



INTERNATIONAL JOURNAL FOR RESEARCH

IN APPLIED SCIENCE & ENGINEERING TECHNOLOGY

Volume: 6 Issue: IV Month of publication: April 2018

DOI: http://doi.org/10.22214/ijraset.2018.4538

www.ijraset.com

Call: © 08813907089 E-mail ID: ijraset@gmail.com



ISSN: 2321-9653; IC Value: 45.98; SJ Impact Factor: 6.887

Volume 6 Issue IV, April 2018- Available at www.ijraset.com

A Significant Computation of Wiener Number and Hyper-Wiener Number of Graphs

P. Gayathri¹, T. Ragavan², K. Vinothini³

^{1, 2,} Assistant Professor, PG and Research Department of Mathematics, A.V.C College (Autonomous), Mannampandal, Tamilnadu, India

³PG and Research Department of Mathematics, A. V. C College (Autonomous), Mannampandal, Tamilnadu,India.³

Abstract: The Wiener index of a graph G is denoted by W(G) and defined as the sum of distances between all pairs of vertices in simple connected graph. Wiener index is used for modelling the shape of organic molecules and for calculating several of their physicochemical properties. In this paper we have considered the popular topological indices Wiener vector, Hyper-Wiener Vector, Wiener Matrix Sequence, Hyper Weiner Matrix sequence, Wiener number and Hyper Wiener number of graphs two connected graphs are computed and presented in a well defined form.

Keywords: Wiener matrix sequence, hyper-Wiener vector, Weighted Wiener polynomial, Wiener polynomial sequence.

I. INTRODUCTION

Let G= (V (G), E (G)) be a simple connected graph of order n and size m. The degree of any vertex is the number of first neighbor of v is denoted by deg(v). The distance of between any two vertices u and v of graph is defined as the length of the shortest path connecting u, v is d (u, v). Topological indices are particularly suitable ,if properties like shape or degree of branching are expected to have an influence on the property predicted. Calculation is often based on the distance matrix of molecular graph. A disadvantage of topological indices is that they are unrelated to observable physical properties. Quantitative structure –Activity and structure property relationships (QSAR/QSPR) use chemo-metric methods to study how a given biological activity or a physicochemical property varies as a function of topological descriptors describing the chemical structure of molecules. With these studies it is possible to replace costly and time taking biological tests or experiments of a given physiochemical property with models involving topological descriptors. In this paper we have considered the two connected graphs and their popular topological indices using the Wiener vector, Hyper-wiener Vector, Wiener Matrix Sequence, Hyper Wiener Matrix Sequence, Wiener polynomial Sequence and Hyper-wiener polynomial, Wiener number and Hyper Wiener number are calculated.

II. WIENER VECTOR AND HYPER WIENER VECTOR

For a connected graph G with n vertices, denoted by 1,2,...n, let $W_k = \sum_{i < j, dij = k} dij$, 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.For a connected graph G with n vertices, denoted by 1,2,...n, let $W_{ij,k} = \max\{d_{ij} - k + 1,0\}$ where d_{ij} is the distance between vertices i and j. Then ${}^kW = \sum_{i < j} W_{ij,k}$, k = 1,2,... are called the higher Wiener numbers of G. The vector

(1W,2W,...) is called the hyper-Wiener vector Of G, denoted by HWV(G).

Let D be the distance matrix of a connected graph of G.

Let $W^{(1)}=D$ for $k=1,2,...W^{(K+1)}$ is obtained from $W^{(k)}$ by leaving zeroes in place and replacing each nonzero entry x of $W^{(k)}$ by x-1. Let D be the distance matrix of a connected graph G, and let $W^1,W^2,...$ be the Wiener matrix sequence of G. The Hyper-Wiener

matrix W^(H) of G is defined as
$$W^{(H)} = \sum_{k=1,2} W^{(K)}$$

From the definitions, we can see that (i, j) entry of $W^{(k)}$ is just equal to d_{ij} -k+1, so the sum of entries of upper triangle of $W^{(k)}$ is just equal to $W^{(k)}$ is just equal to $W^{(k)}$ is just equal to the hyper-Wiener number $W^{(k)}$ is just equal to $W^{(k)}$ in $W^{(k)}$ in $W^{(k)}$ is

ISSN: 2321-9653; IC Value: 45.98; SJ Impact Factor: 6.887 Volume 6 Issue IV, April 2018- Available at www.ijraset.com

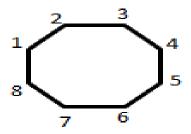


Fig 1: Graph G₁

For graph G₁ in Figure 1, its Wiener matrix sequence, Wiener vector, and hyper-Wiener vector are determined and given below.

$$W^{(1)} = \begin{pmatrix} 0 & 1 & 2 & 3 & 4 & 3 & 2 & 1 \\ 1 & 0 & 1 & 2 & 3 & 4 & 3 & 2 \\ 2 & 1 & 0 & 1 & 2 & 3 & 4 & 3 \\ 3 & 2 & 1 & 0 & 1 & 2 & 3 & 4 \\ 4 & 3 & 2 & 1 & 0 & 1 & 2 & 3 \\ 3 & 4 & 3 & 2 & 1 & 0 & 1 & 2 \\ 2 & 3 & 4 & 3 & 2 & 1 & 0 & 1 \\ 1 & 2 & 3 & 4 & 3 & 2 & 1 & 0 \end{pmatrix}$$

$$W^{(2)} = \begin{pmatrix} 0 & 0 & 1 & 2 & 3 & 2 & 1 & 0 \\ 0 & 0 & 0 & 1 & 2 & 3 & 2 & 1 \\ 1 & 0 & 0 & 0 & 1 & 2 & 3 & 2 \\ 2 & 1 & 0 & 0 & 0 & 1 & 2 & 3 \\ 3 & 2 & 1 & 0 & 0 & 0 & 1 & 2 \\ 2 & 3 & 2 & 1 & 0 & 0 & 0 & 1 \\ 1 & 2 & 3 & 2 & 1 & 0 & 0 & 0 \\ 0 & 1 & 2 & 3 & 2 & 1 & 0 & 0 \end{pmatrix}$$

$$W^{(3)} = \begin{pmatrix} 0 & 0 & 0 & 1 & 2 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 2 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 2 & 1 \\ 1 & 0 & 0 & 0 & 0 & 0 & 1 & 2 \\ 2 & 1 & 0 & 0 & 0 & 0 & 0 & 1 \\ 1 & 2 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 2 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 2 & 1 & 0 & 0 & 0 & 0 \end{pmatrix}$$





ISSN: 2321-9653; IC Value: 45.98; SJ Impact Factor: 6.887 Volume 6 Issue IV, April 2018- Available at www.ijraset.com

$$W^{(H)}(G) = \begin{pmatrix} 0 & 1 & 3 & 6 & 10 & 6 & 3 & 1 \\ 1 & 0 & 1 & 3 & 6 & 10 & 6 & 3 \\ 3 & 1 & 0 & 1 & 3 & 6 & 10 & 6 \\ 6 & 3 & 1 & 0 & 1 & 3 & 6 & 10 \\ 10 & 6 & 3 & 1 & 0 & 1 & 3 & 6 \\ 6 & 10 & 6 & 3 & 1 & 0 & 1 & 3 \\ 3 & 6 & 10 & 6 & 3 & 1 & 0 & 1 \\ 1 & 3 & 6 & 10 & 6 & 3 & 1 & 0 \end{pmatrix}$$

 $WV(G)=(8,16,24,16), \ HWV(G)=(64,36,16,4), \ W=64, \ R=120.$

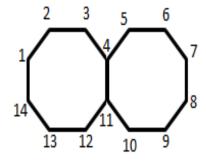


Fig 2: Graph G₂ 6 2 1 2 1



ISSN: 2321-9653; IC Value: 45.98; SJ Impact Factor: 6.887 Volume 6 Issue IV, April 2018- Available at www.ijraset.com

$$W^{(2)} = \begin{pmatrix} 0 & 0 & 1 & 2 & 3 & 4 & 5 & 6 & 5 & 4 & 3 & 2 & 1 & 0 \\ 0 & 0 & 0 & 1 & 2 & 3 & 4 & 5 & 4 & 3 & 2 & 3 & 2 & 1 \\ 1 & 0 & 0 & 0 & 1 & 2 & 3 & 4 & 3 & 2 & 1 & 2 & 3 & 2 \\ 2 & 1 & 0 & 0 & 0 & 1 & 2 & 3 & 2 & 1 & 0 & 1 & 2 & 3 \\ 3 & 2 & 1 & 0 & 0 & 0 & 1 & 2 & 3 & 2 & 1 & 2 & 3 & 4 \\ 4 & 3 & 2 & 1 & 0 & 0 & 0 & 1 & 2 & 3 & 2 & 1 & 2 & 3 & 4 \\ 5 & 4 & 3 & 2 & 1 & 0 & 0 & 0 & 1 & 2 & 3 & 2 & 3 & 4 & 5 \\ 6 & 5 & 4 & 3 & 2 & 1 & 0 & 0 & 0 & 1 & 2 & 3 & 4 & 5 \\ 5 & 4 & 3 & 2 & 3 & 2 & 1 & 0 & 0 & 0 & 1 & 2 & 3 & 4 \\ 4 & 3 & 2 & 1 & 2 & 3 & 2 & 1 & 0 & 0 & 0 & 1 & 2 & 3 \\ 3 & 2 & 1 & 0 & 1 & 2 & 3 & 2 & 1 & 0 & 0 & 0 & 1 & 2 \\ 2 & 3 & 2 & 1 & 2 & 3 & 2 & 1 & 0 & 0 & 0 & 0 & 1 & 2 \\ 2 & 3 & 2 & 1 & 2 & 3 & 4 & 3 & 2 & 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 2 & 3 & 4 & 5 & 6 & 5 & 4 & 3 & 2 & 1 & 0 & 0 \end{pmatrix}$$



ISSN: 2321-9653; IC Value: 45.98; SJ Impact Factor: 6.887 Volume 6 Issue IV, April 2018- Available at www.ijraset.com





ISSN: 2321-9653; IC Value: 45.98; SJ Impact Factor: 6.887 Volume 6 Issue IV, April 2018- Available at www.ijraset.com

$$W^{(H)}(G) = \begin{pmatrix} 0 & 1 & 3 & 6 & 10 & 15 & 21 & 28 & 21 & 15 & 10 & 6 & 3 & 1 \\ 1 & 0 & 1 & 3 & 6 & 10 & 15 & 21 & 15 & 10 & 6 & 10 & 6 & 3 \\ 3 & 1 & 0 & 1 & 3 & 6 & 10 & 15 & 10 & 6 & 3 & 6 & 10 & 6 \\ 6 & 3 & 1 & 0 & 1 & 3 & 6 & 10 & 6 & 3 & 1 & 3 & 6 & 10 \\ 10 & 6 & 3 & 1 & 0 & 1 & 3 & 6 & 10 & 6 & 3 & 6 & 10 & 15 \\ 15 & 10 & 6 & 3 & 1 & 0 & 1 & 3 & 6 & 10 & 6 & 10 & 15 & 21 \\ 21 & 15 & 10 & 6 & 3 & 1 & 0 & 1 & 3 & 6 & 10 & 15 & 21 & 28 \\ 28 & 21 & 15 & 10 & 6 & 3 & 1 & 0 & 1 & 3 & 6 & 10 & 15 & 21 \\ 21 & 15 & 10 & 6 & 10 & 6 & 3 & 1 & 0 & 1 & 3 & 6 & 10 & 15 \\ 15 & 10 & 6 & 3 & 6 & 10 & 6 & 3 & 1 & 0 & 1 & 3 & 6 & 10 \\ 10 & 6 & 3 & 1 & 3 & 6 & 10 & 6 & 3 & 1 & 0 & 1 & 3 & 6 \\ 6 & 10 & 6 & 3 & 6 & 10 & 15 & 10 & 6 & 3 & 1 & 0 & 1 & 3 \\ 3 & 6 & 10 & 6 & 10 & 15 & 21 & 15 & 10 & 6 & 3 & 1 & 0 & 1 \\ 1 & 3 & 6 & 10 & 15 & 21 & 28 & 21 & 15 & 10 & 6 & 3 & 1 & 0 \end{pmatrix}$$

 $WV(G) = \{15,36,66,72,50,36,14\}, HWV(G) = \{289,198,122,64,28,10,2\}, W=289, R=713.$

III. WIENER POLYNOMIAL SEQUENCE AND HYPER-WIENER POLYNOMIAL

Let D be the distance matrix of a graph G, let l be the largest entry of D, let $2d_k$ be the number of such entries of D that are equal to k. The Wiener polynomial W(G,x) of G is then given by

$$W(G, x) = \sum_{k=1}^{l} d_k x^k$$

W(G, x) related to the Wiener index of a graph G, called the Wiener polynomial $W(G, x) = \sum_{\{u,v \subseteq V(G)} x^{d(u,v)}$ where d(u, v)

denotes the distance between vertices u and v. The above two formulae give the same polynomial of G that

$$W = W'(G,1), R = W'(G,1) = \frac{1}{2}W''(G,1)$$
.

A hyper Hosoya polynomial is given by $HH(G,x) = \sum_{k=1}^{l} \left[k + 1/2 \right] d_k x^k$ and showed that R(G) = HH'(G,1). It can be found

that the Wiener vector (W_1, W_2, \ldots) consists of the coefficients of the derivative W'(G, x) of the Wiener polynomial, where W_k is equal to the coefficient kd_{k^k} of x^{k-1} in W'(G, x). The hype-Wiener vector cannot be obtained from the hyper Hosoya polynomial HH (G, x). Let G be a connected graph with G is defined by $W_k(G, x) = \sum_{\{u,v\}\subseteq V(G)} x^{\max[d(u,v)-k+1,0]}$, where G is the diameter of G. The polynomial sequence G is the polynomial sequence G is the diameter of G.

IV. WIENER POLYNOMIAL SEQUENCE OF G

The weighted hyper-wiener number $R_W(G)$ of a graph G is defined as $R_W(G) = \sum_{k=1,2,...} {}^k W_{y_k}$ where y_k is the weight of kW . In

additon we will introduce a novel weighted hyper-wiener polynomial HW(G,x,y) of a graph G, so that the hyper-wiener vector and the weighted hyper-wiener number can be obtained from the polynomial. The Weighted hyper-Wiener polynomial HW(G,x,y) of a



ISSN: 2321-9653; IC Value: 45.98; SJ Impact Factor: 6.887

Volume 6 Issue IV, April 2018- Available at www.ijraset.com

graph G defined as, $HW(G, x, y) = \sum_{k=1,2,...} W_k(G, x) y_k$ where $y = (y_1, y_2,...)$. From the above definition we have that

$$\frac{d}{dx}[HW(G,x,y)]/x = 1 = R_w(G) = \sum_{K=1,2,\dots,k} {}^kW_{Y_K} \text{ where the coefficients of } y_k \text{ in the weighted hyper Wiener number } R_w(G) \text{ are } W_{Y_K}$$

equal to the k^{th} Wiener number . Hence , the hyper –Wiener vector can be given by coefficients of d/dx=[HW(G,x,y]/x=1. In a particular graph, we have d/dx=[HW(G,x,y]/x=1,y=(1,1,1,....)=R(G)

For a graph G_1 in Figure 1, the Wiener vector, the Wiener polynomial sequence, the weighted hyper Wiener polynomial of G_1 are given by

$$W'(G, x) = 16x^3 + 24x^2 + 16x + 8$$

$$WV(G) = (8,16,24,16), W = 64$$

$$W^{(1)}(G,x) = 4x^4 + 8x^3 + 8x^2 + 8x$$

$$W^{(2)}(G,x) = 4x^3 + 8x^2 + 8x + 8$$

$$W^{(3)}(G,x) = 4x^2 + 8x + 16$$

$$W^{(4)}(G,x) = 4x + 24$$

$$HW(G, x, y) = (4x^4 + 8x^3 + 8x^2 + 8)y_1 + (4x^3 + 8x^2 + 8x + 8)y_2 + (4x^2 + 8x + 16)y_3 + (4x + 24)y_4$$

$$\frac{d}{dx} = [HW(G,x,y]/x = 1 = 64y_1 + 36y_2 + 16y_3 + 4y_4]$$

$$\frac{d}{dx}$$
 =[HWG,x,y]/x=1,y=(1,1,1,....)=R(G)= 120.

For a graph G_2 in Figure 2, the Wiener vector, the Wiener polynomial sequence, the weighted hyper Wiener polynomial of G_2 are given by

$$W'(G,x) = 14x^7 + 36x^6 + 50x^5 + 72x^4 + 66X^3 + 36x^2 + 15x$$

$$WV(G) = (15, 36, 66, 72, 50, 36, 14), W = 289$$

$$W^{(1)}(G_{x}x) = 2x^{7} + 6x^{6} + 10x^{5} + 18x^{4} + 22x^{3} + 18x^{2} + 15x$$

$$W^{(2)}(G_x) = 2x^6 + 6x^5 + 10x^4 + 18x^3 + 22x^2 + 18x + 15$$

$$W^{(3)}(G,x) = 2x^5 + 6x^4 + 10x^3 + 18x^2 + 22x + 33$$

$$W^{(4)}(G,x) = 2x^4 + 6x^3 + 10x^2 + 18x + 36$$

$$W^{(5)}(Gx) = 2x^3 + 6x^2 + 10x + 72$$

$$W^{(6)}(G,x)=2x^2+6x+83$$

$$W^{(7)}(G,x)=2x+89$$



ISSN: 2321-9653; IC Value: 45.98; SJ Impact Factor: 6.887 Volume 6 Issue IV, April 2018- Available at www.ijraset.com

$$HW(G,x,y) = (2x^{7} + 6x^{6} + 10x^{5} + 18x^{4} + 22x^{3} + 18x^{2} + 15x)y_{1} + (2x^{6} + 6x^{5} + 10x^{4} + 18x^{3} + 22x^{2} + 18x + 15)y_{2} + (2x^{5} + 6x^{4} + 10x^{3} + 18x^{2} + 22x + 33)y_{3} + (2x^{4} + 6x^{3} + 10x^{2} + 18x + 36)y_{4} + (2x^{3} + 6x^{2} + 10x + 72)y_{5} + (2x^{2} + 6x + 83)y_{6} + (2x + 89)y_{7}$$

$$\frac{d}{dx} = [HW(G,x,y]/x = 1 + 289y_{1} + 198y_{2} + 122y_{3} + 64y_{4} + 28y_{5} + 10y_{6} + 2y_{7} + 2$$

V. CONCLUSION

The topological indices are used to study quantitative structure relationships—property or activity (QSPR/QSAR). The topological invariants such as the Wiener vector, the Hyper-wiener Vector, the Wiener Matrix Sequence, the Hyper Wiener Matrix Sequence, the Wiener polynomial Sequence and the Hyper-wiener polynomial, the Wiener number and the Hyper Wiener number of graphs are derived in this work. These sequences will be helpful for similarity research analysis and multiply regression analysis in the study of structure-property relationship.

REFERENCES

- [1] M. R. Farahani, Omega and related counting polynomials of Triangular Benzenoid G_n and Linear hexagonal chain LH_n, Journal of Chemical Acta 2 (2013), 43-45
- [2] W.Gao, M.R.Farahani, Forgotten topological index of some drug structures, Journal of Saudi Pharmaceutical, 24(3) (2016) 258-264
- [3] M.R.Farahani, A new version of Zagreb index of circumcoronene series of benzenoid, Chemical Physics Research Journal, 6(1) (2013) 27–33
- [4] M.R.Farahani and M.P.Vlad, Computing first and second Zagreb index, first and second Zagreb polynomial of Capra-designed planar benzenoid series Can (C6),StudiaUbbChemia, 58(2) (2013) 133–142
- [5] B.Furtula and I.Gutman, A forgotten topological index, Journal of Mathematical Chemistry, 53(4) (2015) 1184–1190
- [6] W.Gao and M.R.Farahani, Degree-based indices computation for special chemical molecular structures using edge dividing method, Applied Mathematics and Nonlinear Science, 1(1) (2015) 94–117
- [7] W.Gao and W.F.Wang, The fifth geometric-arithmetic index of bridge graph and carbon nanocones, Journal of Difference applications, 23 (2016) 100-109
- [8] P.Gayathri and U.Priyanka, Degree based topological indices of Linear Phenylene, International Journal of Innovative Research in Science, Engineering and Technology, 6(8) (2017) 16986-16997
- [9] L.Yan, Y.Li, W.Gao and J.Li, PI Index for Some Special Graphs, Journal of Chemical and Pharmaceutical Research, 5(11) (2013) 260-265
- [10] M.Ghorbani and M.Ghazi, Computing some topological indices of triangular benzenoid, Digest Journal of Nanomaterials Biostructure, 5(4) (2010) 837–841
- [11] P.Gayathri and K.R.Subramanian, The PI (Padmakar-Ivan) Index of Polyominoes, International Journal of Discrete Mathematics, 1(1) (2016) 1-4, Science Publishing group.
- [12] P. Gayathri, U. Priyanka, S. Sandhiya, S. Sunandha, K.R. Subramanian, M-Polynomials of Penta-Chains, Journal of Ultra Scientist of Physical Sciences, 29(4),(2017) 164-168
- [13] Gayathri1, U. Priyanka and S. Sandhiya, A significant computation for finding PI index of Phenylene, Journal of Ultra Chemistry, 13(3) (2017) 60-6
- [14] P.Gayathri and U.Priyanka, Degree Based Topological Indices of Banana Tree Graph, International Journal of Current Research and Modern Education, Special Issue NCETM, (2017)13-24
- [15] P.Gayathri and T.Ragavan, Wiener Matrix Sequence, Hyper-Wiener Vector, Wiener Polynomial Sequence and Hyper-Wiener Polynomial of Bi-phenylene, International Journal of Innovative Research in Science Engineering and Technology, 6(8) (2017) 16998-17005.
- [16] Gayathri and U.Priyanka, Degree based topological indices of Jahangir graphs, International Journal of Current Advanced Research, 6(11) (2017) 7154-7160
- [17] P.Gayathri and T.Ragavan, Wiener Vector, Hyper-Wiener Vector, Wiener number, Hyper-Wiener number of molecular graphs, Annals of Pure and Applied Mathematics, 15 (1) (2017) 51-65.
- [18] P.Gayathri and U.Priyanka, Degree Based Topological Indices of zig-zag chain, Journal of Mathematics and Informatics Vol. 11, 2017, 83-93, 2017.
- [19] Immadesetty Pothu Raju, "Highly correlated Wiener polarity Index: A model to predict log P", International Journal of Advances in Applied Sciences, Vol. 3. Pp.19-24, 2014.
- [20] A.Behmaram and H.Yousefi-Azari. "Further Results on Wiener Polarity Index of Graphs", Iranian Journal of Mathematical Chemistry, Vol. 2. Pp. 67-70, 2011
- [21] Wiener. H. "Structural determination of paraffin boiling points", Journal of the American Chemical society, 69(1). Pp 17-20, 1947.





10.22214/IJRASET



45.98



IMPACT FACTOR: 7.129



IMPACT FACTOR: 7.429



INTERNATIONAL JOURNAL FOR RESEARCH

IN APPLIED SCIENCE & ENGINEERING TECHNOLOGY

Call: 08813907089 🕓 (24*7 Support on Whatsapp)