International Journal of Mathematical Archive-9(10), 2018, 13-19
Available online through www.ijma.info ISSN 2229 – 5046

ON HYPER TERMINAL WIENER INDEX OF GRAPH

SHAILAJA S. SHIRKOL[1], SHOBHAV.PATIL*[2] AND SUNILKUMAR M.HOSAMANI[3]

[1]Department of Mathematics, SDMCET, Dharwad, Karnataka, India.
[2]Department of Mathematics, KLEDr. MSSCET, Belagavi, Karnataka India.
[3]Department of Mathematics, Rani chennamma university, Belagavi, Karnataka, India.

(Received On: 06-08-18; Revised & Accepted On: 25-09-18)

ABSTRACT

I*n this paper, we initiate the study two new topological indices, terminal type Wiener index and hyper terminal Wiener index defined as* $TW_\lambda = TW_\lambda(G) = \sum_{k\geq 1} d_T(G,k)\cdot k^\lambda$ *and* $HTW = HTW(G) = \frac{1}{2}\sum_{1<i<j<k} [d(v_i,v_j)^2 + d(v_i,v_j)]$ *respectively for graph G.*

MSC (2010): *05C90, 05C35, 05C12.*

Key words: *Wiener index, terminal Wiener index, Hyper Wiener index and Wiener Type index.*

1. INTRODUCTION

In this paper we define two new topological indices Hyper terminal Wiener index and terminal type Wiener index and we compute hyper terminal Wiener index of some chemical class of graphs [1]. For standard on its terminology and notation we follow [2]. The graphs considered here are simple, finite and connected unless mentioned otherwise. Let G be a connected graph, $V(G)$ is the vertex set and $E(G)$ is the edge set of G. Let n the number of vertices, and m the number of edges. The number of edges incident with vertex u is called the degree of vertex u. It is denoted by $deg(u)$. If $deg(u) = 1$ then u is called a pendant vertex. The distance $d(u, v)$ is the length of the shortest path connecting vertices u and v of a graph G, If u and v are equal then $d(u, v) = 0$. The number of pair of vertices of G at a distance k is denoted by $d(G, k)$. Then $d(G, 0) = n$, $d(G, 1) = m$ and $\sum_{k\geq 0} d(G,k) = n(n+1)/2$ [3].

In chemical graph theory the graphs are called as molecular graphs. Molecular graph is simple carbon atom –skeleton of an organic molecules (hydrocarbons). Thus vertices of molecular graph represent the carbon atoms, its edges represent the carbon-carbon bonds. Hence the chemical graph theory deals with analysis of all consequences of connectivity in a chemical system. There are many topological indices put forward to study the chemical system, The oldest molecular structure descriptor was given by Harold Wiener. The Wiener index of a graph see [4] is defined as the sum of distance between all pair of vertices G, It is given by

$$W = W(G) = \sum_{(u,v)\subseteq V(G)} d(u,v)$$

Details on its chemical applications and mathematical properties can be found in [**5, 6, 7**]. Hosoya in [**6**] introduced graph polynomial called as Hosoya polynomial or Wiener polynomial. It is defined as

$$H(G,\lambda) = \sum_{k>1} d(G,k)\cdot \lambda^k$$

where $d(G,k)$ is the number of pair of vertices of the graph G whose distance is k, and λ is some parameter.

Corresponding Author: ShobhaV.Patil*[2]
[2]Department of Mathematics, KLEDr. MSSCET, Belagavi, Karnataka India.

The Hyper -Wiener index was introduced by Milan Radic [8]. Then Klein et. al generalised it for all connected graphs [**9,10,11**] and it is given by

$$WW = WW(G) = \frac{1}{2}\sum_{u<v}[d(u,v)^2 + d(u,v)]$$

The terminal Wiener index of a graph was introduced by I. Gutman *et.al* [**12**] as the sum of the distances between all the pair of pendant vertices.

$$TW = TW(G) = \sum_{1<i<j<k} d(v_i, v_j)$$

The terminal Hosoya Polynomial was introduced by Ramane *et.al* [**13**] as

$$TH(G,\lambda) = \sum_{k\geq 1} d\ (G,k)\cdot\lambda^k$$

The Wiener Type index introduced by I.Gutman *et.al* [6] is defined as

$$H(G,\lambda) = \sum_{k\geq 1} d(G,k)\cdot k^{\lambda}$$

where $d(G, k)$ is the number of pair of vertices of G at a distance is k , and λ is some real number.

In analogy of above topological indices we define two topological indices, terminal type Wiener index TW_λ (G) defined as

$$TW_\lambda = TW_\lambda(G) = \sum_{k\geq 1} d_T(G,k)\cdot k^{\lambda}$$

where $d(G, k)$ is the number of pair of pendant vertices of the graph G whose distance is k, and λ is some real number.
And Hyper terminal Wiener index *HTW(G)* as

$$HTW = HTW(G) = \frac{1}{2}\sum_{1<i<j<k}[d(v_i,v_j)^2 + d(v_i,v_j)]$$

where $d(v_i,v_j)$ is the distance between pair of pendant vertices of the graph G. Evidently

$$TW = TW_1$$

$$HTW = \frac{1}{2}TW_2 + \frac{1}{2}TW_1$$

2. CHEMICAL APPLICABILITY OF *HTW* INDEX

Octane isomers have become a significant set of organic molecules to test the applicability of topological indices. In this section we evaluate Wiener index, hyper terminal Wiener index and terminal Wiener index using strong correlation coefficients acquired from the chemical graphs of octane isomers. We get the experimental results of these isomers at the www.moleculardescriptors.eu (see Table 1). The following physico-chemical features have been modelled: Entropy, Acentric factor (AcenFac), Standard enthalpy of vaporization (DHVAP) Enthalpy of vaporization (HVAP).

Table-1: Topological indices of Octane isomers and their physiochemical properties

Octane isomers	W	HTW	TW	Entropy	AcenFac	DHVAP	HVAP
octane	84	28	7	111.67	0.397898	9.915	73.19
2-methylheptane	79	45	14	109.84	0.377916	9.484	70.3
3-methylheptane	76	42	14	111.26	0.371002	9.521	71.2
4-methylheptane	75	35	14	109.32	0.371504	9.483	70.91
3-ethylhexane	72	40	14	109.43	0.362472	9.476	71.7
2,2-dimethylhexane	71	54	21	103.42	0.339426	8.915	67.7
2,3-dimethylhexane	70	54	22	108.02	0.348247	9.272	70.2
2,4-dimethylhexane	71	59	23	106.98	0.344223	9.029	68.5
2,5-dimethylhexane	74	66	24	105.72	0.35683	9.051	68.6
3,3-dimethylhexane	67	50	21	104.74	0.322596	8.973	68.5
3,4-dimethylhexane	68	53	22	106.59	0.340345	9.316	70.2
3-ethyl-2-methylpentane	67	53	22	106.06	0.332433	9.209	69.7
3-ethyl-3-methylpentane	64	48	21	101.48	0.306899	9.081	69.3
2,2,3-trimethylpentane	63	63	27	101.31	0.300816	8.826	67.3
2,2,4-trimethylpentane	66	72	32	104.09	0.30537	8.402	64.87
2,3,3-trimethylpentane	62	62	27	102.06	0.293177	8.897	68.1
2,3,4-trimethylpentane	65	70	32	102.39	0.317422	9.014	68.37
2,2,3,3-trimethylbutane	58	72	40	93.06	0.25394	8.14	66.2

Table-2: Correlation coefficient between topological indices and physicochemical properties

Indices/Property	Entropy	AcenFac	DHVAP	HVAP
W	0.877	0.964	0.822	0.689
HTW	0.741	0.771	0.87	0.889
TW	0.878	0.899	0.929	0.878

For the octane isomers hyper terminal Wiener index shows good correlation for enthalpy of vaporization (HVAP) compared to Wiener index and terminal Wiener index (see Table 2). The variation with respect to Entropy, Acentric factor (AcenFac), standard Enthalpy of vaporization (DHVAP), variation remain almost same for all the *n*-octane isomers. The correlation of hyper terminal Wiener index with HVAP is shown in Figure 1.

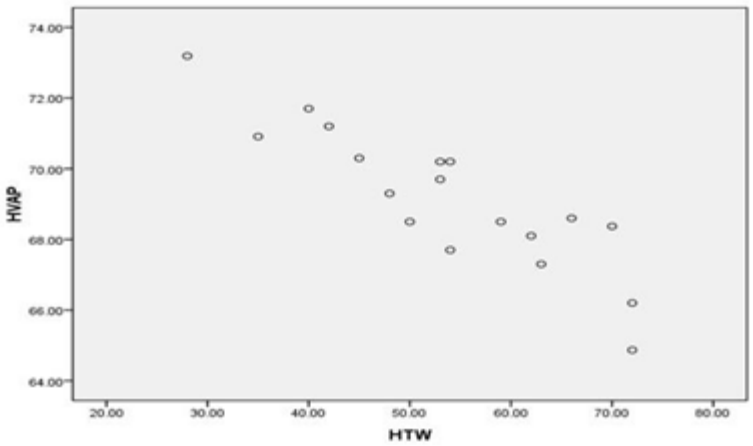

Figure1. Correlation of Hyper Terminal Wiener index and HVAP

3. MAIN RESULTS

Preposition 1: If P_n is path on *n* vertices then $HTW(P_n) = \frac{n(n-1)}{2}$

Proof: Let $G = P_n$ be a path tree on *n* vertices. Let $V(P_n) = \{v_1, v_2, v_3 ... v_n\}$ such that $\deg(v_i) = \deg(v_n) = 1$ and $\deg(v_i) = 2; 2 \le i \le n-1$. Then clearly $d(v_1, v_n) = n-1$ .Therefore

$$HTW(P_n) = \frac{1}{2}[(n-1)^2 + (n-1)]$$
$$= \frac{1}{2}(n-1)[n-1+1]$$
$$= \frac{1}{2}n(n-1)$$

Preposition 2: If S_n is star tree on *n* vertices then $HTW(S_n) = \frac{3}{2}(n-1)(n-2)$

Proof: Let $G = S_n$ be a star graph on *n* vertices. Let $V(S_n) = \{v_1, v_2, v_3 ... v_n\}$ such that $\deg(v_1) = n-1$ and $\deg(v_i) = 1; 2 \le i \le n-1$. Then clearly *G* contains *n*-1 pendant vertices and further $d(v_i, v_j) = 2$ *where* $v_i, v_j \in V(S_n) - \{v_1\}$ Hence

$$HTW(S_n) = \frac{1}{2}[{}^{n-1}C_2(2^2 + 2)]$$
$$= \frac{3}{2}(n-1)(n-2)$$

Preposition 3: Let Y_n has vertex set $V=\{v_1, v_2,.... v_n\}$ such that $\deg(v_1)=\deg(v_{n-1})=\deg(v_n)=1$ and $\deg(v_i)=2; 2\le i\le n-3$, then $HTW(Y_n)=n^2-3n+5$

Proof: Let Y-tree, Y_n $(n \ge 4)$ be a tree as defined in the preposition and the edge set will be the edge set $E=\{ v_1 v_2, v_2 v_3,....., v_{n-2} v_{n-1}, v_{n-2}v_n\}$. Further $d(v_1.v_n)=d(v_1.v_{n-1})=n-2$ and $d(v_{n-1}.v_n)=2$ then

$$HTW(Y_n)=\frac{1}{2}\Big[2\{(n-2)^2+(n-2)\}+(2^2+2)\Big]\lim_{x\to\infty}$$
$$=\frac{1}{2}\Big[2(n^2+4-4n+n-2)+6\Big]$$
$$=n^2-3n+5$$

Now we find HTW of a graph representing the molecular structure of 2-Methyl pentane as shown in Figure 2.

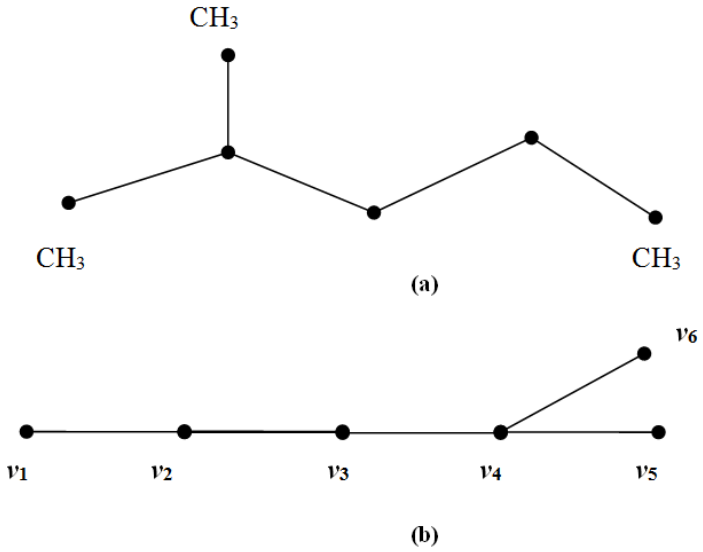

Figure-2

$$HTW(Y_6)=\frac{1}{2}[(4^2+4)+(4^2+4)+(2^2+2)]=23$$
$$HTW(Y_6)=6^2-(3\times 6)+5=23$$

Preposition 4: The hyper terminal Wiener index of $P_n^+(n\ge 4)$ with 2n vertices is

$$HTW(P_n^+)=\sum_{l=1}^{n-1}(n-l)(l^2+5l+6)$$

Proof: Let the vertex set $P_n^+(n\ge 4)$ be $V=\{v_1, v_2,....v_n, v_{n+1}...,v_{2n-1}, v_{2n}\}$ and Edge set $E=\{v_1v_2, v_2v_3,...,v_{n-1}, v_n\}\cup\{v_i, v_{n+i}: 1\le i\le n\}$,

Then $\deg(v_1)=\deg(v_n)=2$, $\deg(v_i)=3; 2\le i\le n-1$ and $\deg(v_j)=1;\ n+1\le i\le 2n$. Clearly $P_n^+(n\ge 4)$ contains n pendant vertices $v_{n+1}, v_{n+2},..., v_{2n}$ .The distance between pendant vertices is given by

$$d(v_{n+1}, v_{n+2})=d(v_1, v_2)+2$$
$$d(v_{n+1}, v_{n+3})=d(v_1, v_3)+2$$
$$\vdots$$
$$d(v_{n+1}, v_{2n})=d(v_1, v_n)+2$$

Similarly

$$d(v_{n+2}, v_{n+2}) = d(v_2, v_2) + 2$$
$$d(v_{n+2}, v_{n+3}) = d(v_2, v_3) + 2$$
$$\vdots$$
$$d(v_{n+2}, v_{2n}) = d(v_2, v_n) + 2$$

In the same way we can calculate the distance between all pendant vertices and hyper terminal Wiener index of $P_n^+(n \geq 4)$ as follows

$$HTW(P_n^+) = \frac{1}{2}\Big[(n-1)(3^2+3) + (n-2)(4^2+4) + (n-3)(5^2+5) + \ldots\ldots\ldots\ldots + (n-(n-1))((n+1)^2 + (n+1))\Big]$$
$$= \frac{1}{2}\sum_{l=1}^{n-1}(n-l)[(l+2)^2 + (l+2)]$$
$$= \frac{1}{2}\sum_{l=1}^{n-1}(n-l)(l^2+5l+6)$$

Now we find *HTW* of a graph representing the molecular structure of (3, 4, 5) trimethylheptane as shown in Figure 3.

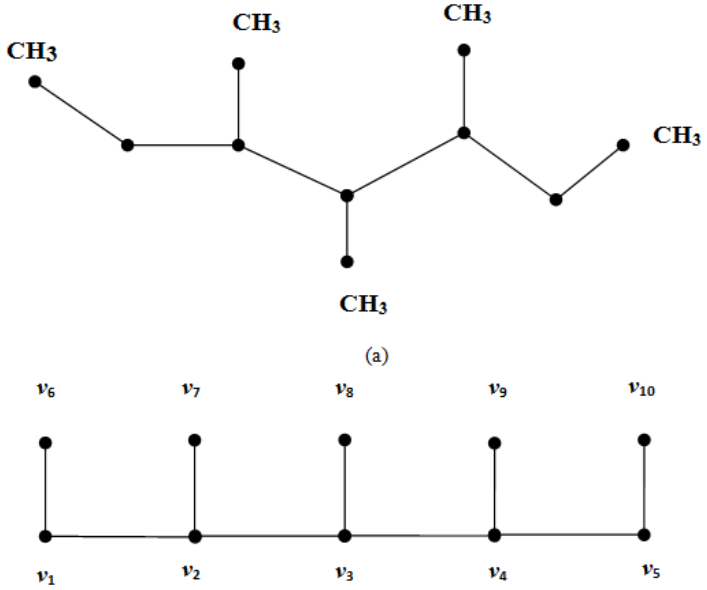

Figure-3.

$$HTW(P_5^+) = \frac{1}{2}\Big[4(3^2+3) + 3(4^2+4) + 2(5^2+5) + 1(6^2+6)\Big] = 105$$
$$HTW(P_5^+) = \frac{1}{2}\sum_{1}^{4}(5-l)(l^2+5l+6)$$
$$= \frac{1}{2}\Big[4(12) + 3(20) + 2(30) + 1(42)\Big] = 105$$

Preposition 5: The hyper terminal Wiener index of (1,4) –biregular caterpillar graph *G* with (3*n*-4) vertices is

$$HTW(G) = \frac{1}{2}\Big[n^2 + 5n + 12\Big] + 2\sum_{l=2}^{n-2}(n-l)(l^2+3l+2)$$

Proof: Let the vertex set and the edge set (1,4)-bi-regular caterpillar graph *G* be

$V=\{v_1, v_2, \ldots, v_n, v_{n+1}, \ldots v_{2(n-1)}, v_{2n}, v_{2n+1}, \ldots v_{3n-4},\}$ and

$E=\{v_1v_2,\ v_2\ v_3,\ldots\ldots,\ v_{n-1},v_n\}\cup\{\ v_2,v_{n+1},\ v_2,v_{n+2},\ldots\ v_{n-1},v_{2n},\ v_{n-1},v_{3n-4}\ \}$ and the degree of every vertex of G is given by $\deg(v_1)=\deg(v_j)=1: n+1\le j\le 3n-4,\ \deg(v_i)=4; 2\le i\le n-1$.Hence G has $2n$-2 pendant vertices. Therefore hyper terminal Wiener index of (1,4)-bi-regular caterpillar graph G is

$$HTW(G)=\frac{1}{2}\left[\begin{array}{r}\{(n-2)+4\}(2^2+2)+4(n-2)(3^2+3)+4(n-3)(4^2+4)+4(n-4)(5^2+5)+....\\ ...4(n-(n-2))((n-1)^2+(n-1))+1((n-1)^2+(n-1))\end{array}\right]$$

$$=\frac{1}{2}\left[6(n+2)+4\sum_{l=2}^{n-2}(n-l)[(l+1)^2+(l+1)]+(n^2-2n+1+n-1)\right]$$

$$=\frac{1}{2}\left[n^2+5n+12+4\sum_{l=2}^{n-2}(n-l)(l+1)(l+2)\right]$$

$$=\frac{1}{2}\left[n^2+5n+12\right]+2\sum_{l=2}^{n-2}(n-l)(l^2+3l+2)$$

Now we find *HTW* of a graph representing molecular structure of (2, 2, 3, 3, 4, 4)-hexamethylpentane representing (1, 4) bi-regular caterpillar graph with 11 vertices as shown in Figure 4.

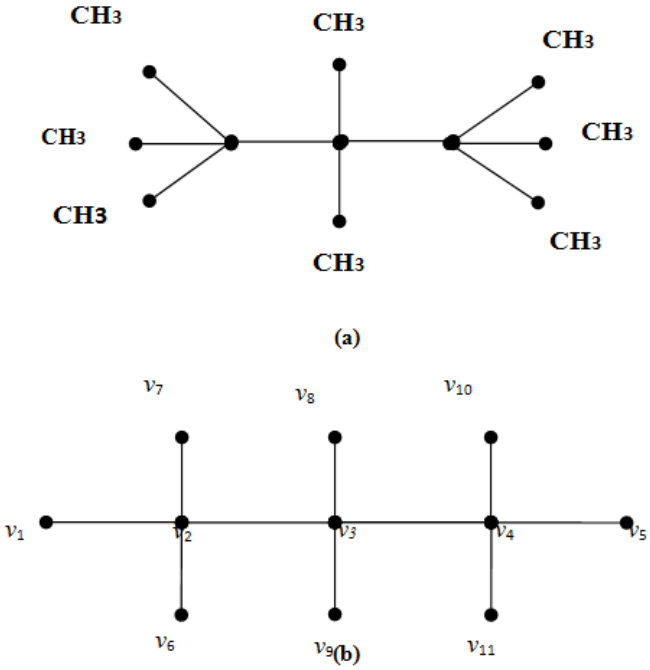

Figure-4

$$HTW(G)=\frac{1}{2}\left[7(2^2+2)+12(3^2+3)+9(4^2+4)\right]=183$$

$$HTW(G)=\frac{1}{2}\left[5^2+5(5)+12\right]+2\sum_{l=2}^{3}(5-l)(l^2+3l+2)$$

$$=31+2\left[3(12)+2(20)\right]=31+152=183$$

REFERENCES

1. Baskar Babujee and Senbagamalar J, Wiener index for special trees isomorphic to hydrocarbons, Acta Cienci, vol 25, no 2, (2009). 575-558.
2. F.Harary, Graph Theory, Addison Wesley Reading (Mass) 1969.
3. I. Gutman, Some relation between distance based polynomials of tree, Bulletin T.CXXXI de l'Academie serbe des science et des arts (2005).
4. H. Wiener, Structural determination of para n boiling points, J. Am. Chem. Soc 69, 17 (1947).

5. A. A. Dobrynin, R. Entringer and I. Gutman, Wiener index of trees: theory and applications, Acta Appl. Math. 66 (2001), 211-249.
6. H. Hosoya, On some counting polynomials in chemistry. Discrete Applied Mathematics, 19 (1988), 239-257.
7. I. Gutman, Y. N. Yeh, S. L. Lee and Y. L. Luo Some recent results in the theory of the Wiener number, Indian J. Chem. 32A(1993), 651-661.
8. Randic,M.Novel molecular descriptor for structureproperty studies, Chemical Physics Letters, 211(10), (1993), 478-483.
9. D. J. Klein, I. Lukovits and I. Gutman, On the de nition of the hyper wiener index for cycle containing structure, J. Chem. Inf. Comput. Sci. 35(1995), 50-52.
10. I. Gutman, Relation between Hyper-Wiener and Wiener index, Chem. Phys. Lett. 364(2002), 352-356.
11. I. Gutman and B Fortula, Hyper Wiener index vs Wiener index .Two highly correlated structure-descriptors, G Monatsh. Chem.134 (2003), 975-981.
12. I Gutman, Boris Fortula and Miroslav Petrovic, Terminal Wiener index, J. Math Chem (2009), 522-531.
13. K. P. Narayankar, S. B. Lokesh, S. S. Shirkol and H. S. Ramane, Terminal Hosoya polynomial of thorn graphs, Scientia Magna. 9, (2013). 37-42.

Source of support: Nil, Conflict of interest: None Declared.