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# THE TOPOLOGICAL INDICES AND PHYSICAL PROPERTIES OF n-HEPTANE ISOMERS

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**ABSTRACT**

In chemistry the structural characteristics of a molecule are responsible for its properties. Topological indices have important role in theoretical chemistry. Topological index is a numerical value associated with chemical constitution for correlation of chemical structure with various physical properties.

In this study, some physical and chemical properties as Acentric factor (Acen fac), Entropy (S), Enthalpy of vaporization (HVAP) and Standard enthalpy of vaporisation (DHVAP), Density (ρ) , Boiling point (bp), Refractive index have been Appeared. The Topological Indices: Wiener Numbers (*W*), Hosoya Indices (*Z*), Randic Indices (χ), Balaban Indices (*J*), Harary Numbers (*H*) of n-heptane isomers have been used. The topological indices are used in QSPR/QSAR studies to modeling physic-chemical properties of molecules. The correlation coefficients and regression equations among the physical Properties and topological indices of n- heptane isomers is studied. We have also studied multiple correlation coefficients (Multiple *R*), Analysis of variance (*ANOVA*), and multiple linear regression (*Y*).

**Keywords:** Topological indices, physical properties, regression analysis, Isomers.

## 1. INTRODUCTION

The graph theory is a significant part of applied mathematics and chemical graph theory which is a branch of graph theory has many applications related to chemistry. A special class of chemical graphs is molecular graphs. In these graphs, vertices correspond to individual atoms, and edges correspond to bonds between them. It provides many information on chemical compounds using an important tool called the topological index [1,2]. Topological indices are graph invariants that play an important role in chemistry, pharmaceutical sciences, materials science, engineering etc. The boiling point (bp) is a measure of the forces of attraction between like molecules. A topological index which is a numerical quantity derived from the chemical graph of a molecule which is used to modeling chemical and physical properties of molecules in QSPR/QSAR researches [3].

Among several types of topological indices, vertex degree based [4] topological indices are most investigated and widely used. The oldest topological indices are Wiener index (*W*) and Wiener polarity indices ($W_p$**)** are distance based topological indices. Hosoya Indices (*Z*), Randic Indices ( χ ) which is used in molecular branching [5 ], Balaban Indices (J) is the average distance-sum connectivity index. Harary Numbers (*H*) is the sum of squares of reciprocal distances in a molecular graph. The Harary index is a more discriminating index than the Wiener number, but it is not unique.

Let *G=(V, E)* be a molecular graph which is simple connected graph. The vertex (atom) set *V(G)* and edge (bond) set *E(G).* The *d(u, v)* denotes the distance between vertices *u* and *v* of *G* is the length of the shortest path connecting them. The degree $d_G(u)$ of a vertex *u* is the number of vertices adjacent to *u.* For a positive integer *k*, the open *k*-neighbourhood of *v* in the graph *G*,
denoted by $N_k(v) = \{ u \in V(G) : d(u, v)=k \}$. The *k*- distance degree of a vertex *v* of *G* is defined as [6], the number of vertices in the open k-neighbourhood of *v* and denoted as $d_k(v) = |N_k(v)|$ . For a vertex *v*, *e*(*v*) denotes the number of edges in the shortest path between the vertex *v* and the farthest vertex from *v*. The *e*(*v*) is called the eccentricity of *v*. For a graph *G*, maximum eccentricity is called a diameter of *G* and denoted as *D*, and minimum eccentricity is called a radius of *G* and denoted as *r*.

One of the oldest graph invariants are the Wiener index, which was formally introduced by Harold Wiener [7] in 1947. The Wiener index is defined as the sum of distances between any two atoms in the molecules, in terms of bonds and denoted by *W(G).*

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

Wiener polarity index [7] of a simple connected graph is denoted by $W_p(G)$ and defined as,

$$W_p(G) = \frac{1}{2}\sum_{v \in V(G)} d_3(u) \quad (2)$$

The authors in [8], defined generalised Wiener polarity index as,

$$W_k(G) = \frac{1}{2}\sum_{v \in V(G)} d_k(u) \quad (3)$$

From equation 2 and 3, $W_p(G) = W_3(G)$ and $W_1(G) = m$ = number of edges of any connected graph *G*.

The first and second Zagreb indices of a simple connected graph *G* is defined as,

$$M_1(G) = \sum_{v \in V(G)} d_1(v)^2 \quad (4)$$

$$M_2(G) = \sum_{uv \in E(G)} d_1(u) d_1(v) \quad (5)$$

The *k*-total distance degree of a vertex *v* of *G* as, for $k \leq D$

$$d_{tk}(v) = \sum_{i=1}^{k} d_i(v) \quad (6)$$

For $k = r$, *k*-total distance degree is called as 'total radius distance degree'. For $k = D$, *k*-total distance degree is called as 'total diameter distance degree'.

Clearly for any vertex *v* of *G*, $\sum_{i=1}^{e(v)} d_i(v)$ = n-1 and for $e(v) < k$, $d_k(v) = 0$.

The k- total Wiener polarity index as defined in [9] is

$$W_k^s(G) = \frac{1}{2}\sum_{v \in V(G)} d_{tk}(v) = W_1(G) + W_2(G) + \ldots\ldots + W_k(G) \quad (7)$$

The Randic index , $\chi(G)$ [5] of a simple connected graph *G* is defined as,

$$\chi(G) = \sum_{uv \in E(G)} [d_1(u) d_1(v)]^{-1/2} \quad (8)$$

The Hosoya Index, $Z(G)$ was introduce by Hosoya [10] of a simple connected graph *G*, is defined as, the total number of matchings of *G*. Let *m(G, k)* be the number of *k*-matchings of *G* and set *m(G, 0)* = 1. The Hosoya index can be formulated as

$$Z(G) = \sum_{k \geq 0} m(G, k) \quad (9)$$

Balaban Index, $J(G)$ is the average-distance sum connectivity [11] of a graph *G*, is defined as

$$J(G) = \frac{m}{m-n+2}\sum_{uv \in E(G)} \frac{1}{\sqrt{W(u)\,W(v)}} \quad (10)$$

where the sum is taken over all edges *uv* of *G*. The denominator m − n + 2 in the definition is used in order to have better comparability between acyclic and cyclic graphs with the same number of vertices. Recall that the cyclomatic number μ of *G*, which is the minimum number of edges that must be removed from *G* in order to transform it to an acyclic graph, is defined by

μ = m − n + 1. Thus Balaban index (often also referred to as J index) is sometimes given as

$$J(G) = = \frac{m}{\mu+1}\sum_{uv \in E(G)} \frac{1}{\sqrt{W(u)\,W(v)}} \quad (11)$$

$w(u)$ (resp. $w(v)$) denotes the sum of distances from *u* (resp. *v*) to all the other vertices of *G*.

The Harary Numbers, $H(G)$ was introduce by Plavsic D, et al. [12]

$$H(G) = \frac{1}{2}\sum_{i=1}^{N}\sum_{j=1}^{N}(D_{ij})^{-2} \quad (12)$$

where $D(G)$ is distance matrix of *G* and $\frac{1}{D(G)} = D^{-1}(G)$, $D^{-2}(G)$ is the matrix whose elements are the square of the reciprocal distance in *G* .

Some topological indices of n-heptane isomers from [13] and some physical properties from [14-16] very good correlated.

In table-1 we have studied about the physico-chemical properties, Entropy (S ), Acentric Factor (Acent Fac.),

Enthalpy of vaporization (HVAP), Standard enthalpy of vaporisation (DHVAP), Boiling point (bp ◦C) , Density

(ρ) and Refractive Index of n-heptane isomers.

In table-2 we have studied about the topological indices, Wiener Numbers (*W*), Hosoya Indices (*Z*), Randic Indices ($\chi$),

Balaban Indices (*J*), Harary Numbers (*H*), First Zagreb index ($M_1$), Second Zagreb index ($M_2$), Wiener polarity index ($W_p$ ) and 3- total Wiener polarity index ( $W_3^*$ ) of n-heptane isomers .

**Table-1**. Some physical properties of n-heptane isomers.

| **Molecule** | **Entropy $JK^{-1}mol^{-1}$** | **Acen. Frac** | **HVAP** | **DHVAP** | **Boiling Point bp** | **Density ρ** | **Refractive Index** |
|---|---|---|---|---|---|---|---|
| Heptane | 328.57 | 0.3460 | 36.6 | 36.00 | 98.4 | 0.684 | 1.3878 |
| 2-methylhexane | 323.34 | 0.3298 | 34.8 | 34.98 | 90.0 | 0.677 | 1.3848 |
| 3-methylhexane | 309.60 | 0.3240 | 35.0 | 35.16 | 92.0 | 0.686 | 1.3887 |
| 2,2- dimethylpentane | 300.29 | 0.2886 | 31.0 | 32.56 | 79.2 | 0.674 | 1.3822 |
| 2,3- dimethylpentane | 297.10 | 0.2986 | 34.5 | 34.30 | 89.8 | 0.695 | 1.3919 |
| 2,4- dimethylpentane | 303.17 | 0.3059 | 32.7 | 33.02 | 80.5 | 0.673 | 1.3815 |
| 3,3- dimethylpentane | 305.60 | 0.2697 | 33.2 | 33.15 | 86.1 | 0.694 | 1.3909 |
| 3-ethylpentane | 314.56 | 0.3101 | 34.1 | 35.32 | 93.5 | 0.698 | 1.3934 |
| 2,2,3-trimethylbutane | 292.25 | 0.2510 | 32.4 | 32.04 | 80.9 | 0.690 | 1.3894 |

**Table-2**. Topological indices of n-heptane isomers.

| | ***W*** | ***Z*** | ***χ*** | ***J*** | ***H*** | ***$M_1$*** | ***$M_2$*** | ***$W_p$*** | ***$W_3^*$*** |
|---|---|---|---|---|---|---|---|---|---|
| A = Heptane | 56 | 21 | 3.4142 | 2.4475 | 7.9897 | 22 | 20 | 4 | 15 |
| B = 2-methylhexane | 52 | 18 | 3.2701 | 2.6783 | 8.2119 | 24 | 22 | 4 | 16 |
| C = 3-methylhexane | 50 | 19 | 3.3081 | 2.8318 | 8.2831 | 24 | 23 | 5 | 17 |
| D = 2,2- dimethylpentane | 46 | 14 | 3.0607 | 3.1545 | 8.6319 | 28 | 26 | 4 | 18 |
| E = 2,3- dimethylpentane | 46 | 17 | 3.1807 | 3.1442 | 8.5417 | 26 | 26 | 6 | 19 |
| F = 2,4- dimethylpentane | 48 | 15 | 3.1259 | 2.9532 | 8.4444 | 26 | 24 | 4 | 17 |
| G =3,3- dimethylpentane | 44 | 17 | 3.1213 | 3.3604 | 8.7292 | 28 | 28 | 6 | 20 |
| H =3-ethylpentane | 48 | 20 | 3.3461 | 2.9923 | 8.3542 | 24 | 24 | 6 | 18 |
| I =2,2,3-trimethylbutane | 42 | 13 | 2.9434 | 3.5412 | 8.9167 | 30 | 30 | 6 | 21 |

**Table-3**. The correlation coefficients between the physical Properties and topological indices of n-heptane isomers

| | **Entropy** | **Acentric factor** | **HVAP** | **DHVAP** | **Boiling point** | **Density** | **Refractive index** |
|---|---|---|---|---|---|---|---|
| ***W*** | 0.9069 | 0.9649 | 0.7417 | 0.8344 | 0.7288 | -0.3208 | -0.2048 |
| $W_3^*$ | 0.8298 | -0.9576 | -0.5994 | -0.7212 | -0.5435 | 0.5173 | 0.4156 |
| $W_p$ | -0.4763 | -0.5910 | -0.0675 | -0.1561 | 0.0416 | 0.9207 | 0.8718 |
| $M_1$ | -0.8672 | -0.9681 | -0.8442 | -0.9567 | -0.8554 | 0.0491 | 0.2303 |
| $M_2$ | -0.8713 | -0.9920 | -0.7193 | -0.8411 | -0.6931 | 0.3401 | 0.2303 |
| ***Z*** | 0.8269 | 0.7851 | 0.8758 | 0.9641 | 0.9630 | 0.3213 | 0.4228 |
| ***H*** | -0.8952 | -0.9907 | -0.7981 | -0.8997 | -0.7802 | 0.2235 | 0.1082 |
| ***J*** | -0.8820 | -0.9857 | -0.7418 | -0.8305 | -0.6953 | 0.3586 | 0.2450 |
| ***X*** | 0.8626 | 0.8985 | 0.8515 | 0.9811 | 0.9204 | 0.1321 | 0.2412 |

**Table 4**. Regression equations of some topological indices and some physical properties of n-heptane isomers.

| | **Entropy** | **Acentric factor** | **HVAP** | **DHVAP** | **Boiling point** bp |
|---|---|---|---|---|---|
| ***W*** | -5.7325X+336.9387 | 0.006778X+ -0.0227 | 0.304167X+19.21111 | 0.275556x+20.83222 | 1.134722x+33.35556 |
| $M_1$ | -4.11108X+414.25 | -0.01137X+0.5956 | -0.55431X+48.1 | -0.52802x+47.67 | -2.22586X+145.2 |
| $M_2$ | -3.41218X+392.8217 | -0.00962X+0.540992 | -0.39015X+43.4780 | -0.38346X+43.56007 | -1.48971X+124.7338 |
| ***Z*** | 3.66817X+245.5091 | 0.008624X+0.155065 | 0.538113X+24.6030 | 0.497906X+25.5391 | 2.344717X+47.70151 |
| ***H*** | -38.013X+629.7082 | -0.10418X+1.183572 | -4.69422X+73.5048 | -4.44784X+71.66925 | -18.1863X+241.6029 |
| ***J*** | -31.554X+403.3001 | -0.08731X+0.565577 | -3.67523X+44.8790 | -3.45876X+44.47491 | -13.6519X+128.9348 |
| ***χ*** | 69.0118X+87.66399 | 0.178008X -0.26641 | 9.435963X+3.64695 | 9.13821X+4.846569 | 40.41668X -41.3787 |

**Table 5.** Regression Analysis

| **Regression Statistics** | |
|---|---|
| Multiple R | 0.995688589 |
| R Square | 0.991395765 |
| Adjusted R Square | 0.965583061 |
| Standard Error | 2.232734928 |
| Observations | 9 |

| *ANOVA* | | | | | | |
|---|---|---|---|---|---|---|
| | **Degree of Freedom *df*** | **Sum of Square *SS*** | **Mean Sum of Square *MS*** | **Variance Test *F*** | | |
| Regression | 6 | 1148.786012 | 191.4643353 | 38.40728037 | | |
| Residual | 2 | 9.970210515 | 4.985105258 | | | |
| Total | 8 | 1158.756222 | | | | |
| | | | | | | |
| | **Coefficients** | **Standard Error** | **t-Stat** | **P-value** | **Lower 95%** | **Upper 95%** |
| **Intercept** | 25377.83889 | 5086.669882 | 4.989087062 | 0.037905594 | 3491.664844 | 47264.01294 |
| $X_1$ | -2230.673075 | 406.3813361 | -5.489113 | 0.031623225 | -3979.190839 | -482.15531 |
| $X_2$ | 2.65508439 | 1.986698567 | 1.336430415 | 0.313163457 | -5.892989622 | 11.2031584 |
| $X_3$ | 55.32623911 | 11.08315672 | 4.991920669 | 0.037864986 | 7.639264596 | 103.0132136 |
| $X_4$ | 0.932570862 | 1.000516543 | 0.932089397 | 0.449689069 | -3.372304374 | 5.237446098 |
| $X_5$ | 5422.946248 | 1560.029029 | 3.47618291 | 0.073720695 | -1289.31691 | 12135.20941 |
| $X_6$ | -21737.91374 | 4565.02508 | -4.76183884 | 0.041382944 | -41379.63136 | -2096.19612 |

**Multiple Linear regression:** $Y = 25377.8388 - 2230.6731\ X_1 + 2.6551\ X_2 + 55.3262\ X_3 + 0.9326\ X_4 + 5422.9462\ X_5 - 21737.9137 X_{6.}$, where, Y= Entropy.

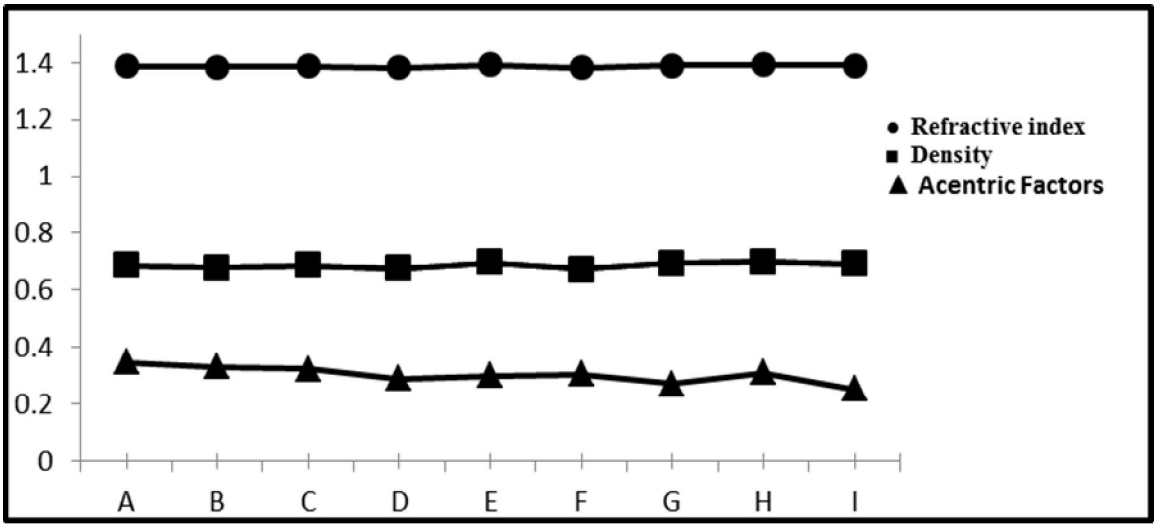


**Fig-1**. Graph of physical properties of *n*- heptane isomers.

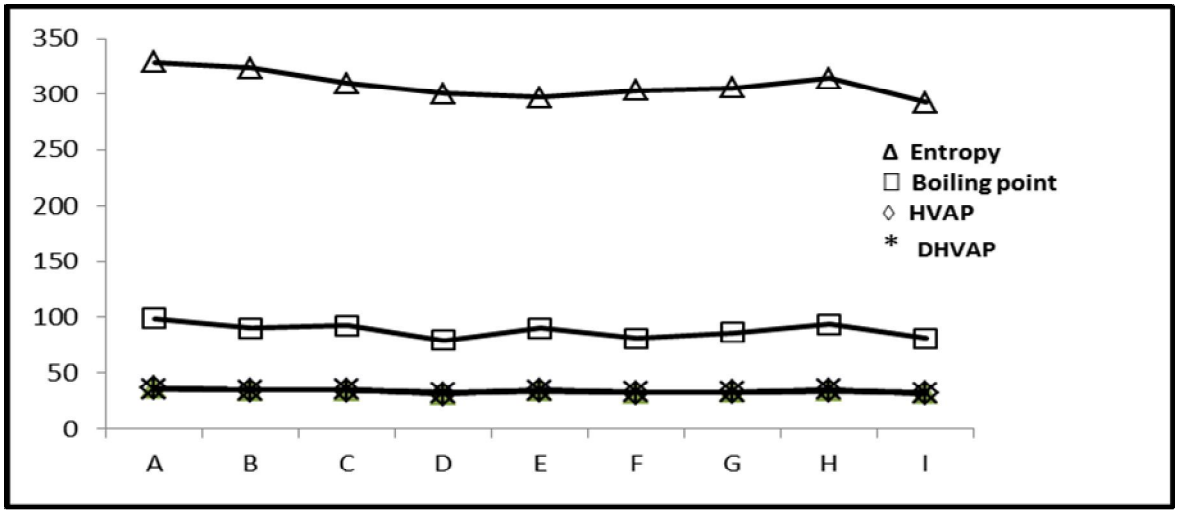


**Fig-2.** Graph of physical properties of *n*- heptane isomers.

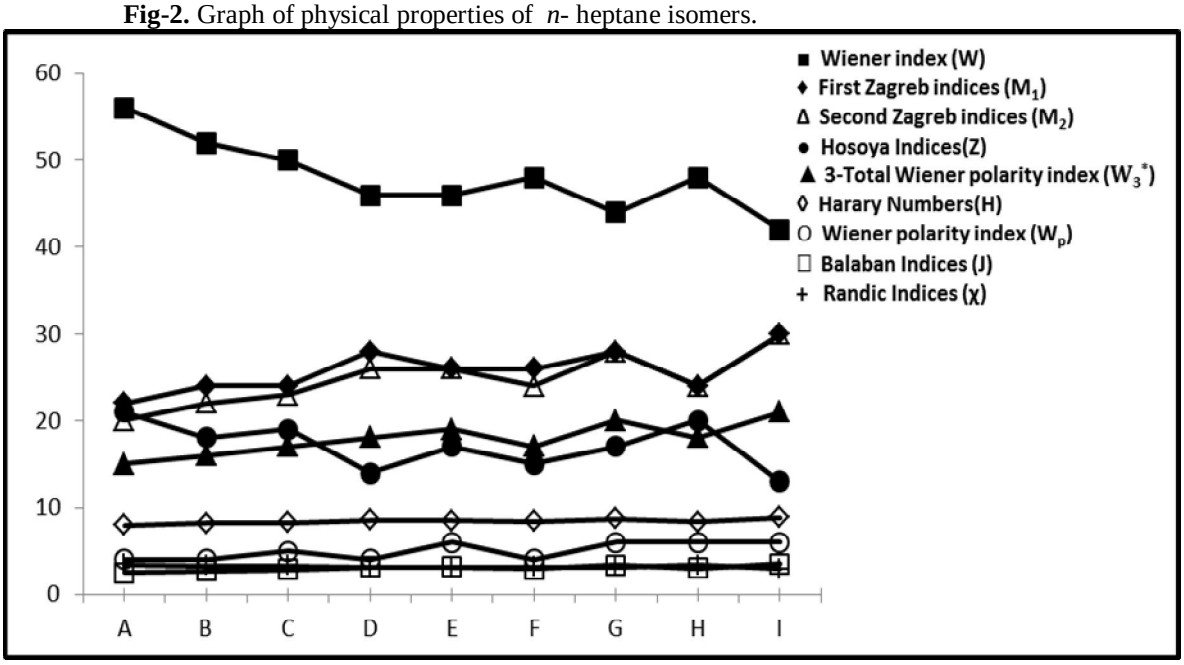


**Fig-3**. Graph of Topological indices of n-heptane isomers.

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## CONCLUSION

We analyzed that, topological indices, Wiener index (*W)*, First Zagreb indices ($M_1$), Hosoya Index (*Z)*, Harary Numbers (*H)*, Randic Indices ( $\chi$ ) are very good correlated to physical properties such as Entropy, Acentric factor, HVAP, DHVAP, Boiling Point( bp). The multiple correlation R = 0.995688 is closer to 1, hence there is strong relation between dependent & independent variables *R* square = 0.99139 which is coefficient of determination, it is closer to 1 hence the existing multiple linear regression equation will provide best predictions. In ANOVA table the regression coefficient is significant i.e none of the coefficient is zero.

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