# WIENER AND HYPER-WIENER INDEX OF DUTCH WINDMILL GRAPHS

Raghisa KHALID[1], Nazeran IDREES[2*]

*In theoretical chemistry and chemical graph theory as well, the vertex degree and distance based topological indices have captured much attention by the researchers. Topological indices are found to be very useful in biochemistry, chemistry and nanotechnology in structure-property relationship, structure-activity relationship and pharmaceutical drug design. In this paper distance based topological indices like Wiener index and hyper-Wiener index of Dutch windmill graph $D_m^n$ are computed by analysing the shortest path among each two vertices and the general formulas are derived for the above-mentioned family of graphs.*

**Keywords**: Wiener index, hyper-Wiener index, Dutch windmill graph $D_m^n$

## 1. Introduction

In chemical graph theory we study the structure of molecules and is considered an important tool to understand the molecular structure and synthesis of complex, functional organic molecules. The arrangement of molecules and modeling unknown structures with desired properties is provided by the topological classification of chemical structure. A real number associated to a graph by a function is said to be topological index $TI$. In theoretical chemistry, distance based molecular structure descriptors have used for demonstrating physical, biological and other properties of chemical compounds. Topological indices are the molecular descriptors which are being widely used to illustrate the chemical compound and predict certain physiochemical properties like boiling point, stability, molecular weight, enthalpy of formation and many others in QSAR/QSPR studies. For some interesting applications of Wiener index in QSAR/ QSPR studies, we refer the readers to [1-3]

In this paper all molecular graphs are finite, connected, loopless and without parallel edges. Let $F$ be a graph with $n$ vertices and $m$ edges. The length of shortest path among the two vertices is termed as the distance among two vertices $q$ and $r$, signified as $d(q,r)$. Using these expressions, some topological

[1] Department of Mathematics, Government College University Faisalabad, Pakistan, E-mail: kraghisa@yahoo.com
[2*] Department of Mathematics, Government College University Faisalabad, Pakistan, corresponding author, E-mail: nazeranjawwad@gmail.com

indices are defined in the following way.

The first distance based topological index is the Wiener index, which was presented by Wiener [4]. Firstly, Wiener index was used as tool for predicting the boiling points of paraffin but later strong connection among Wiener index and the chemical properties of a compound was found.

**Definition 1.** The Wiener index (i.e., the entire distance or the transmission number) is defined as the sum of the distance among all unordered pairs of vertices in any graph $F$.

$$W(F) = \sum_{\{q,r\} \subseteq V(F)} d(q,r) \qquad (1)$$

Here $d(q,r)$ denote the distance between vertices $q$ and $r$ in $F$.
As a kind of extension of the Wiener index, the hyper-Wiener index of acyclic graphs was proposed by Randic [5]. It was used as a structure invariant for predicting physiochemical properties of organic compounds.

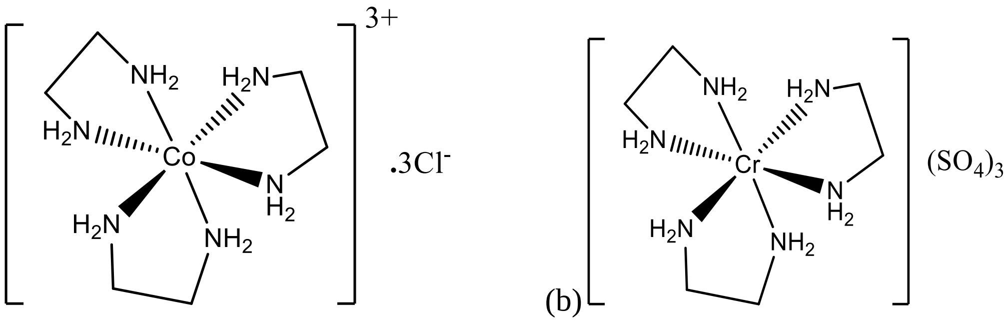
**Definition 2.** For a molecular graph $F$, the hyper-Wiener index is defined as

$$WW(F) = \frac{1}{2}W(F) + \frac{1}{2}\sum_{\{q,r\} \subseteq V(F)} d(q,r)^2 \qquad (2)$$

where $d(q,r)$ denotes the distance between vertices $q$ and $r$ in the graph $F$.
Wiener and hyper- Wiener indices have attracted a lot of attention by researchers in recent past. Wu [6] presented the lower and upper bounds for Wiener index of line graph $W\left(L\left(G\right)\right)$ in terms of a graph invariant called Gutman index of $G$. Later on Gao and Shi [7] determined the Hyper-Wiener index of gear fan graph, gear wheel graph and their r-corona graphs. After that, Cai et al. [8] obtained the second minimum hyper-Wiener indices among all the trees with $n$ vertices and diameter $d$ and characterized the corresponding extremal graphs. Some other results on Wiener and hyper-Wiener index include [9,10].

## 2. Main results

The Dutch windmill graph $D_m^n$ is the graph obtained by $m$ number of cycle graph $C_n$ having $n$-vertices, with a node in common, and therefore corresponds to the usual windmill graph. Structures of many different chemical graphs correspond to Dutch windmill graphs. See, for example, the compounds given below




(a) (b)

Fig. 1: (a)Tris(ethylenediamine)cobalt(III) chloride; (b)Tris(ethylenediamine)Chromium(III) sulphate

The distance based topological indices like Wiener index and hyper-Wiener index for Dutch windmill graph are computed in this section.

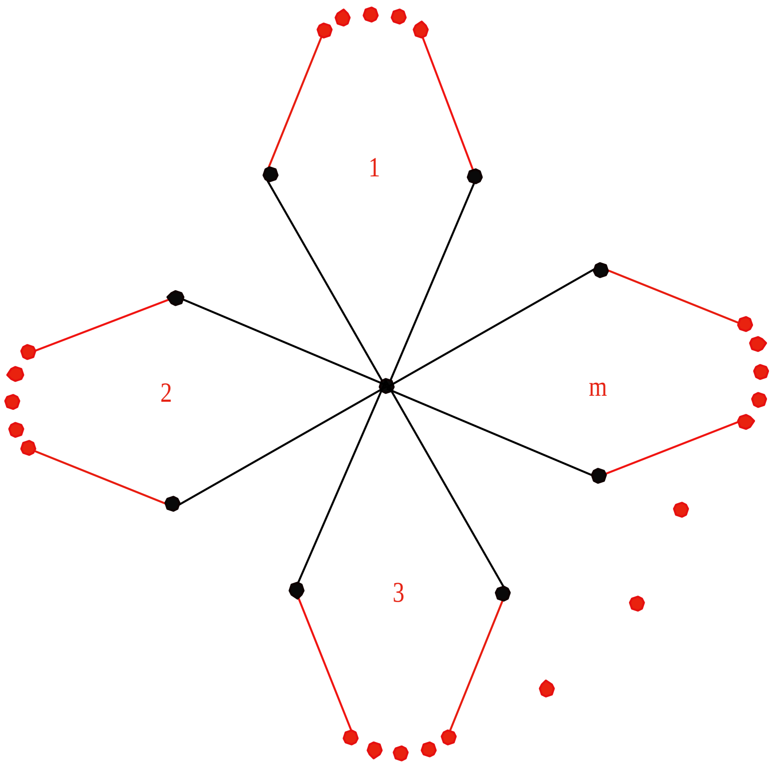



Fig. 2: A representation of Dutch windmill graph $D_m^n$

**Theorem 2.1**

The Wiener index of Dutch windmill graph is given by

$$WD_{2m}^{n} = m^2 n\left[(2m-1)n-(m-1)\right], \text{ when } m \text{ is even,}$$

$$WD^n_{2m+1} = \frac{m(m+1)}{2} n\left[4mn - (2m-1)\right]$$, when $m$ is odd.

**Proof:**

Consider a Dutch windmill graph $D^n_m$. Any Dutch windmill graph $D^n_m$ have $mn$ edges and $(n-1)m+1$ vertices. For each pair $q,r$ of vertices, let $d(q,r)$ represent the distance among the vertices $q$ and $r$. We found the shortest path among all the pair of vertices such that $q$ and $r$ of Dutch windmill graph $D^n_m$.

**Case 1:** m is even:- As we know that Wiener index is given by equation 1 as

$$W(F) = \sum_{\{q,r\} \subseteq V(F)} d(q,r)$$

From Table 1, we have,

$$WD^n_{2m} = m^2 n\left[(2m-1)n - (m-1)\right].$$

**Case 2:** m is odd:- As we know that Wiener index is given by

$$W(F) = \sum_{\{q,r\} \subseteq V(F)} d(q,r)$$

From Table 2, we have

$$WD^n_{2m+1} = \frac{m(m+1)}{2} n\left[4mn - (2m-1)\right].$$

Here the proof of the theorem 2.1 is completed.

**In general case for $D^n_m$:** We analysed the distances between the vertices of chemical graphs of $D^n_m$ for different values of $m$ and $n$, and computed the Wiener index. The results are summarized in tables below.

*Table 1*

**Wiener index of $D^n_m$ where $n \geq 2$ and $m \geq 3$, $m$ is even**

| | |
|---|---|
| $WD^n_4$ | $12n^2 - 4n$ |
| $WD^n_6$ | $45n^2 - 18n$ |
| $WD^n_8$ | $112n^2 - 48n$ |
| - | - |
| - | - |
| - | - |
| $WD^n_{2m}$ | $m^2 n\left[(2m-1)n - (m-1)\right]$ |

*Table 2*

**General term for Wiener index of $D_m^n$ where $n \geq 2$, $m \geq 3$ and $m$ is odd**

| | |
|---|---|
| $WD_3^n$ | $4n^2 - n$ |
| $WD_5^n$ | $24n^2 - 9n$ |
| $WD_7^n$ | $72n^2 - 30n$ |
| $WD_9^n$ | $160n^2 - 70n$ |
| - | - |
| - | - |
| $WD_{2m+1}^n$ | $\frac{m(m+1)}{2} n\left[4mn - (2m-1)\right]$ |

**Theorem 2.2**

The hyper-Wiener index of Dutch windmill graph $D_m^n$ is given as follows when $3 \leq m \leq 7$:

$$WW(D_3^n) = 6n^2 - 3n\,,$$

$$WW(D_4^n) = 23n^2 - 13n\,,$$

$$WW(D_5^n) = 50n^2 - 30n\,,$$

$$WW(D_6^n) = \frac{221n^2 - 137n}{2}\,,$$

$$WW(D_7^n) = 312n^2 - 214n\,.$$

**Proof:**

Consider a Dutch windmill graph $D_m^n$. For each pair $q, r$ of vertices, let $d(q,r)$ represent the distance among the vertices $q$ and $r$. Firstly, we calculate the Wiener index of Dutch windmill graph and secondly, we take square of each shortest path among all the pair of vertices of Dutch windmill graph $D_m^n$.

As we know that hyper-Wiener index is given by equation 2 as

$$WW(F) = \frac{1}{2}W(F) + \frac{1}{2}\sum_{\{q,r\} \subseteq V(F)} d(q,r)^2$$

From Tables 3,4,5,6 and 7 we can get the hyper-Wiener index of Dutch windmill graph $D_m^n$ when $3 \leq m \leq 7$,

$$WW(D_3^n) = 6n^2 - 3n\,,$$

$$WW(D_4^n) = 23n^2 - 13n\ ,$$

$$WW(D_5^n) = 50n^2 - 30n\,,$$

$$WW(D_6^n) = \frac{221n^2 - 137n}{2}\ ,$$

$$WW(D_7^n) = 312n^2 - 214n\,.$$

Here the proof of the theorem 2.2 is completed.

*Table 3*

**Hyper-Wiener index for $D_3^n$**

| | |
|---|---|
| $WW\left(D_3^2\right)$ | 18 |
| $WW\left(D_3^3\right)$ | 45 |
| $WW\left(D_3^4\right)$ | 84 |
| - | - |
| - | - |
| - | - |
| $WW\left(D_3^n\right)$ | $6n^2 - 3n$ |

*Table 4*

**Hyper-Wiener index for $D_4^n$**

| | |
|---|---|
| $WW\left(D_4^2\right)$ | 66 |
| $WW\left(D_4^3\right)$ | 168 |
| $WW\left(D_4^4\right)$ | 316 |
| - | - |
| - | - |
| - | - |
| $WW\left(D_4^n\right)$ | $23n^2 - 13n$ |

*Table 5*

**Hyper-Wiener index for $D_5^n$**

| | |
|---|---|
| $WW\left(D_5^2\right)$ | 140 |
| $WW\left(D_5^3\right)$ | 360 |
| $WW\left(D_5^4\right)$ | 680 |
| - | - |

| | |
|---|---|
| - | - |
| - | - |
| $WW\left(D_5^n\right)$ | $50n^2-30n$ |

*Table 6*

**Hyper-Wiener index for $D_6^n$**

| | |
|---|---|
| $WW\left(D_6^2\right)$ | 305 |
| $WW\left(D_6^3\right)$ | 789 |
| $WW\left(D_6^4\right)$ | 1494 |
| - | - |
| - | - |
| - | - |
| $WW\left(D_6^n\right)$ | $\frac{221n^2-137n}{2}$ |

*Table 7*

**Hyper-Wiener index for $D_7^n$**

| | |
|---|---|
| $WW\left(D_7^2\right)$ | 820 |
| $WW\left(D_7^3\right)$ | 2166 |
| $WW\left(D_7^4\right)$ | 4136 |
| - | - |
| - | - |
| - | - |
| $WW\left(D_7^n\right)$ | $312n^2-214n$ |

## 3. Conclusion

Wiener index and hyper-Wiener index are very important topological indices in chemical modeling of compounds. We have found closed formulas for Wiener and hyper-Wiener indices of family of Dutch windmill graphs. These indices can be employed for quantitative structure activity relations of chemical compounds whose chemical graphs correspond to Dutch windmill graphs.

## REFERENCES

[1] *V Verma, K Singh, D Kumar, B Narasimhan*, "QSAR studies of antimicrobial activity of 1,

3-disubstituted-1H-naphtho [1, 2-e][1, 3] oxazines using topological descriptors." in Arabian Journal of Chemistry 10 (2017): S747-S756.

[2] *J. C. Dearden*,"The Use of Topological Indices in QSAR and QSPR Modeling", in Advances in QSAR Modeling. Springer, Cham, 2017. 57-88.

[3] *Z. Meryam, M. El Marraki, and M. Essalih*, "Some tools of QSAR/QSPR and drug development: Wiener and Terminal Wiener indices", in Cloud Technologies and Applications (CloudTech), 2015 International Conference on. IEEE, 2015.

[4] *H. Wiener*, "Structural determination of paraffin boiling points", Journal of the American Chemical Society, **69** (1947), 17.

[5] *M. Randić*, "Novel molecular descriptor for structure—property studies", in Chemical physics letters, **211** (1993), no. (4-5), 478-483.

[6] *B. Wu*, "Wiener index of line graphs", in MATCH Commun. Math. Comput. Chem, **64**, no. 3, 2010, 699-706.

[7] *W. Gao and L. Shi*, "Hyper-wiener index of gear fan and gear wheel related graph", IJCS, (2015), **2** (2015), no. 5, 52-58.

[8] *G. Cai, G. Yu, J. Cao, A. Alsaedi and F. Alsaadi*, "The Hyper-Wiener Index of Trees of Order with Diameter", Discrete Dynamics in Nature and Society, 2016.

[9] *A. Chen, X. Xiong and F. Lin*, "Distance-based topological indices of the tree-like polyphenyl systems", Applied Mathematics and Computation, **281** (2016), 233-242.

[10] *W. Gao, M. R. Farhani, M. Imran and M. R. Khanna*, "Distance-based topological polynomials and indices of friendship graphs", SpringerPlus, **5** (2016), no. 1, 1563.