = R D, is a square n*n symmetric matrix whose entries $(RD)_{ij}$ are equal to the reciprocal of the distance between vertices i and j for non-diagonal elements and are equal to zero , for the diagonal elements , [4,5].

$(RD)_{Ij} = 0$ for $i = j$

and $= d_{ij}^{-1}$ for $i \neq j$

Reciprocal distance matrix allows the calculation of a Wiener number, analogue called Harare index [6].Regression involves comparison between two or more variables .It is basis of correlation analysis. Two variables are said to be correlated when the movements or changes in one are followed directly or indirectly by movements or changes in the other and when the greater the magnitude of change in one, the greater it is other, also. For practical purposes, topological indices having the absolute value of the correlation coefficient less than 0.8 are characterized as useless. The standard formulae for coefficient of correlation and regression equations given by Elhance and H.K.Das [7, 8] and source data for reciprocal degree distance, acentric factor and entropy (s) of the octane isomers [5], are used for calculations. In this paper the coefficient of correlation, regression equations, standard error of coefficient of correlation of isomers of octane are computed.

2. RESULTS AND DISCUSSION

Hydrogen suppressed molecular graph is constructed by representing each atom of a molecule by a vertex and bonds between atoms by edges. The molecular graph of octane with vertex degree indicated and of 2,2,3,3-tetramethyl butane are shown in fig.(1) (a), (b) .

The values of reciprocal degree distance, acentric factor and entropy (s) of isomers of octane are represented in table (1), source data [5].The reciprocal distance matrix of a square matrix for

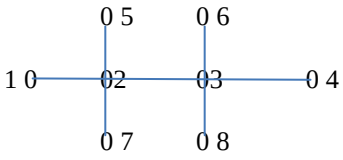
2,2,3,3-tetramethyl butane is represented in fig.(2).The computed values of r,r^2 , $b_{x\ y}$, $b_{y\ x}$,standard error of the coefficient of correlation, standard error of the regression coefficient of y on x ,and regression equations of acentric factor and entropy are given in table (2). The r^2 values computed using the formulae [8, 9, 10, and 11] agrees well with the value given by L.Pourfaraj [5].The regression equations between x and y shows average relationship between two series and reveals the probable change in a dependent variable as compared to as certain change in other variable. The correlation coefficient over 0.9 for topological index is preferred in designing quantitative structure–property relations [12].

1 2 2 2 2 2 2 1 (degree)

0 0 0 0 0 0 0 0

1 2 5 4 5 6 7 8

(a) *Molecular graph of octane with vertex degree indicated.*



(b) *Molecular graph of 2, 2,3,3-tetra methyl butane.*

Fig, (1): *Molecular graph of octane (a) and 2,2,3,3-tetra methyl butane(b).*

1	2	3	4	5	6	7	8
1	0	1	1/2	1/3	1/2	1/3	1/2	1/3
2	1	0	1	1/2	1/2	1/3	1/2	1/3
3	1/2	1	0	1	1/2	1	1/2	1
4	1/3	1/2	1	0	1/3	1/2	1/3	1/3
5	1/2	1	1/2	1/3	0	1/3	1/2	1/3
6	1/3	1/2	1	1/2	1/3	0	1/3	1/2
7	1/2	1	1/2	1/3	1/2	1/3	0	1/3
8	1/3	1/2	1	1/2	1/3	1/2	1/3	1

Fig.(2):*Reciprocal distance matrix of square matrix for 2,2,3,3-tetra methyl butane.*

Table (1): Reciprocal degree distance, acentric factor, entropy(s), x and y of all octane

Isomer	**Reciprocal degree distance**	**Acentric factor**	**X**	**Entropy(s)**	**y**
octane	99.57	0.3978	0.06218	111	+6
2-methyl heptane	104.33	0.3779	0.04220	109.8	4.84
3-methyl heptane	106.2	0.3710	0.03528	111.3	6.26
4-methyl heptane	112.27	0.3715	0.03579	109.3	4.32
3-ethyl hexane	108.6	0.3625	0.02676	109.4	4.43
2,2-dimethyl hexane	113.4	0.3395	0.00371	103.4	-2.42
2,3-dimethyl hexane	112.27	0.3483	0.01253	108.02	3.02
2,4-dimethyl hexane	112.27	0.3442	0.00851	106.9	3.98
2,5-dimethyl hexane	109.2	0.3568	0.02115	105.7	0.72
3,3-dimethyl hexane	116.47	0.3226	-0.0132	104.7	-1.74
3,4-dimethyl hexane	113.8	0.3404	0.00463	106.6	1.59
2-methyl3-ethyl pentane	114.33	0.3324	-0.0033	106.1	1.06
3-methyl3ethyl pentane	119	0.3069	-0.0289	101.5	4.48
2,2,3-trimethyl pentane	121.67	0.3009	-0.0349	101.3	-4.31
2,2,4-trimethyl pentane	118.67	0.3054	-0.0304	104.1	-0.94
2,3,3-trimethyl pentane	122.67	0.2932	-0.0426	102.1	-1.09
2,3,4-trimethyl pentane	118	0.3174	-0.0183	102.4	-3.06
2,2,3,3-tetramethylbutane	130	0.2553	-0.0805	93.06	-11.9

Table (2): Correlation coefficient and regression equations of isomers of octane

r^2 (Correlation coefficient)	**b_{xy} (Regression coefficient of x on y)**	**$b_{y\ x}$ (Regression coefficient of y on x)**	**Standard error of the coefficient of correlation**	**Standard error of the regression of y on x**	**Regression equation y on x**	**Regression equation x on y**
r = 0.9519 r^2 = 0.9063	0.0197	45.96	0.023	-5.3	y - 46x = 90	x - 0.02y = 1.73

3. CONCLUSION

The matrix representation of molecular graph is used to study topological indices. The vertices and edges consist of data structure that stores important information. The statistical parameters are used to study the quantitative structure property relationship (QSPR) of the isomers of octane.

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