Asian Journal of Chemistry; Vol. 26, No. 11 (2014), 3397-3400

ASIAN JOURNAL OF CHEMISTRY

http://dx.doi.org/10.14233/ajchem.2014.17534

Wiener Index of Gear Fan Graph and Gear Wheel Graph

WEI GAO[1,*] and LI SHI[2]

[1]School of Information Science and Technology, Yunnan Normal University, Kunming, P.R. China
[2]Institute of Medical Biology, Chinese Academy of Medical Sciences & Peking Union Medical College, Kunming 650092, P.R. China

*Corresponding author: Tel/Fax: +86 871 66435256; E-mail: gaowei@ynnu.edu.cn

Received: 17 February 2014; *Accepted*: 18 April 2014; *Published online*: 25 May 2014; AJC-15257

Chemical compounds and drugs are often modeled as graphs where each vertex represents an atom of molecule and covalent bounds between atoms are represented by edges between the corresponding vertices. This graph derived from a chemical compounds is often called its molecular graph and can be different structures. An indicator defined over this molecular graph, the Wiener index, has been shown to be strongly correlated to various chemical properties of the compounds. The Wiener index of a graph is defined as the sum of distances between all pairs of vertices of the graph. It has been found extensive applications in chemistry. In this paper, we determine the Wiener index of gear fan graph, gear wheel graph and their *r*-corona graphs.

Keywords: Chemical graph theory, Organic molecules, Wiener index, Gear fan graph, Gear wheel graph, *r*-Corona graph.

INTRODUCTION

Wiener index, Szeged index and PI index are introduced to reflect certain structural features of organic molecules. The Wiener index is the sum of distances between all pairs of vertices in a (connected) graph. It is an important topological index in chemistry since Harold Wiener defined it in 1947. It is used for the structure of molecule. Scientists found that there is a very close relation between the physical, chemical characteristics of many compounds and the topological structure of that. The Wiener index is such a topological index and it has been widely used in Chemistry fields. After several years, mathematician began to pay attention to the Wiener index and study it from the mathematical point of view. In such background, since each structural feature of organic molecule can be expressed as a graph, chemical graph theory as a branch of combinatorial chemistry is introduced to research the structure of molecule from graph theory standpoint. Some conclusion for PI index can refer to Yan *et al.*[1].

The graphs considered in this paper are simple and connected. The vertex and edge sets of G are denoted by V(G) and E(G), respectively. The Wiener index is defined as the sum of distances between all unordered pair of vertices of a graph G, *i.e.*,

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

where d(u, v) is the distance between u and v in G.

Several papers contributed to determine the Wiener index of special graphs. A polyomino system is a finite 2-connected plane graph such that each interior face (say a cell) is surrounded by a regular square of length one. Furthermore, a polyomino chain is a polyomino system, in which the joining of the centers of its adjacent regular squares forms a path $c_1c_2\ldots c_n$, where c_i is the center of the i-th square (i = 1, 2, …, n). A generalized polyomino chain is defined as follows: a generalized polyomino chain of length 1 is a unit square, a generalized polyomino chain of length k + 1 can be obtained by attaching a new unit square to a generalized polymino chain of length k, there are two ways attaching the new unit square: either attaching with two vertices of degree 2, or attaching with a vertex of degree 2 and a vertex of degree 3. The helical polyomino system Z(km, (k – 1)n) and Z(km, kn) are geometrically non-planar polyomino systems. Pan[2] determined the wiener index of W[Z(km, kn)] and W[Z((k+1)m, kn)]. Chen *et al.*[3] gained the exact expression for general pepoid graph. Xing and Cai[4] characterized the tree with third-minimum wiener index and introduce the method of obtaining the order of the Wiener indices among all the trees with given order and diameter, respectively. A tricyclic graph is a connected graph with n vertices and n + 2 edges. Wan and Ren[5] studied the Wiener index of tricyclic graph τ_n^3 which have at most a common vertex between any two circuits and the smallest, the second-smallest Wiener indices of the tricyclic graphs are given. The Hyper-Wiener index WW is one of the recently distance-based graph invariants. That WW clearly encodes the compactness of a structure and the WW of G is define as:

$$WW(G)=\frac{1}{2}\left(\sum_{\{u,v\}\subseteq V(G)} d(u,v)^2+\sum_{\{u,v\}\subseteq V(G)} d(u,v)\right)$$

Pan[6] deduced the formula of Wiener number and Hyper-Wiener number of two types of polyomino systems. More results on Wiener index can refer to[7-14].

$W(P_n)=\frac{n(n-1)(n+1)}{6}$ is determined by Dobrymin *et al.*[15]. The graph Fn = {v} Pn is called a fan graph and the graph Wn = {v} Cn is called a wheel graph, where Pn is a path with n vertices and Cn is a cycle with n vertices. Graph Ir(G) is called *r*-crown graph of G which splicing r hang edges for every vertex in G. The vertex set of hang edges that splicing of vertex v is called *r*-hang vertices, note v*. By adding one vertex in every two adjacent vertices of the fan path Pnof fan graph Fn, the resulting graph is a subdivision graph called gear fan graph, denote as $\tilde{F}_n$. By adding one vertex in every two adjacent vertices of the wheel cycle Cn of wheel graph Wn, the resulting graph is a subdivision graph, called gear wheel graph, denoted as $\tilde{W}_n$.

In this paper, we present the Wiener index of $I_r(F_n)$ and $I_r(W_n)$ first; then, the wiener index of gear fan graph and gear wheel graph are determined; at last, the wiener index of *r*-corona graph for $\tilde{F}_n$ and $\tilde{W}_n$ are derived.

Main results and proof

Theorem 1: $W(I_r(F_n)) = r^2(2n^2 + n + 1) + r(3n^2-n + 3) + (n^2-n + 1)$.

Proof: Let Pn = $v_1v_2\ldots v_n$ and the r hanging vertices of vi be $v_i^1, v_i^2, \ldots, v_i^r$ (1 ≤ in). Let v be a vertex in Fnbeside Pn and the r hanging vertices of v be $v^1, v^2, \ldots, v^4$.

By the definition of Wiener index, we have

$$W(I_r(F_n))=\sum_{i=1}^{r}d(v,v^i)+\sum_{i=1}^{n}d(v,v_i)$$

$$+\sum_{i=1}^{n}\sum_{j=1}^{r}d(v,v_i^j)+\sum_{i=1}^{n}\sum_{j=1}^{r}d(v_i,v^j)$$

$$+\sum_{i=1}^{n}\sum_{j=1}^{r}\sum_{k=1}^{r}d(v_i^j,v^k)+\sum_{i=1}^{n-1}\sum_{j=1+1}^{n}d(v_i,v_j)+\sum_{i=1}^{n}\sum_{j=1}^{r}d(v_i,v_i^j)$$

$$+\sum_{i=1}^{n}\sum_{j\in\{1,2,\ldots,n\}}\sum_{k=1}^{r}d(v_i,v_j^k)+\sum_{i=1}^{n}\sum_{j=1}^{r-1}\sum_{k=j+1}^{r}d(v_i^j,v_i^k)$$

$$+\sum_{i=1}^{n-1}\sum_{j=i+1}^{n}\sum_{k=1}^{r}\sum_{t=1}^{r}d(v_i^k,v_j^t)$$

$= r + n + 2nr + 2nr + 3nr^2 + (n-1)^2 + nr + r(3n^2-5n + 2)$
$+ nr(r-1) + r^2(n-1)(2n-1)$
$= r^2(2n^2 + n + 1) + r(3n^2-n + 3) + (n^2-n+1)$.

In this way, we get the decision.

Theorem 2: $W(I_r(W_n)) = r^2(2n^2 + n) + r(3n^2-n + 1) + (n^2-n)$.

Proof: Let Cn = $v_1v_2\ldots vn$ and $v_i^1, v_i^2, \ldots, v_i^r$ be the r hanging vertices of vi (1 ≤ i ≤ n). Let v be a vertex in Wn beside Cn and $v^1, v^2, \ldots, v^r$ be the r hanging vertices of v.

By the definition of Wiener index, we have

$$W(I_r(W_n))=\sum_{i=1}^{r}d(v,v^i)+\sum_{i=1}^{n}d(v,v_i)$$

$$+\sum_{i=1}^{n}\sum_{j=1}^{r}d(v,v_i^j)+\sum_{i=1}^{n}\sum_{j=1}^{r}d(v_i,v^j)$$

$$+\sum_{i=1}^{n}\sum_{j=1}^{r}\sum_{k=1}^{r}d(v_i^j,v^k)+\sum_{i=1}^{n-1}\sum_{j=i+1}^{n}d(v_i,v_j)+\sum_{i=1}^{n}\sum_{j=1}^{r}d(v_i,v_i^j)$$

$$+\sum_{i=1}^{n}\sum_{j\in\{1,2,\ldots,n\}-i}\sum_{k=1}^{r}d(v_i,v_j^k)$$

$$+\sum_{i=1}^{n}\sum_{j=1}^{r-1}\sum_{k=j+1}^{r}d(v_i^j,v_i^k)+\sum_{i=1}^{n-1}\sum_{j=i+1}^{n}\sum_{k=1}^{r}\sum_{t=1}^{r}d(v_i^k,v_j^t)$$

$= r + n + 2nr + 2nr + 3nr^2 + n(n-2) + nr + r(3n^2-5n) + nr(r-1) + r^2n(2n-3)$
$= r^2(2n^2 + n) + r(3n^2-n + 1) + (n^2-n)$.

Hence, we derivethe desire conclusion.

Theorem 3: $W(\tilde{F}_n) = 6n^2-13n + 10$.

Proof: Let Pn = $v_1v_2\ldots$ vn and $v_{i,i+1}$ be the adding vertex between vi and vi + 1. Let v be a vertex in Fn beside Pn. By virtue of the definition of Wiener index, we get

$$W(\tilde{F}_n)=\sum_{i=1}^{n}d(v,v_i)+\sum_{i=1}^{n-1}d(v,v_{i,i+1})$$

$$+\sum_{i=1}^{n-1}\sum_{j=i+1}^{n}d(v_i,v_j)+\sum_{i=1}^{n}\sum_{j=1}^{n-1}d(v_i,v_{j,j+1})$$

$$+\sum_{i=1}^{n-2}\sum_{j=i+1}^{n-1}d(v_{i,i+1},v_{j,j+1})$$

$= n + 2(n-1) + n(n-1) + (3n^2-7n + 4) + 2(n-2)^2$
$= 6n^2-13n + 10$.

Thus, the desire result is given.

Theorem 4: $W(\tilde{F}_n) = 6n^2-6n$.

Proof: Let Cn = $v_1v_2\ldots$vn and v be a vertex in Wn beside Cn. Let $v_{i,i+1}$ be the adding vertex between viand vi + 1. In view of the definition of Wiener index, we deduce

$$W(\tilde{W}_n)=\sum_{i=1}^{n}d(v,v_i)+\sum_{i=1}^{n}d(v,v_{i,i+1})$$

$$+\sum_{i=1}^{n-1}\sum_{j=i+1}^{n}d(v_i,v_j)+\sum_{i=1}^{n}\sum_{j=1}^{n}d(v_i,v_{j,j+1})$$

$$+\sum_{i=1}^{n-1}\sum_{j=i+1}^{n} d(v_{i,i+1)}, v_{j,j+1})$$

= n + 2n + n(n-1) + (3n²-4n) + n(2n-4)

= 6n² – 6n.

Hence, we get the desire conclusion.

Theorem 5: $W(I_r(\tilde{F}_n)) = r^2(10n^2\text{-}13n + 9) + r(16n^2\text{-}28n + 21) + (6n^2\text{-}13n + 10)$.

Proof: Let Pn = v1v2 …vn and $v_{i,i+1}$ be the adding vertex between viand vi + 1. Let $v_i^1, v_i^2, \ldots, v_i^r$ be the r hanging vertices of vi $(1 \le i \le n)$. Let $v^1_{i,i+1}, v^2_{i,i+1}, \ldots, v^r_{i,i+1}$ be the r hanging vertices of $v_{i,i+1}(1 \le i \le n\text{-}1)$. Let v be a vertex in Fn beside Pn and the r hanging vertices of v be v^1, v2, …, v^4.

By virtue ofthe definition of Wiener index, we get

$$W(I_r(\tilde{F}_n)) = \sum_{i=1}^{r} d(v, v^i) + \sum_{i=1}^{n} d(v, v_i)$$

$$+\sum_{i=1}^{n}\sum_{j=1}^{r} d(v, v_i^j) + \sum_{i=1}^{n}\sum_{j=1}^{r} d(v_i, v^j)$$

$$+\sum_{i=1}^{n}\sum_{j=1}^{r}\sum_{k=1}^{r} d(v_i^j, v^k) + \sum_{i=1}^{n-1}\sum_{j=i+1}^{n} d(v_i, v_j)$$

$$+\sum_{i=1}^{n}\sum_{j=1}^{r} d(v_i, v_i^j) + \sum_{i=1}^{n}\sum_{j\in\{1,2,\ldots,n\}}\sum_{k=1}^{r} d(v_i, v_j^k)$$

$$+\sum_{i=1}^{n}\sum_{j=1}^{r-1}\sum_{k=j+1}^{r} d(v_i^j, v_i^k) + \sum_{i=1}^{n-1}\sum_{j=i+1}^{n}\sum_{k=1}^{r}\sum_{t=1}^{r} d(v_i^k, v_j^t)$$

$$+\sum_{i=1}^{n-1} d(v, v_{i,i+1}) + \sum_{i=1}^{n-1}\sum_{j=1}^{r} d(v, v^j_{i,i+1})$$

$$+\sum_{i=1}^{r}\sum_{j=1}^{n-1} d(v^i, v_{j,j+1}) + \sum_{i=1}^{r}\sum_{j=1}^{n-1}\sum_{k=1}^{r} d(v^i, v^k_{j,j+1})$$

$$+\sum_{i=1}^{n}\sum_{j=1}^{n-1} d(v_i, v_{j,j+1}) + \sum_{i=1}^{n}\sum_{j=1}^{n-1}\sum_{k=1}^{r} d(v_i, v^k_{j,j+1})$$

$$+\sum_{i=1}^{n}\sum_{j=1}^{r}\sum_{k=1}^{n-1} d(v_i^j, v_{k,k+1}) + \sum_{i=1}^{n}\sum_{j=1}^{r}\sum_{k=1}^{n-1}\sum_{t=1}^{r} d(v_i^j, v^r_{k,k+1})$$

$$+\sum_{i=1}^{n-2}\sum_{j=i+1}^{n-1} d(v_{i,i+1}, v_{j,j+1}) + \sum_{i=1}^{n-1}\sum_{j=1}^{r} d(v_{i,i+1}, v^j_{i,i+1})$$

$$+\sum_{i=1}^{n-1}\sum_{j\in\{1,2,\ldots,n-1\}-i}\sum_{k=1}^{r} d(v_{i,i+1}, v^k_{j,j+1}) + \sum_{i=1}^{n-1}\sum_{j=1}^{r-1}\sum_{k=j+1}^{r} d(v^j_{i,i+1}, v^k_{i,i+1})$$

$$+\sum_{i=1}^{n-2}\sum_{j=i+1}^{n-1}\sum_{k=1}^{r}\sum_{t=1}^{r} d(v^k_{i,i+1}, v^t_{j,j+1})$$

= r + n + 2nr + 2nr + 3nr² + n(n-1) + nr + 3n(n-1)r + nr(r-1) + 2r²n(n-1) + 2(n-1) + 3r(n-1) + 3r(n-1) + 4r²(n-1) + (n-1)(3n-4) + 4r(n-1)² + 4r(n-1)² + r²(5n-4)(n-1) + 2(n-2)² + r(n-1) + r(5n²-19n + 18) + r(n-1)(r-1) + (n-2)(3n-5)r²

= r²(10n²-13n + 9) + r(16n²-28n + 21) + (6n²-13n + 10).

Thus, the result is hold.

Theorem 6: $W(I_r(\tilde{W}_n)) = r^2(10n^2\text{-}4n) + r(16n^2\text{-}8n + 1) + (6n^2\text{-}6n)$.

Proof: Let Cn = v_1v_2…vn and v be a vertex in Wn beside Cn. $v_{i,i+1}$ be the adding vertex between viand vi + 1. Let v^1, v^2, …, v^r be the r hanging vertices of v and $v_i^1, v_i^2, \ldots, v_i^r$ be the r hanging vertices of vi $(1 \le i \le n)$. Let $v_{n,n+1}$ = and $v^1_{i,i+1}, v^2_{i,i+1}, \ldots, v^r_{i,i+1}$ be the r hanging vertices of $(1 \le i \le n)$. In view of the definition of Wiener index, we deduce

$$W(I_r(\tilde{W}_n)) = \sum_{i=1}^{r} d(v, v^i) + \sum_{i=1}^{n} d(v, v_i) + \sum_{i=1}^{n}\sum_{j=1}^{r} d(v, v_i^j)$$

$$+\sum_{i=1}^{n}\sum_{j=1}^{r} d(v_i, v^j) + \sum_{i=1}^{n}\sum_{j=1}^{r}\sum_{k=1}^{r} d(v_i^j, v^k) + \sum_{i=1}^{n-1}\sum_{j=i+1}^{n} d(v_i, v_j)$$

$$+\sum_{i=1}^{n}\sum_{j=1}^{r} d(v_i, v_i^j) + \sum_{i=1}^{n}\sum_{j\in\{1,2,\ldots,n\}-i}\sum_{k=1}^{r} d(v_i, v_j^k)$$

$$+\sum_{i=1}^{n}\sum_{j=1}^{r-1}\sum_{k=j+1}^{r} d(v_i^j, v_i^k) + \sum_{i=1}^{n-1}\sum_{j=i+1}^{n}\sum_{k=1}^{r}\sum_{t=1}^{r} d(v_i^k, v_j^t)$$

$$+\sum_{i=1}^{n} d(v, v_{i,i+1}) + \sum_{i=1}^{n}\sum_{j=1}^{r} d(v, v^j_{i,i+1}) + \sum_{i=1}^{r}\sum_{j=1}^{n} d(v^i, v_{j,j+1})$$

$$+\sum_{i=1}^{r}\sum_{j=1}^{n}\sum_{k=1}^{r} d(v^i, v^k_{j,j+1}) + \sum_{i=1}^{n}\sum_{j=1}^{n} d(v_i, v_{j,j+1})$$

$$+\sum_{i=1}^{n}\sum_{j=1}^{n}\sum_{k=1}^{r} d(v_i, v^k_{j,j+1}) + \sum_{i=1}^{n}\sum_{j=1}^{r}\sum_{k=1}^{n} d(v_i^j, v_{k,k+1})$$

$$+\sum_{i=1}^{n}\sum_{j=1}^{r}\sum_{k=1}^{n}\sum_{t=1}^{r} d(v_i^j, v^r_{k,k+1}) + \sum_{i=1}^{n-1}\sum_{j=i+1}^{n} d(v_{i,i+1}, v_{j,j+1})$$

$$+\sum_{i=1}^{n}\sum_{j=1}^{r} d(v_{i,i+1}, v^j_{i,i+1}) + \sum_{i=1}^{n}\sum_{j\in\{1,2,\ldots,n\}-1}\sum_{k=1}^{r} d(v_{i,i+1}, v^k_{j,j+1})$$

$$+\sum_{i=1}^{n}\sum_{j=1}^{r-1}\sum_{k=j+1}^{r} d(v^j_{i,i+1}, v^k_{i,i+1}) + \sum_{i=1}^{n-1}\sum_{j=i+1}^{n}\sum_{k=1}^{r}\sum_{t=1}^{r} d(v^k_{i,i+1}, v^t_{j,j+1})$$

= r + n + 2nr + 2nr + 3nr² + n(n-1) + nr + 3n(n-1)r-nr(r-1) + 2n(n-1)r² + 2n + 3rn + 3rn + 4r²n + n(3n-4) + 4rn(n-1) + 4rn(n-1) + r²n(5n-4) + 2n(n-2) + rn + r(5n²-9n) + nr(r-1) + (3n²-5n)r²

= r²(10n²-4n) + r(16n²-8n + 1) + (6n²-6n).

As conclusion, we obtainthe finalconclusion.

Conclusion

Combinatorial chemistry is a new powerful technology in molecular recognition and drug design. It is a wet-laboratory methodology purposedto massively parallel screening of chemical compounds for the founding of compounds that have certain biological activities. The power of trickdraws from the interaction between computational modeling and experimental design.

Fan graph, wheel graph, gear fan graph, gear wheel graph and their *r*-corona graphs are common structural features of organic molecules. The contributions of our paper are determining the Wiener index of these special structural features of organic molecules.

ACKNOWLEDGEMENTS

This work was supported in part by the Ph.D. start funding to first author.

REFERENCES

1. L. Yan, Y.F. Li, W. Gao and J.S. Li, *J. Chem. Pharm. Res*., **5**, 260 (2013).
2. Y.J. Pan, J. Math. *Stu*., **42**, 280 (2009).
3. D.Q. Chen, X. Dong and Z. Fan, *J. Wuhan Inst. Chem. Tech*., **27**, 82 (2012).
4. B.H. Xing and G.X. Cai, *OR Tran*., **15**, 36 (2011).
5. H. Wan and H.Z. Ren, *J. Math. Stu*., **45**, 207 (2012).
6. Y.J. Pan, *J. Math. Stu*., **46**, 260 (2013).
7. D. Stevanovic, *Match Commun. Math. Comput. Chem.*, **60**, 71 (2008).
8. Y. Hong, H.Q. Liu and X.Y. Wu, *Hacet. J. Math. Stat*, **40**, 63 (2011).
9. X.D. Zhang and Q.Y. Xiang, *Match Commun. Math. Comput. Chem*., **60**, 623 (2008).
10. G. Cash, S. Klav•ar and M. Petkovšek, *J. Chem. Inf. Comput. Sci*., **42**, 571 (2002).
11. E. Castro, I. Gutman, D. Marino and P. Peruzzo, *J. Serb. Chem. Soc*., **67**, 647 (2002).
12. B. Wu, *Match Commun. Math. Comput. Chem*., **64**, 699 (2010).
13. A. Vijayabarathi and G.S.G.N. Anjaneyulu, *Int. J. Chem. Tech. Res*., **5**, 1847 (2013).
14. P. Dankelmann, I. Gutman, S. Mukwembi and H.C. Swart, *Discrete Math*., **309**, 3452 (2009).
15. A.A. Dobrynin, R. Entringer and I. Gutman, *Acta Appl. Math*., **66**, 211 (2001).