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Hyper-Wiener Index, Hyper-Hosoya Polynomial For Tree Of Isomers Of Pentane

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Abstract:

The organic compounds exclusively composed of carbon and hydrogen atoms. The 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. The Wiener Index W(G), Hyper-Wiener Index WW(G) and Hosoya Polynomial H($G; x$), Hyper-Hosoya Polynomial H H($G; x$) of a tree Graph is used to mathematical model of molecules in order to gain insight into physical properties of the chemical compounds. Some physical properties such as the boiling point, density are related to geometric structure of the compound. We examine the physical properties of pentane (C_5H_{12}). The (C_5H_{12}) has three different structural isomers with a linear structure of 5 carbon atoms, pentane, isopentane and neopentane with branched structure.

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Keywords:- Hyper Wiener Index, Hyper Hosoya Polynomial, tree,Isomers, Chemical graph theory.

1 Introduction:

The Wiener index Wof graph G is W(G) = 1

distance matrix of a graph. Many authores write W(G) = ∑di,j , i > j.

Randic introduced [1]an extension of Wiener index for trees known as Hyper-Wiener

Index WW(G). Klein et al.[2] generalized this extension to cyclic structures.

WW(G) = 1

∑di,j or lower traingular part of the

2 ∑d 2 i,j + 2 1 ∑di,j , i > j (1.1) 2

In 1988, Hosoya [4] introduced the term Wiener polynomial of a graph or Hosoya polynomial [3].

$$H(G;x) = \sum_{k=1}^{m} d(G;k)x^k \tag{1.2}$$

where $d(G;x)$ is the number of pair of vertices in the graph G of distance k and m is maximum value of k.

The $$H'(G;x) = \sum_{k=1}^{m} kd(G;k)x^{k-1} \tag{1.3}$$

is called first derivative of Hosoya polynomial [5]. The first derivative evaluated at $x = 1$ is equals to Wiener Index[3] i.e., $W(G) = H'(G;1)$.

The Hyper-Wiener Index $$WW(G) = H'(G;1) + \frac{1}{2}H''(G;1) \tag{1.4}$$

where $H''(G;1)$ is the second derivative at $x = 1$, of the Hosoya polynomial. The derivation is shown by Cash [5].

The Hyper-Hosoya polynomial $HH(G;x)$ which has the property that its first deriva-tive evaluated at $x = 1$, equals to Hyper Wiener Index [5]. i.e. $WW(G) = HH'(G;1)$. Also

$$HH(G;x) = \frac{1}{2}\left[H(G;x) + xH'(G;x)\right] + c \tag{1.5}$$

where c is constant of integration. But by both Hosoya[4]and Sagan[8], the constant term was zero(summation over 0 k m). The $HH(G;x)$ may be expressed by [5] as

$$HH(G;x) = \sum_{k=0}^{m} \frac{k+1}{2} d(G;k)x^k \tag{1.6}$$

where k; m and $d(G;x)$ are as in equation (1.2).

In Work of [6]has been demonstrated that if T is any n vertex tree different from P_n (path) and S_n(star) then $W(S_n) < W(T) < W(P_n)$.

The boiling point decreases in a general way as the compactness of the molecule increases if the relative molecular mass is same. The boiling point decreases with increasing branching. The quantitative structure-activity relationship showed that it is correlated with critical point, density, surface tension, and viscosity of its liquid phase and van der Waals surface area of the molecule. Ahire et. al [10] observed that the relation of the Wiener index of isomers of C_5H_{12} are closely correlated with the boiling points and densities of alkane molecules. . The Wiener index, Hosoya index and Wiener polynomial of these isomers are in the order: pentane > isopentane > neopentane. Similarly the values of density and boiling point are follows same trend. The present paper is aimed to contribute the equations (1.2) to (1.6) for tree graphs of isomers of C_5H_{12} and observing relation between them.

Figure-1. The chemical graph (carbon tree) for pentane is five vertex path graph.

Figure- 1.

Figure-2. The chemical graph (carbon tree) for isopentane is five vertex path graph.

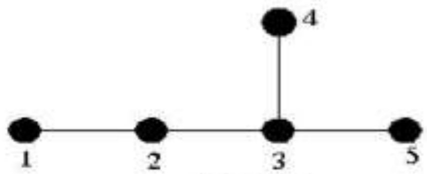

Figure- 2

Figure-3. The chemical graph (carbon tree) for neopentane is five vertex path graph.

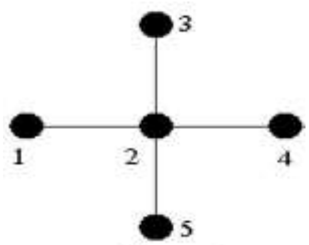

Figure-3

The $W(G_1)$ of pentane(figure-1) is $1+2+3+4+1+2+3+2+1+1 = 20$

The $W(G_2)$ of isopentane(figure-2) is $1+2+3+3+1+2+2+1+1+2 = 18$

The $W(G_3)$ of neopentane(figure-3) is $1+2+2+2+1+1+1+2+2+2 = 16$

The $H(G_1; x)$ for pentane (figure-1) is $x^4 + 2x^3 + 3x^2 + 4x$

The $H(G_2; x)$ for isopentane (figure-2) is $2x^3 + 4x^2 + 4x$

The $H(G_3; x)$ for neopentane (figure-3) is $6x^2 + 4x:$

) $H'(G_1; x) = 4x^3 + 6x^2 + 6x + 4;$ $H'(G_2; x) = 6x^2 + 8x + 4,$ $H'(G_3; x) = 12x + 4$

Hyper-Wiener Index

The Hyper-Wiener Index $WW(G_1)$ from equation (1.2) is

$$WW(G_1) = \frac{1}{2}\sum d_{i;j}^2 + \frac{1}{2}\sum d_{i;j}; \quad i > j$$

$$= \frac{1}{2}\left[(1^2 + 2^2 + 3^2 + 4^2 + 1^2 + 2^2 + 3^2 + 2^2 + 1^2 + 1^2) + \frac{1}{2}(20)\right]$$

$$= 35$$

The Hyper-Wiener Index $WW(G_1)$ from equation (1.4) is

$$WW(G_1) = H'(G_1; 1) + \frac{1}{2}H''(G_1; 1)$$
$$= 20 + \frac{1}{2}[2(3) + 3(2)(2) + 4(3)(1)]$$
$$= 35$$

Similarly $WW(G_2) = 28$
$WW(G_3) = 22$

Hyper-Hosoya Polynomial

The Hyper-Hosoya polynomial $HH(G_1; x)$ from equation (1.5)

$$HH(G_1; x) = \frac{1}{2}\left[H(G_1; x) + xH'(G_1; x)\right]$$
$$= \frac{1}{2}\left[(x^4 + 2x^3 + 3x^2 + 4x) + x\left[\left(\frac{d}{dx}\right)x^4 + 2x^3 + 3x^2 + 4x\right]\right]$$
$$= \frac{5}{2}x^4 + 4x^3 + \frac{9}{2}x^2 + 4x$$

The Hyper-Hosoya polynomial $HH(G_1; x)$ from equation (1.6)

$$HH(G_1; x) = \sum_{k=0}^{m} \binom{k+1}{2} d(G_1; k)x^k$$
$$= 0 + 4x + \binom{3}{2}3x^2 + \binom{4}{2}2x^3 + \binom{5}{2}x^4$$
$$= \frac{5}{2}x^4 + 4x^3 + \frac{9}{2}x^2 + 4x$$

) $HH(G_1; 1) = 15$

Similarly $HH(G_2; x) = 4x^3 + 6x^2 + 4x$: Hence $HH(G_2; 1) = 14$
$HH(G_3; x) = 9x^2 + 4x$: Hence $HH(G_3; 1) = 13$

Conclusion

Hyper-Wiener index of C_5H_{12} are in the order: pentane > isopentane > neopentane. The relation $W(S_n) < W(T) < W(P_n)$ is satisfied as Figure-1 is Path, Figure-2 is tree and Figure-3 is star. We observe that Hyper-Wiener index for all these graphs satisfies same relation.i.e. $WW(S_n) < WW(T) < WW(P_n)$.
At $x = 1$, $HH(S_n) < HH(T) < HH(P_n)$.

References

[1] *M.Randic; Novel Molecular Descriptor for Structure-Properties Studies,* Chem.Phys.Lett. 211 (1993),pp.478-483.

[2] *D.J.Klein, I.Lukovits and I.gutman; On the Definition of the Hyper-Wiener Index for Cycle-containing Structures,* J. Chem.Inf Comput.Sci., 35 (1995),pp.50-52.

I.Gutman and D.Stevanovic, Hosoya Polynomials of trees with up to 10 vertices., Zb.Rad. (Kragujevac)21 (1999),pp.111-119.

[3] *H.Hosoya;On Some Counting Polynomials in Chemistry.*, Disc. Appl.math. 19(1988),pp.239-257.

[4] *G.G.Cash, Relationship Between the Hosoya Polynomial and the Hyper-Wiener Index.*, Appl.Maths.lett. 15 (2002),pp.893-895.

[5] *A.A.Dobrynin, R.Entringer and I.Gutman ; Wiener Index of Trees: Theory and Applications.*, Acta Appl.Math., 66(2001),pp.211-249.

[6] *H.B.Walikar, H.S.Ramane, L.Sindagi, S.S.Shirakol and I.Gutman; Hosoya Poly-nomial of thorn Trees, Rods, Rings, and Stars.*, Kragujevac J. Sci., 28(2006),pp.47-56.

[7] *B.E.Sagan, Y.N.Yeh and P.Zhang ; The Wiener Polynomial of a Graph.*,Internat. J. Quantum Chem.60(1996),pp.959-969.

[8] *M.Bersohn;A Fast Algorithm for Calculation of the Discrete Matrix of a Molecule.*, J. Comput. Chem.4 (1983),pp.110-113.

[9] *K.S.Ahire and R.B.Sawant; Wiener Index, Wiener Polynomial and Hosoya In-dex in Isomers of Organic Compounds* Bull. of Marathwada Maths. Soc. Vol. 14(2)(2013),pp.1-4.

[10] *H. Wiener; Structural Determination of Paraffin Boiling Points,* J. Amer.Chem. Soc. 69 (1947),pp.17-20.

[11] *J.Devillers and balaban; Eiditors, Topological Indices and Related Developers in QSAR and QSPR,* Golden and Breech, Amsterdam, (1999).

[13] *S.Klavzar, P.Ziget and I.Gutman; An Algorithm for the Calculations of the Hyper-Wiener index of Benzenoid Hydrocarbons.*,Comput. Chem.24 (2000),pp.229-233.

[14] *R.F. Ma, L.Shi, Y.Y.Duan, L.Z.Han, X.Liu; Saturated liquid viscosity of cy-clopentane and isopentane*, J.Chines Uni.25(2010), pp.155-161.

[15] *M.Diudea; Wiener and Hyper-Wiener numbers in a Single matrix.*, J. Chem.Inf Comput. Sci. 36 (1996),pp.833-836.

[16] *I.Gutman; E.Estrada and O.Ivanciuc, Some Properties of the Wiener Polynomial of Trees*.,Graph Theory Notes, New York 36(1999),pp.7-13.

[17] *B.Yang,C.Ye,L.Yan; On the Hosoya index of graphs,* Appl.Math.J.Chines Uni.25,(2010),pp.155-161.

[18] *I.Gutman; Relation Between Hyper-Wiener and Wiener Index* ., Chem. Phys. Lett. 364 (2002),pp.352-356.

[19] *D.Bonchev, D.J. Klein ; On the Wiener Number of thorn Trees, Stars, Rings and Roads*.,Croat. Chem. Acta 75(2002),pp.613-620.