ISSN : 0974 - 7435 Volume 10 Issue 12

2014

BioTechnology

An Indian Journal

FULL PAPER

BTAIJ, 10(12), 2014 [6230-6235]

Hyper-wiener index of hexagonal mobius graph

Jiayong Dou[1]*, Yaya Wang[1], Wei Gao[2]

[1]Department of Information Engineering, Binzhou Polytechnic, Binzhou, (CHINA)

[2]School of Information Science and Technology, Yunnan Normal University, Kunming, (CHINA)

ABSTRACT

Hyper-Wiener index is an important topological index in theoretical chemistry. Physical chemical properties of material are closely related to this index. Hexagonal Mobius graphs are one type of molecular graphs embedded into the Mobius strip such that each face is a hexagon. In this paper, we obtain the Hyper-Wiener index of the two classes of hexagonal Mobius graphs.

KEYWORDS

Chemical graph theory; Organic molecules; Hyper-Wiener index; Hexagonal mobius graph; Automorphism.

INTRODUCTION

The Hyper-Wiener index, as an extension of Wiener index, is an important topological index in Chemistry. It is used for the structure of molecule. There is a very close relation between the physical, chemical characteristics of many compounds and the topological structure of that. The Hyper-Wiener index is such a topological index and it has been widely used in Chemistry fields.

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.

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:

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

Some conclusions for Hyper-Wiener index and Wiener index can refer to[1-5]. Pan[6] deduced the formula of Wiener number and Hyper-Wiener number of two types of polyomino systems. Tang[7] studied the Wiener indices of unicycles graphs. Firstly, it gave a formulation for calculating the Wiener index of an unicycles graphs according its struction. And then, in terms of this formulation, it characterized the graphs with the largest, the smallest, the second largest, the second smallest, the third largest and the third smallest Wiener indies among all the unicycles graphs. Xing et al.,[8] determined the n-vertex unicyclic graphs of cycle length r with the smallest and the largest Hyper-Wiener indices for $3 \le r \le n$, and the n-vertex unicyclic graphs with the smallest, the second smallest, the largest and the second largest Hyper-Wiener indices for $n \ge 5$. Yuan[9] learned the special class of unicyclic graph. Feng et al.,[10] determined the extremal bicyclic graphs with maximal and minimal hyper-Wiener index. Chen[11] investigated the properties of the Wiener index of unicyclic graphs, which are used to give a lower bound for the Wiener index of unicylic graphs of order 2β having perfect matching. Moreover, all extremal unicyclic graphs which attain the lower bound were characterized. Qi and Zhou[12] determined the minimum Hyper-Wiener index of unicylic graphs with given number of vertices and matching number, and characterized the extremal graphs. Feng and llic[13] presented sharp bounds for the Zagreb indices, Harary index and hyper-Wiener index of graphs with a given matching number, and we also completely determine the extremal graphs. Also, Du and Zhou[14] determined the minimum Wiener indices of trees and unicyclic graphs with given number of vertices and matching number respectively, and the extremal graphs are characterized.

Let G=(V, E) and H=(V', E') be two graphs. $G \times H$ is a such graph, its vertex set is $V \times V'$, there exist an edge between (a, x) an (b, y) if and only if one of following condition holds: (1) $ab \in E$ and x=y; (2) a=b and $xy \in E'$. Let $V(P_k)$={0,1,…,k-1}. The hexagonal Mobius graph with length 2k and width 2 denoted by $H_{2,2k}$ is defined as follows: deleting edges {(0, 2j+1) (1, 2j+1)|$0 \le j \le k$-1} from $P_2 \times P_{2k}$, then adding edges (1,0)(0,2k-1) and (0,0)(1,2k-1). The hexagonal Mobius graph with length 2k+1 and width 3 denoted by $H_{3,2k+1}$ is defined as follows: deleting edges {(0, 2j) (1, 2j)|$0 \le j \le k$} from $P_3 \times P_{2k+1}$, then adding edges (0,0)(2,2k), (1,0)(1,2k) and (2,0)(0,2k).

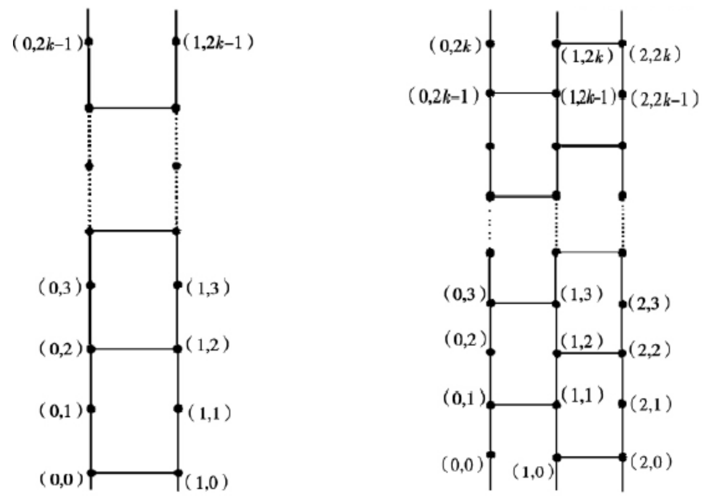

Figure 1 : $H_{2,2k}$ and $H_{3,2k+1}$

In this paper, we determine the Hyper-Wiener index of above two hexagonal Mobius graphs.

Main results and proof

Theorem 1. $WW(H_{2,2k}) = \begin{cases} 8, & k=1 \\ 70, & k=2 \\ k(4\sum_{i=1}^{k} i^2 + 2) + 2k^2(k+1), & k \geq 3 \end{cases}$.

Proof. When k=1 and k=2, $H_{2,2}$ and $H_{2,4}$ are isomorphism to following graphs (see Figure 2.), respectively. By the definition of Hyper-wiener index and directly computing, we have $WW(H_{2,2})$=8 and $WW(H_{2,4})$=70.

When $k \geq 3$, the vertices of $H_{2,2k}$ have two orbits under its automorphism group, and all the 2k vertices with degree 2 in one orbit and all the 2k vertices with degree 3 in the other orbit.

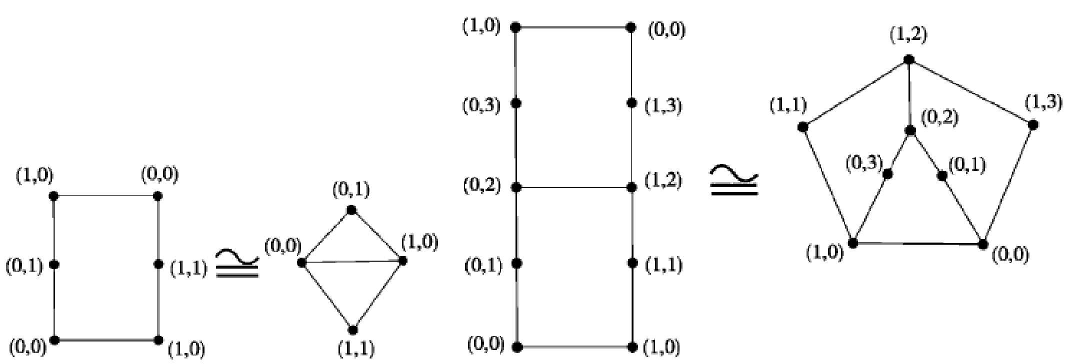

Figure 2 : The graphs isomorphism to $H_{2,2}$ and $H_{2,4}$, respectively.

- Taking any vertex v with degree 2, the sum of distance square from v to other vertex is calculated by (see left graph of Figure 3.)

$$2\times 2(1^2+2^2+\cdots+k^2)-2^2+3^2=4\sum_{i=1}^{k} i^2+5\,.$$

- Taking any vertex v with degree 3, the sum of distance square from v to other vertex is calculated by (see right graph of Figure 3.)

$$2\times 2(1^2+2^2+\cdots+k^2)-1^2=4\sum_{i=1}^{k} i^2-1\,.$$

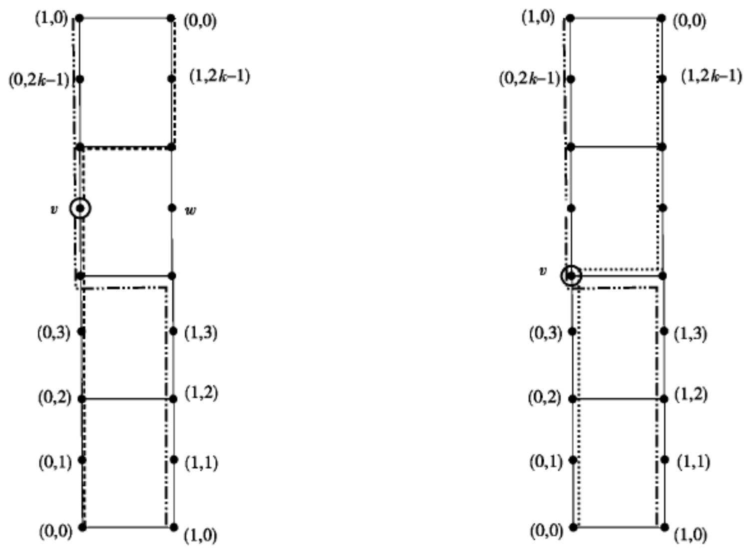

Figure 3 : Distance computing by taking any vertex with degree 2 or 3 from $H_{2,2k}$ respectively.

Hence, we infer

$$WW(H_{2,2k})=\frac{1}{2}\{\frac{1}{2}\{2k\times(4\sum_{i=1}^{k}i^2+5)+2k\times(4\sum_{i=1}^{k}i^2-1)\}+\frac{1}{2}\{2k\times[2k(k+1)+1]+2k\times[2k(k+1)-1]\}\}$$

$$=\frac{1}{2}\{\{k(8\sum_{i=1}^{k}i^2+4)\}+\{4k^2(k+1)\}\}=k(4\sum_{i=1}^{k}i^2+2)+2k^2(k+1)\,.\ \square$$

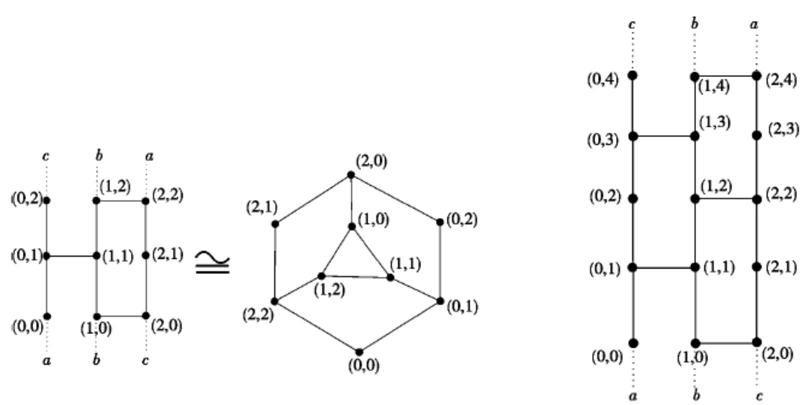

Figure 4 : The graph isomorphism to $H_{3,3}$ and the structure of $H_{3,5}$, respectively.

Theorem 2. $$WW(H_{3,2k+1}) = \begin{cases} 102, & k=1 \\ 465, & k=2 \\ \dfrac{2k+1}{4}\{18\sum_{i=1}^{k} i^2 + (25k^2+57k+88)\}, & k \geq 3 \end{cases}.$$

Proof. When k=1, $H_{3,3}$ is isomorphism to left graph of Figure 4. By the definition of Hyper-wiener index and directly computing, we have $WW(H_{3,3})$=102. When k=2, the structure of $H_{3,5}$ is showed in right graph of Figure 4. We yield $WW(H_{3,5})$ =465.

When $k \geq 3$, the vertices of $H_{3,2k+1}$ have three orbits under its automorphism group, and all the vertices with degree 2 and degree in boundary in the first and second orbit respectively, and all the inner vertices with degree 3 in the third orbit.

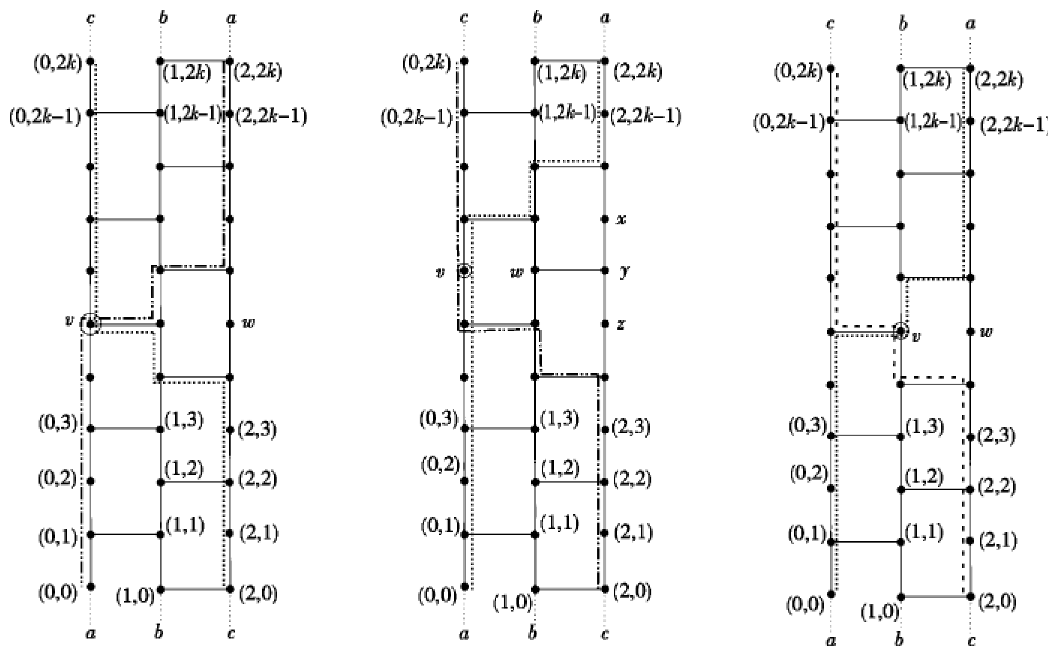

Figure 5 : Distance computing by taking any vertex from $H_{3,2k+1}$.

- There are 2k+1 vertices with degree 3 in boundary. Taking any vertex v, the sum of distance square from v to other vertex is calculated by (see middle graph of Figure 5.)

$$\{2\times 2(1^2+2^2+\cdots+(k+1)^2)-1^2\} + \{2(1^2+2^2+\cdots+(k+1)^2)-1^2\} - (2^2+1^2+2^2)+4^2 = 6\sum_{i=1}^{k+1} i^2 + 5 .$$

- There are 2k+1 vertices with degree 2 in boundary. Taking any vertex v, the sum of distance square from v to other vertex is calculated by (see left graph of Figure 5.)

$$\{2\times 2(1^2+2^2+\cdots+(k+1)^2)-2^2+3^2+4^2+5^2+5^2\}+\{2(2^2+\cdots+(k+1)^2)-(2^2+2^2+3^2+3^2)\}=6\sum_{i=1}^{k+1}i^2+45\,.$$

• There are $2k+1$ inner vertices with degree 3. Taking any vertex v, the sum of distance square from v to other vertex is calculated by (see right graph of Figure 5.)

$$\{2\times 2(1^2+2^2+\cdots+(k+1)^2)-1^2\}+\{2(1^2+2^2+\cdots+k^2)-(1^2+1^2)\}+3^2=6\sum_{i=1}^{k}i^2+4(k+1)^2+6\,.$$

Hence, we infer

$$WW(H_{3,2k+1})=\frac{1}{2}\{\frac{2k+1}{2}[6\sum_{i=1}^{k+1}i^2+5+6\sum_{i=1}^{k+1}i^2+45+6\sum_{i=1}^{k}i^2+4(k+1)^2+6]+\frac{2k+1}{2}(k+1)(9k+16)\}$$

$$=\frac{2k+1}{4}\{18\sum_{i=1}^{k}i^2+(25k^2+57k+88)\}\,.\ \square$$

ACKNOWLEDGEMENTS

First, we thank the reviewers for their constructive comments in improving the quality of this paper. This work was supported in part by Binzhou Polytechnic Fund (2011XYKT01) and (2013XYKT08). We also would like to thank the anonymous referees for providing us with constructive comments and suggestions.

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