

Certain General Zagreb Indices and Zagreb Polynomials of Molecular Graphs

Yun Gao^{1, *}, Wei Gao², Li Liang²

¹Department of Editorial, Yunnan Normal University, Kunming, China

²School of Information Science and Technology, Yunnan Normal University, Kunming, China

Abstract

Chemical compounds and drugs are often modelled 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. In this paper, by virtue of mathematical derivation, we determine the fourth, fifth and sixth general Zagreb indices and Zagreb polynomials of fan molecular graph, wheel molecular graph, and gear fan molecular graph, gear wheel molecular graph, and their r -corona molecular graphs. The results obtained in our paper illustrate the promising application prospects for chemistry and pharmacy science.

Keywords

Chemical Graph Theory, General Zagreb Index, Zagreb Polynomial, R-Corona Molecular Graph

Received: April 15, 2015 / Accepted: May 10, 2015 / Published online: June 8, 2015

© 2015 The Authors. Published by American Institute of Science. This Open Access article is under the CC BY-NC license.

<http://creativecommons.org/licenses/by-nc/4.0/>

1. Introduction

Wiener index, edge Wiener index, Hyper-wiener index, Geometric-arithmetic index and Zagreb indices are introduced to reflect certain structural features of organic molecules. Several papers contributed to determine the distance-based index of special molecular graphs (See Yan et al., [1-2], Gao et al., [3-4], Gao and Shi [5], Gao and Wang [6], Xi and Gao [7-8], Xi et al., [9], Gao et al., [10] for more detail). The notation and terminology used but undefined in this paper can be found in [11].

Let P_n and C_n be path and cycle with n vertices. The molecular graph $F_n = \{v\} \vee P_n$ is called a fan molecular graph and the molecular graph $W_n = \{v\} \vee C_n$ is called a wheel molecular graph. Molecular graph $I_r(G)$ is called r -crown molecular graph of G which splicing r hang edges for every vertex in G . By adding one vertex in every two adjacent vertices of the fan path P_n of fan molecular graph F_n , the resulting molecular graph is a subdivision molecular graph called gear fan

molecular graph, denote as \tilde{F}_n . By adding one vertex in every two adjacent vertices of the wheel cycle C_n of wheel molecular graph W_n , The resulting molecular graph is a subdivision molecular graph, called gear wheel molecular graph, denoted as \tilde{W}_n .

The eccentricity $ec(u)$ of vertex $u \in V(G)$ is the maximum distance between u and any other vertex in G . In [12], Gao introduced the following general indices and polynomials:

The general fourth Zagreb index: $Zg_4^k(G) = \sum_{u \in E(G)} (ec(u) + ec(v))^k$

The general fifth Zagreb index: $Zg_5^k(G) = \sum_{v \in V(G)} ec(v)^k$

The general sixth Zagreb index: $Zg_6^k(G) = \sum_{u \in E(G)} (ec(u)ec(v))^k$

* Corresponding author

E-mail address: gaoyun@ynnu.edu.cn (Yun Gao)

The fourth Zagreb polynomial: $Zg_4(G, x) = \sum_{uv \in E(G)} x^{ec(u)+ec(v)} = \sum_{i=1}^r 6^k + \sum_{i=1}^n 6^k + \sum_{i=1}^{n-1} 9^k + \sum_{i=1}^n \sum_{j=1}^r 12^k$

The fifth Zagreb polynomial: $Zg_5(G, x) = \sum_{v \in V(G)} x^{ec(v)^2} = (n+r)6^k + (n-1)9^k + nr \cdot 12^k$

The sixth Zagreb polynomial: $Zg_6(G, x) = \sum_{uv \in E(G)} x^{ec(u)ec(v)}$
 $Zg_6(I_r(F_n), x) = \sum_{i=1}^r x^{ec(v)+ec(v^i)} + \sum_{i=1}^n x^{ec(v)+ec(v_i)} + \sum_{i=1}^{n-1} x^{ec(v_i)+ec(v_{i+1})}$
 $+ \sum_{i=1}^n \sum_{j=1}^r x^{ec(v_i)+ec(v_j^i)}$

Here, k is a real number.

In this paper, we present these indices and polynomials of $I_r(F_n)$, $I_r(W_n)$, $I_r(\tilde{F}_n)$ and $I_r(\tilde{W}_n)$.

2. Main Results and Proofs

Theorem 1.

$$Zg_4^k(I_r(F_n)) = (n+r)5^k + (n-1)6^k + nr7^k,$$

$$Zg_5^k(I_r(F_n)) = 2^k + (n+r)3^k + nr4^k,$$

$$Zg_6^k(I_r(F_n)) = (n+r)6^k + (n-1)9^k + nr \cdot 12^k,$$

$$Zg_4(I_r(F_n), x) = (n+r)x^5 + (n-1)x^6 + nrx^7,$$

$$Zg_5(I_r(F_n), x) = x^4 + (n+r)x^9 + nrx^{16},$$

$$Zg_6(I_r(F_n), x) = (n+r)x^6 + (n-1)x^9 + nrx^{12}.$$

Proof. Let $P_n = v_1 v_2 \dots v_n$ and the r hanging vertices of v_i be $v_i^1, v_i^2, \dots, v_i^r$ ($1 \leq i \leq n$). Let v be a vertex in F_n beside P_n , and the r hanging vertices of v be v^1, v^2, \dots, v^r . By the definition of general Zagreb indices and Zagreb polynomials, we have

$$\begin{aligned} Zg_4^k(I_r(F_n)) &= \sum_{i=1}^r (ec(v) + ec(v^i))^k + \sum_{i=1}^n (ec(v) + ec(v_i))^k + \\ &\sum_{i=1}^{n-1} (ec(v_i) + ec(v_{i+1}))^k + \sum_{i=1}^n \sum_{j=1}^r (ec(v_i) + ec(v_j^i))^k \\ &= \sum_{i=1}^r 5^k + \sum_{i=1}^n 5^k + \sum_{i=1}^{n-1} 6^k + \sum_{i=1}^n \sum_{j=1}^r 7^k \\ &= (n+r)5^k + (n-1)6^k + nr7^k. \end{aligned}$$

$$\begin{aligned} Zg_5^k(I_r(F_n)) &= ec(v)^k + \sum_{i=1}^n ec(v_i)^k + \sum_{i=1}^r ec(v^i)^k + \\ &\sum_{i=1}^n \sum_{j=1}^r ec(v_j^i)^k = 2^k + (n+r)3^k + nr4^k. \end{aligned}$$

$$\begin{aligned} Zg_6^k(I_r(F_n)) &= \sum_{i=1}^r (ec(v)ec(v^i))^k + \sum_{i=1}^n (ec(v)ec(v_i))^k + \\ &\sum_{i=1}^{n-1} (ec(v_i)ec(v_{i+1}))^k + \sum_{i=1}^n \sum_{j=1}^r (ec(v_i)ec(v_j^i))^k \end{aligned}$$

$$\begin{aligned} &= \sum_{i=1}^r 6^k + \sum_{i=1}^n 6^k + \sum_{i=1}^{n-1} 9^k + \sum_{i=1}^n \sum_{j=1}^r 12^k \\ &= (n+r)6^k + (n-1)9^k + nr \cdot 12^k \\ Zg_4(I_r(F_n), x) &= \sum_{i=1}^r x^{ec(v)+ec(v^i)} + \sum_{i=1}^n x^{ec(v)+ec(v_i)} + \sum_{i=1}^{n-1} x^{ec(v_i)+ec(v_{i+1})} \\ &+ \sum_{i=1}^n \sum_{j=1}^r x^{ec(v_i)+ec(v_j^i)} \\ &= \sum_{i=1}^r x^5 + \sum_{i=1}^n x^5 + \sum_{i=1}^{n-1} x^6 + \sum_{i=1}^n \sum_{j=1}^r x^7 \\ &= (n+r)x^5 + (n-1)x^6 + nrx^7. \end{aligned}$$

$$\begin{aligned} Zg_5(I_r(F_n), x) &= x^{ec(v)^2} + \sum_{i=1}^n x^{ec(v_i)^2} + \sum_{i=1}^r x^{ec(v^i)^2} + \sum_{i=1}^n \sum_{j=1}^r x^{ec(v_j^i)^2} = \\ &x^4 + (n+r)x^9 + nrx^{16}. \end{aligned}$$

$$\begin{aligned} Zg_6(I_r(F_n), x) &= \sum_{i=1}^r x^{ec(v)ec(v^i)} + \sum_{i=1}^n x^{ec(v)ec(v_i)} + \sum_{i=1}^{n-1} x^{ec(v_i)ec(v_{i+1})} + \\ &\sum_{i=1}^n \sum_{j=1}^r x^{ec(v_i)ec(v_j^i)} = \sum_{i=1}^r x^6 + \sum_{i=1}^n x^6 + \sum_{i=1}^{n-1} x^9 + \sum_{i=1}^n \sum_{j=1}^r x^{12} \\ &= (n+r)x^6 + (n-1)x^9 + nrx^{12}. \end{aligned}$$

Corollary 1.

$$Zg_4^k(F_n) = n5^k + (n-1)6^k,$$

$$Zg_5^k(F_n) = 2^k + n3^k,$$

$$Zg_6^k(F_n) = n6^k + (n-1)9^k,$$

$$Zg_4(F_n, x) = nx^5 + (n-1)x^6,$$

$$Zg_5(F_n, x) = x^4 + nx^9,$$

$$Zg_6(F_n, x) = nx^6 + (n-1)x^9.$$

Theorem 2.

$$Zg_4^k(I_r(W_n)) = (n+r)5^k + n6^k + nr7^k,$$

$$Zg_5^k(I_r(W_n)) = 2^k + (n+r)3^k + nr4^k,$$

$$Zg_6^k(I_r(W_n)) = (n+r)6^k + n9^k + nr \cdot 12^k,$$

$$Zg_4(I_r(W_n), x) = (n+r)x^5 + nx^6 + nrx^7,$$

$$Zg_5(I_r(W_n), x) = x^4 + (n+r)x^9 + nrx^{16},$$

$$Zg_6(I_r(W_n), x) = (n+r)x^6 + nx^9 + nrx^{12}.$$

Proof. Let $C_n = v_1 v_2 \dots v_n$ and $v_i^1, v_i^2, \dots, v_i^r$ be the r hanging

vertices of v_i ($1 \leq i \leq n$). Let v be a vertex in W_n beside C_n , and v^1, v^2, \dots, v^r be the r hanging vertices of v . By the definition of general Zagreb indices and Zagreb polynomials, we have

$$\begin{aligned} Zg_4^k(I_r(W_n)) &= \sum_{i=1}^r (ec(v) + ec(v^i))^k + \sum_{i=1}^n (ec(v) + ec(v_i))^k + \\ &\sum_{i=1}^n (ec(v_i) + ec(v_{i+1}))^k + \sum_{i=1}^n \sum_{j=1}^r (ec(v_i) + ec(v_i^j))^k \\ &= \sum_{i=1}^r 5^k + \sum_{i=1}^n 5^k + \sum_{i=1}^n 6^k + \sum_{i=1}^n \sum_{j=1}^r 7^k \\ &= (n+r)5^k + n6^k + nr7^k. \end{aligned}$$

$$\begin{aligned} Zg_5^k(I_r(W_n)) &= ec(v)^k + \sum_{i=1}^n ec(v_i)^k + \sum_{i=1}^r ec(v^i)^k + \\ &\sum_{i=1}^n \sum_{j=1}^r ec(v_i^j)^k = 2^k + (n+r)3^k + nr4^k. \end{aligned}$$

$$\begin{aligned} Zg_6^k(I_r(W_n)) &= \sum_{i=1}^r (ec(v)ec(v^i))^k + \sum_{i=1}^n (ec(v)ec(v_i))^k + \\ &\sum_{i=1}^n (ec(v_i)ec(v_{i+1}))^k + \sum_{i=1}^n \sum_{j=1}^r (ec(v_i)ec(v_i^j))^k \\ &= \sum_{i=1}^r 6^k + \sum_{i=1}^n 6^k + \sum_{i=1}^n 9^k + \sum_{i=1}^n \sum_{j=1}^r 12^k \\ &= (n+r)6^k + n9^k + nr \cdot 12^k. \end{aligned}$$

$$\begin{aligned} Zg_4(I_r(W_n), x) &= \sum_{i=1}^r x^{ec(v)+ec(v^i)} + \sum_{i=1}^n x^{ec(v)+ec(v_i)} + \sum_{i=1}^n x^{ec(v_i)+ec(v_{i+1})} \\ &+ \sum_{i=1}^n \sum_{j=1}^r x^{ec(v_i)+ec(v_i^j)} = \sum_{i=1}^r x^5 + \sum_{i=1}^n x^5 + \sum_{i=1}^n x^6 + \sum_{i=1}^n \sum_{j=1}^r x^7 = \\ &(n+r)x^5 + nx^6 + nrx^7. \end{aligned}$$

$$\begin{aligned} Zg_5(I_r(W_n), x) &= x^{ec(v)^2} + \sum_{i=1}^n x^{ec(v_i)^2} + \sum_{i=1}^r x^{ec(v^i)^2} + \sum_{i=1}^n \sum_{j=1}^r x^{ec(v_i^j)^2} \\ &= x^4 + (n+r)x^9 + nrx^{16}. \end{aligned}$$

$$\begin{aligned} Zg_6(I_r(W_n), x) &= \sum_{i=1}^r x^{ec(v)ec(v^i)} + \sum_{i=1}^n x^{ec(v)ec(v_i)} + \sum_{i=1}^n x^{ec(v_i)ec(v_{i+1})} + \\ &\sum_{i=1}^n \sum_{j=1}^r x^{ec(v_i)ec(v_i^j)} \\ &= \sum_{i=1}^r x^6 + \sum_{i=1}^n x^6 + \sum_{i=1}^n x^9 + \sum_{i=1}^n \sum_{j=1}^r x^{12} \\ &= (n+r)x^6 + nx^9 + nrx^{12}. \end{aligned}$$

Corollary 2.

$$Zg_4^k(W_n) = n5^k + n6^k,$$

$$Zg_5^k(W_n) = 2^k + n3^k,$$

$$Zg_6^k(W_n) = n6^k + n9^k,$$

$$Zg_4(W_n, x) = nx^5 + nx^6,$$

$$Zg_5(W_n, x) = x^4 + nx^9,$$

$$Zg_6(W_n, x) = nx^6 + nx^9.$$

Theorem 3.

$$Zg_4^k(I_r(\tilde{F}_n)) = (r+n)7^k + (nr+2n-2)9^k + (n-1)r \cdot 11^k,$$

$$Zg_5^k(I_r(\tilde{F}_n)) = 3^k + (n+r)4^k + (nr+n-1)5^k + (n-1)r6^k,$$

$$Zg_6^k(I_r(\tilde{F}_n)) = (r+n) \cdot 12^k + (nr+2n-2) \cdot 20^k + (n-1)r \cdot 30^k,$$

$$Zg_4(I_r(\tilde{F}_n), x) = (r+n)x^7 + (nr+2n-2)x^9 + (n-1)rx^{11},$$

$$Zg_5(I_r(\tilde{F}_n), x) = x^9 + (n+r)x^{16} + (nr+n-1)x^{25} + (n-1)rx^{36},$$

$$Zg_6(I_r(\tilde{F}_n), x) = (r+n)x^{12} + (nr+2n-2)x^{20} + (n-1)rx^{30}.$$

Proof. Let $P_n = v_1 v_2 \dots v_n$ and $v_{i,i+1}$ be the adding vertex between v_i and v_{i+1} . Let $v_i^1, v_i^2, \dots, v_i^r$ be the r hanging vertices of v_i ($1 \leq i \leq n$). Let $v_{i,i+1}^1, v_{i,i+1}^2, \dots, v_{i,i+1}^r$ be the r hanging vertices of $v_{i,i+1}$ ($1 \leq i \leq n-1$). Let v be a vertex in F_n beside P_n , and the r hanging vertices of v be v^1, v^2, \dots, v^r . By virtue of the definition of general Zagreb indices and Zagreb polynomials, we get

$$\begin{aligned} Zg_4^k(I_r(\tilde{F}_n)) &= \sum_{i=1}^r (ec(v) + ec(v^i))^k + \sum_{i=1}^n (ec(v) + ec(v_i))^k + \\ &\sum_{i=1}^n \sum_{j=1}^r (ec(v_i) + ec(v_i^j))^k + \sum_{i=1}^{n-1} (ec(v_i) + ec(v_{i,i+1}))^k + \\ &\sum_{i=1}^{n-1} (ec(v_{i,i+1}) + ec(v_{i+1}))^k + \sum_{i=1}^{n-1} \sum_{j=1}^r (ec(v_{i,i+1}) + ec(v_{i,i+1}^j))^k \\ &= \sum_{i=1}^r 7^k + \sum_{i=1}^n 7^k + \sum_{i=1}^n \sum_{j=1}^r 9^k + \sum_{i=1}^{n-1} 9^k + \sum_{i=1}^{n-1} 9^k + \sum_{i=1}^{n-1} \sum_{j=1}^r 11^k \\ &= (r+n)7^k + (nr+2n-2)9^k + (n-1)r \cdot 11^k. \end{aligned}$$

$$Zg_5^k(I_r(\tilde{F}_n)) = ec(v)^k + \sum_{i=1}^n ec(v_i)^k + \sum_{i=1}^r ec(v^i)^k +$$

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

$$= 3^k + (n+r)4^k + (nr+n-1)5^k + (n-1)r6^k.$$

$$\begin{aligned} Zg_6^k(I_r(\tilde{F}_n)) &= \sum_{i=1}^r (ec(v)ec(v^i))^k + \sum_{i=1}^n (ec(v)ec(v_i))^k + \\ & \sum_{i=1}^n \sum_{j=1}^r (ec(v_i)ec(v_i^j))^k + \sum_{i=1}^{n-1} (ec(v_i)ec(v_{i,i+1}))^k + \\ & \sum_{i=1}^{n-1} (ec(v_{i,i+1})ec(v_{i+1}))^k + \sum_{i=1}^{n-1} \sum_{j=1}^r (ec(v_{i,i+1})ec(v_{i,i+1}^j))^k \\ &= \sum_{i=1}^r 12^k + \sum_{i=1}^n 12^k + \sum_{i=1}^n \sum_{j=1}^r 20^k + \sum_{i=1}^{n-1} 20^k + \sum_{i=1}^{n-1} 20^k + \sum_{i=1}^{n-1} \sum_{j=1}^r 30^k \\ &= (r+n) \cdot 12^k + (nr+2n-2) \cdot 20^k + (n-1)r \cdot 30^k. \end{aligned}$$

$$\begin{aligned} Zg_4(I_r(\tilde{F}_n), x) &= \sum_{i=1}^r x^{ec(v)+ec(v^i)} + \sum_{i=1}^n x^{ec(v)+ec(v_i)} + \\ & \sum_{i=1}^n \sum_{j=1}^r x^{ec(v_i)+ec(v_i^j)} + \sum_{i=1}^{n-1} x^{ec(v_i)+ec(v_{i,i+1})} + \sum_{i=1}^{n-1} x^{ec(v_{i,i+1})+ec(v_{i+1})} + \\ & \sum_{i=1}^{n-1} \sum_{j=1}^r x^{ec(v_{i,i+1})+ec(v_{i,i+1}^j)} \\ &= \sum_{i=1}^r x^7 + \sum_{i=1}^n x^7 + \sum_{i=1}^n \sum_{j=1}^r x^9 + \sum_{i=1}^{n-1} x^9 + \sum_{i=1}^{n-1} x^9 + \sum_{i=1}^{n-1} \sum_{j=1}^r x^{11} \\ &= (r+n)x^7 + (nr+2n-2)x^9 + (n-1)rx^{11}. \end{aligned}$$

$$\begin{aligned} Zg_5(I_r(\tilde{F}_n), x) &= x^{ec(v)^2} + \sum_{i=1}^n x^{ec(v_i)^2} + \sum_{i=1}^r x^{ec(v^i)^2} + \sum_{i=1}^n \sum_{j=1}^r x^{ec(v_i^j)^2} + \\ & \sum_{i=1}^{n-1} x^{ec(v_{i,i+1})^2} + \sum_{i=1}^{n-1} \sum_{j=1}^r x^{ec(v_{i,i+1}^j)^2} \\ &= x^9 + (n+r)x^{16} + (nr+n-1)x^{25} + (n-1)rx^{36}. \end{aligned}$$

$$\begin{aligned} Zg_6(I_r(\tilde{F}_n), x) &= \sum_{i=1}^r x^{ec(v)ec(v^i)} + \sum_{i=1}^n x^{ec(v)ec(v_i)} + \sum_{i=1}^n \sum_{j=1}^r x^{ec(v_i)ec(v_i^j)} \\ &+ \sum_{i=1}^{n-1} x^{ec(v_i)ec(v_{i,i+1})} + \sum_{i=1}^{n-1} x^{ec(v_{i,i+1})ec(v_{i+1})} + \sum_{i=1}^{n-1} \sum_{j=1}^r x^{ec(v_{i,i+1})ec(v_{i,i+1}^j)} \\ &= \sum_{i=1}^r x^{12} + \sum_{i=1}^n x^{12} + \sum_{i=1}^n \sum_{j=1}^r x^{20} + \sum_{i=1}^{n-1} x^{20} + \sum_{i=1}^{n-1} x^{20} + \sum_{i=1}^{n-1} \sum_{j=1}^r x^{30} \\ &= (r+n)x^{12} + (nr+2n-2)x^{20} + (n-1)rx^{30}. \end{aligned}$$

Corollary 3.

$$Zg_4^k(\tilde{F}_n) = n7^k + (2n-2)9^k,$$

$$Zg_5^k(\tilde{F}_n) = 3^k + n4^k + (n-1)5^k,$$

$$Zg_6^k(\tilde{F}_n) = n12^k + (2n-2) \cdot 20^k,$$

$$Zg_4(\tilde{F}_n, x) = nx^7 + (2n-2)x^9,$$

$$Zg_5(\tilde{F}_n, x) = x^9 + nx^{16} + (n-1)x^{25},$$

$$Zg_6(\tilde{F}_n, x) = nx^{12} + (2n-2)x^{20}.$$

Theorem 4.

$$Zg_4^k(I_r(\tilde{W}_n)) = (r+n)7^k + (nr+2n)9^k + nr \cdot 11^k,$$

$$Zg_5^k(I_r(\tilde{W}_n)) = 3^k + (n+r)4^k + (nr+n)5^k + nr6^k,$$

$$Zg_6^k(I_r(\tilde{W}_n)) = (r+n)12^k + (nr+2n)20^k + nr \cdot 30^k,$$

$$Zg_4(I_r(\tilde{W}_n), x) = (r+n)x^7 + (nr+2n)x^9 + nrx^{11},$$

$$Zg_5(I_r(\tilde{W}_n), x) = x^9 + (n+r)x^{16} + (nr+n)x^{25} + nrx^{36},$$

$$Zg_6(I_r(\tilde{W}_n), x) = (r+n)x^{12} + (nr+2n)x^{20} + nrx^{30}.$$

Proof. Let $C_n = v_1v_2 \dots v_n$ and v be a vertex in W_n beside C_n . $v_{i,i+1}$ be the adding vertex between v_i and v_{i+1} . Let v^1, v^2, \dots, v^r be the r hanging vertices of v and $v_i^1, v_i^2, \dots, v_i^r$ be the r hanging vertices of v_i ($1 \leq i \leq n$). Let $v_{n,n+1} = v_{1,n}$ and $v_{i,i+1}^1, v_{i,i+1}^2, \dots, v_{i,i+1}^r$ be the r hanging vertices of $v_{i,i+1}$ ($1 \leq i \leq n$). In view of the definition of general Zagreb indices and Zagreb polynomials, we deduce

$$\begin{aligned} Zg_4^k(I_r(\tilde{W}_n)) &= \sum_{i=1}^r (ec(v) + ec(v^i))^k + \sum_{i=1}^n (ec(v) + ec(v_i))^k + \\ & \sum_{i=1}^n \sum_{j=1}^r (ec(v_i) + ec(v_i^j))^k + \sum_{i=1}^n (ec(v_i) + ec(v_{i,i+1}))^k + \\ & \sum_{i=1}^n (ec(v_{i,i+1}) + ec(v_{i+1}))^k + \sum_{i=1}^n \sum_{j=1}^r (ec(v_{i,i+1}) + ec(v_{i,i+1}^j))^k \\ &= \sum_{i=1}^r 7^k + \sum_{i=1}^n 7^k + \sum_{i=1}^n \sum_{j=1}^r 9^k + \sum_{i=1}^n 9^k + \sum_{i=1}^n 9^k + \sum_{i=1}^n \sum_{j=1}^r 11^k \\ &= (r+n)7^k + (nr+2n)9^k + nr \cdot 11^k. \end{aligned}$$

$$\begin{aligned} Zg_5^k(I_r(\tilde{W}_n)) &= ec(v)^k + \sum_{i=1}^n ec(v_i)^k + \sum_{i=1}^r ec(v^i)^k + \\ & \sum_{i=1}^n \sum_{j=1}^r ec(v_i^j)^k + \sum_{i=1}^n ec(v_{i,i+1})^k + \sum_{i=1}^n \sum_{j=1}^r ec(v_{i,i+1}^j)^k \\ &= 3^k + (n+r)4^k + (nr+n)5^k + nr6^k. \end{aligned}$$

$$\begin{aligned} Zg_6^k(I_r(\tilde{W}_n)) &= \sum_{i=1}^r (ec(v)ec(v^i))^k + \sum_{i=1}^n (ec(v)ec(v_i))^k + \\ & \sum_{i=1}^n \sum_{j=1}^r (ec(v_i)ec(v_i^j))^k + \sum_{i=1}^n (ec(v_i)ec(v_{i,i+1}))^k + \\ & \sum_{i=1}^n (ec(v_{i,i+1})ec(v_{i+1}))^k + \sum_{i=1}^n \sum_{j=1}^r (ec(v_{i,i+1})ec(v_{i,i+1}^j))^k \end{aligned}$$

$$= \sum_{i=1}^r 12^k + \sum_{i=1}^n 12^k + \sum_{i=1}^n \sum_{j=1}^r 20^k + \sum_{i=1}^n 20^k + \sum_{i=1}^n 20^k + \sum_{i=1}^n \sum_{j=1}^r 30^k$$

$$= (r+n)12^k + (nr+2n)20^k + nr \cdot 30^k.$$

$$\begin{aligned} Zg_4(I_r(\tilde{W}_n), x) &= \sum_{i=1}^r x^{ec(v)+ec(v^i)} + \sum_{i=1}^n x^{ec(v)+ec(v_i)} + \\ &\sum_{i=1}^n \sum_{j=1}^r x^{ec(v_i)+ec(v_j^i)} + \sum_{i=1}^n x^{ec(v_i)+ec(v_{i+1})} + \sum_{i=1}^n x^{ec(v_{i+1})+ec(v_{i+1})} + \\ &\sum_{i=1}^n \sum_{j=1}^r x^{ec(v_{i+1})+ec(v_{i+1}^j)} \end{aligned}$$

$$= \sum_{i=1}^r x^7 + \sum_{i=1}^n x^7 + \sum_{i=1}^n \sum_{j=1}^r x^9 + \sum_{i=1}^n x^9 + \sum_{i=1}^n x^9 + \sum_{i=1}^n \sum_{j=1}^r x^{11}$$

$$= (r+n)x^7 + (nr+2n)x^9 + nr x^{11}.$$

$$\begin{aligned} Zg_5(I_r(\tilde{W}_n), x) &= x^{ec(v)^2} + \sum_{i=1}^n x^{ec(v_i)^2} + \sum_{i=1}^r x^{ec(v^i)^2} + \sum_{i=1}^n \sum_{j=1}^r x^{ec(v_j^i)^2} \\ &+ \sum_{i=1}^n x^{ec(v_{i+1})^2} + \sum_{i=1}^n \sum_{j=1}^r x^{ec(v_{i+1}^j)^2} \end{aligned}$$

$$= x^9 + (n+r)x^{16} + (nr+n)x^{25} + nr x^{36}.$$

$$\begin{aligned} Zg_6(I_r(\tilde{W}_n), x) &= \sum_{i=1}^r x^{ec(v)ec(v^i)} + \sum_{i=1}^n x^{ec(v)ec(v_i)} + \sum_{i=1}^n \sum_{j=1}^r x^{ec(v_i)ec(v_j^i)} \\ &+ \sum_{i=1}^n x^{ec(v_i)ec(v_{i+1})} + \sum_{i=1}^n x^{ec(v_{i+1})ec(v_{i+1})} + \sum_{i=1}^n \sum_{j=1}^r x^{ec(v_{i+1})ec(v_{i+1}^j)} \end{aligned}$$

$$= \sum_{i=1}^r x^{12} + \sum_{i=1}^n x^{12} + \sum_{i=1}^n \sum_{j=1}^r x^{20} + \sum_{i=1}^n x^{20} + \sum_{i=1}^n x^{20} + \sum_{i=1}^n \sum_{j=1}^r x^{30}$$

$$= (r+n)x^{12} + (nr+2n)x^{20} + nr x^{30}.$$

Corollary 4.

$$Zg_4^k(\tilde{W}_n) = n7^k + 2n9^k,$$

$$Zg_5^k(\tilde{W}_n) = 3^k + n4^k + n5^k,$$

$$Zg_6^k(\tilde{W}_n) = n12^k + 2n20^k,$$

$$Zg_4(\tilde{W}_n, x) = nx^7 + 2nx^9,$$

$$Zg_5(\tilde{W}_n, x) = x^9 + nx^{16} + nx^{25},$$

$$Zg_6(\tilde{W}_n, x) = nx^{12} + 2nx^{20}.$$

3. Conclusions

In this paper, we mainly present the fourth, fifth and sixth Zagreb index and Zagreb polynomial of fan molecular graph,

wheel molecular graph, and gear fan molecular graph, gear wheel molecular graph, and their r-corona molecular graphs.

Acknowledgements

First, we thank the reviewers for their constructive comments in improving the quality of this paper. This work was supported in part by the PhD initial funding of the second author. We also would like to thank the anonymous referees for providing us with constructive comments and suggestions.

References

- [1] L. Yan, Y. Li, W. Gao, J. S. Li, On the extremal hyper-wiener index of graphs, Journal of Chemical and Pharmaceutical Research, 2014, 6(3): 477-481.
- [2] L. Yan, W. Gao, J. S. Li, General harmonic index and general sum connectivity index of polyomino chains and nanotubes, Journal of Computational and Theoretical Nanoscience, In press.
- [3] W. Gao, L. Liang, Y. Gao, Some results on wiener related index and shultz index of molecular graphs, Energy Education Science and Technology: Part A, 2014, 32(6): 8961-8970.
- [4] W. Gao, L. Liang, Y. Gao, Total eccentricity, adjacent eccentric distance sum and Gutman index of certain special molecular graphs, The Bio Technology: An Indian Journal, 2014, 10(9): 3837-3845.
- [5] W. Gao, L. Shi, Wiener index of gear fan graph and gear wheel graph, Asian Journal of Chemistry, 2014, 26(11): 3397-3400.
- [6] W. Gao, W. F. Wang, Second atom-bond connectivity index of special chemical molecular structures, Journal of Chemistry, Volume 2014, Article ID 906254, 8 pages, <http://dx.doi.org/10.1155/2014/906254>.
- [7] W. F. Xi, W. Gao, Geometric-arithmetic index and Zagreb indices of certain special molecular graphs, Journal of Advances in Chemistry, 2014, 10(2): 2254-2261.
- [8] W. F. Xi, W. Gao, λ -Modified extremal hyper-Wiener index of molecular graphs, Journal of Applied Computer Science & Mathematics, 2014, 18 (8): 43-46.
- [9] W. F. Xi, W. Gao, Y. Li, Three indices calculation of certain crown molecular graphs, Journal of Advances in Mathematics, 2014, 9(6): 2696-2304.
- [10] Y. Gao, W. Gao, L. Liang, Revised Szeged index and revised edge Szeged index of certain special molecular graphs, International Journal of Applied Physics and Mathematics, 2014, 4(6): 417-425.
- [11] J. A. Bondy, U. S. R. Mutry, Graph Theory, Spring, Berlin, 2008.
- [12] W. Gao, The fourth geometric-arithmetic index of benzenoid series, In press.