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THE HOSOYA INDEX AND THE MERRIFIELD-SIMMONS INDEX OF SOME GRAPHS

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ABSTRACT. The Hosoya index and the Merrifield-Simmons index are two types of graph invariants used in mathematical chemistry. In this paper, we give some formulas to compute these indices for some classes of corona product and link of two graphs. Furthermore, we obtain exact formulas of Hosoya and Merrifield-Simmons indices for the set of bicyclic graphs, caterpillars and dual star.

1. Introduction

In this paper, we follow the standard notation in graph theory in [1]. Let $G = (V, E)$ be a simple connected graph of order n and size m . Two distinct edges in a graph G are independent if they are not incident with a common vertex in G . A set of pairwise independent edges in G is called a matching. A k -matching of G is a set of k mutually independent edges. In theoretical chemistry molecular structure descriptors are used for modeling physico-chemical, phar-macologic, toxicologic, biological and other properties of chemical compounds. For detailed information on the chemical applications, we refer to [1, 2, 6, 7, 17]. The Hosoya index also known as the Z -index, of a graph is the total number of matchings in it. This graph invariant was introduced by Haruo Hosoya in 1971 [9]. Let $m(G, k)$ be the number of its k -matchings and $m(G, 0) = 1$ for any graph G . Then $Z(G)$ is defined as follows:

$$Z(G) = \sum_{k=0}^{\lfloor \frac{n}{2} \rfloor} m(G, k).$$

Some papers related to this index can be found in [10, 11, 18, 20].

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Two vertices of G are said to be independent if they are not adjacent in G . The Merrifield-Simmons index of G , denoted by $i(G)$, is defined as the number of subsets of the vertex set, in which any two vertices are non adjacent, that is the number of independent vertex set of G [15]. The Merrifield-Simmons index is one of the most popular topological indices in chemistry, which was extensively studied in a monograph [14]. There have been many papers studying the Merrifield-Simmons index, for example see [12, 13, 21, 22].

The cyclomatic number of a connected graph G is defined as $c(G) = m - n + 1$. A graph G with $c(G) = k$ is called a k cyclic graph, for $c(G) = 2$, we named G as a bicyclic graph. Let $B(n)$ be the set of all bicyclic graphs with n vertices. For any graph $G \in B(n)$, there are two fundamental cycles C_p and C_q in G . $C_{p,q,l}$ is the set of $G \in B(n)$ in which the two cycles in G are linked by a path of length $l > 0$.

If $E' \subseteq E$ and $W \subseteq V$, then $G - E'$ and $G - W$ denote the subgraphs of G obtained by deleting the edges of E' and the vertices of W , respectively. For the neighborhood of a vertex v in a graph G , the notation $N_G(v)$ is used which is defined as $N_G(v) = \{u | uv \in E(G)\}$, and $N_G[v] = N_G(v) \cup \{v\}$. For given graphs G and H , their corona product, $G \circ H$ is obtained by taking $|V(G)|$ copies of H and joining each vertex of the i -th copy with vertex $u_i \in V(G)$. Suppose G and H are two graphs with disjoint vertex sets. For given vertices $y \in V(G)$ and $z \in V(H)$ a link of G and H by vertices y and z is defined as the graph $(G \sim H)(y, z)$ obtained by joining y and z by an edge in the union of these graphs [5]. The join $G + H$ of graphs G and H is the graph union $G \cup H$ together with all the edges joining $V(G)$ and $V(H)$.

The complement of a graph G is a graph H on the same vertices such that two vertices of H are adjacent if and only if they are not adjacent in G . The graph H is usually denoted by \bar{G} . A caterpillar or caterpillar tree is a tree in which all the vertices of the caterpillar are within distance 1 of a central path. It is easy the corona product of the path P_n and the empty graph \bar{K}_p is a class of caterpillars. We denote this graph by $ca(n, p)$.

Fibonacci numbers are terms of the sequence defined in a quite simple recursive fashion. We define Fibonacci numbers: $F_0 = 0$, $F_1 = 1$, and for $n \geq 2$, $F_n = F_{n-1} + F_{n-2}$.

Throughout this paper, C_n , K_n , P_n and S_n denote the cycle, complete, path and star graphs on n vertices respectively. Our other notations are standard and taken mainly from [4, 8, 17].

In [3, 19], the Hosoya and Merrifield-Simmons index of corona product of a path and a cycle with the graph K_2 were computed. In [16], these indices were computed for $P_n \circ K_1$, $P_n \circ \bar{K}_i$ and $C_n \circ \bar{K}_i$. In this paper we generalize the previous results. In fact we compute these indices for $P_n \circ G$ and $C_n \circ G$, where G is an arbitrary graph.

2. Hosoya Index

In this section, we give some formulas for Hosoya index of some classes of corona product and link of two graphs. Furthermore, we obtain exact formula for the set of bicyclic graphs, caterpillars and dual star graphs. We state the following Lemmas:

Lemma 2.1. [7] *Let $G = (V(G), E(G))$ be a graph. Then*

- i) If G_1, G_2, \dots, G_m are the components of the graph G , then $Z(G) = \prod_{i=1}^m Z(G_i)$.*
- ii) If $e = xy \in E(G)$, then $Z(G) = Z(G - e) + Z(G - \{x, y\})$.*
- iii) If $x \in V(G)$, then $Z(G) = Z(G - \{x\}) + \sum_{y \in N_G(x)} Z(G - \{x, y\})$.*
- iv) $Z(S_n) = n$; $Z(P_n) = F_{n+1}$ for any $n > 0$; $Z(C_n) = F_{n-1} + F_{n+1}$ for any $n \geq 3$.*

Lemma 2.2. [7] *Let $G = (V(G), E(G))$ be a graph. Then*

- i) If G_1, G_2, \dots, G_m are the components of the graph G , then $i(G) = \prod_{k=1}^m i(G_k)$.*
- ii) If $e = xy \in E(G)$, then $i(G) = i(G - \{x, y\}) + i(G - N_G[x]) + i(G - N_G[y])$.*
- iii) If $x \in V(G)$, then $i(G) = i(G - \{x\}) + i(G - N_G[x])$.*
- iv) $i(S_n) = 2^{n-1}$; $i(P_n) = F_{n+2}$ for any $n > 0$; $i(C_n) = F_{n-1} + F_{n+1}$ for any $n \geq 3$.*

Let G be a graph. We denote the corona product of the path $P_n = v_1v_2 \dots v_n$ and the graph G , by G_n , i.e., $G_n = P_n \circ G$.

Theorem 2.3. *Let G be a graph. Then*

$$Z(G_n) = \frac{k_1(k_1 - r_2) + k_2}{\sqrt{k_1^2 + 4k_2}} \left(\frac{k_1 + \sqrt{k_1^2 + 4k_2}}{2} \right)^{n-1} + \frac{k_1(r_1 - k_1) - k_2}{\sqrt{k_1^2 + 4k_2}} \left(\frac{k_1 - \sqrt{k_1^2 + 4k_2}}{2} \right)^{n-1},$$

where $k_1 = Z(G) + \sum_{x \in V(G)} Z(G - x)$, $k_2 = Z^2(G)$ and $r_1 = \frac{k_1 + \sqrt{k_1^2 + 4k_2}}{2}$, $r_2 = \frac{k_1 - \sqrt{k_1^2 + 4k_2}}{2}$.

Proof. By Lemma 2.1, parts (ii) and (iii), we have

$$\begin{aligned} Z(G_n) &= Z(G_n - v_1v_2) + Z(G_n - \{v_1, v_2\}) \\ &= Z(G + v_1)Z(G_{n-1}) + Z^2(G)Z(G_{n-2}) \\ &= \left(Z(G) + \sum_{x \in N_{G+v_1}(v_1)} Z((G + v_1) - \{v_1, x\}) \right) Z(G_{n-1}) + Z^2(G)Z(G_{n-2}) \\ &= \left(Z(G) + \sum_{x \in V(G)} Z(G - x) \right) Z(G_{n-1}) + Z^2(G)Z(G_{n-2}). \end{aligned}$$

In order to solve the recursive formula, let $k_1 = Z(G) + \sum_{x \in V(G)} Z(G - x)$ and $k_2 = Z^2(G)$. Thus the characteristic equation is $r^2 - k_1r - k_2 = 0$. Since the roots of this equation are $r_1 = \frac{k_1 + \sqrt{k_1^2 + 4k_2}}{2}$, $r_2 = \frac{k_1 - \sqrt{k_1^2 + 4k_2}}{2}$, we have:

$$Z(G_n) = c_1r_1^n + c_2r_2^n. \quad (n \geq 3)$$

By using Lemma 2.1, parts (ii) and (iii), one can see that $Z(G_1) = k_1$ and $Z(G_2) = k_1^2 + k_2$. Thus we have the following equation

$$(2.1) \quad \begin{cases} Z(G_n) = c_1 r_1^n + c_2 r_2^n \\ Z(G_1) = k_1 \\ Z(G_2) = k_1^2 + k_2 \end{cases} .$$

By using the initial conditions, we have $c_1 = \frac{k_1(r_2-r_1)-k_1(k_1-r_1)-k_2}{r_1(r_2-r_1)}$ and $c_2 = \frac{k_1(k_1-r_1)+k_2}{r_2(r_2-r_1)}$. So by substitution r_1, r_2, c_1 and c_2 in the equation (2.1), we have:

$$\begin{aligned} Z(G_n) &= \frac{k_1(k_1 - r_2) + k_2}{\sqrt{k_1^2 + 4k_2}} \left(\frac{k_1 + \sqrt{k_1^2 + 4k_2}}{2} \right)^{n-1} \\ &+ \frac{k_1(r_1 - k_1) - k_2}{\sqrt{k_1^2 + 4k_2}} \left(\frac{k_1 - \sqrt{k_1^2 + 4k_2}}{2} \right)^{n-1}. \end{aligned}$$

□

In the next corollary, we substitute the graph G , by the graph K_2 in Theorem 2.3. In [3], the following corollary was proved in [3; Theorem 1], but we conclude it from Theorem 2.3.

Corollary 2.4.

$$Z(P_n \circ K_2) = \frac{2 + \sqrt{2}}{4} (2 + 2\sqrt{2})^n + \frac{2 - \sqrt{2}}{4} (2 - 2\sqrt{2})^n.$$

Corollary 2.5. *For the caterpillar $ca(n, p)$, we have:*

$$\begin{aligned} Z(ca(n, p)) &= \frac{(p + 1)(p + 1 - r_2) + 1}{\sqrt{p^2 + 2p + 5}} \left(\frac{(p + 1) + \sqrt{p^2 + 2p + 5}}{2} \right)^{n-1} \\ &+ \frac{(p + 1)(r_1 - p - 1) - 1}{\sqrt{p^2 + 2p + 5}} \left(\frac{(p + 1) - \sqrt{p^2 + 2p + 5}}{2} \right)^{n-1}, \end{aligned}$$

where $r_1 = \frac{1+p+\sqrt{p^2+2p+5}}{2}$ and $r_2 = \frac{1+p-\sqrt{p^2+2p+5}}{2}$.

Proof. The proof is straightforward from Theorem 2.3 and these facts that $k_1 = Z(\bar{K}_p) + \sum_{x \in V(G)} Z(\bar{K}_p - x) = p + 1$ and $k_2 = Z^2(\bar{K}_p) = 1$. □

Let G be a graph and C_n be the cycle $C_n : v_1 v_2 \dots v_n v_1$. We denote the graph $C_n \circ G$ by G'_n . In the next theorem, we give an exact formula for the Hosoya index of the graph G'_n .

Theorem 2.6. *Let G be a graph. Then*

$$\begin{aligned} Z(G'_n) &= \frac{k_1(k_1 - r_2) + k_2}{\sqrt{k_1^2 + 4k_2}} \left(\frac{k_1 + \sqrt{k_1^2 + 4k_2}}{2}\right)^{n-1} \\ &+ \frac{k_1(r_1 - k_1) - k_2}{\sqrt{k_1^2 + 4k_2}} \left(\frac{k_1 - \sqrt{k_1^2 + 4k_2}}{2}\right)^{n-1} \\ &+ \frac{k_2k_1(k_1 - r_2) + k_2^2}{\sqrt{k_1^2 + 4k_2}} \left(\frac{k_1 + \sqrt{k_1^2 + 4k_2}}{2}\right)^{n-3} \\ &+ \frac{k_1k_2(r_1 - k_1) - k_2^2}{\sqrt{k_1^2 + 4k_2}} \left(\frac{k_1 - \sqrt{k_1^2 + 4k_2}}{2}\right)^{n-3} \end{aligned}$$

where $k_1 = Z(G) + \sum_{x \in V(G)} Z(G - x)$, $k_2 = Z^2(G)$ and $r_1 = \frac{k_1 + \sqrt{k_1^2 + 4k_2}}{2}$, $r_2 = \frac{k_1 - \sqrt{k_1^2 + 4k_2}}{2}$.

Proof. By Lemma 2.1, parts (ii) and (iii), we have

$$\begin{aligned} Z(G'_n) &= Z(G'_n - v_1v_2) + Z(G'_n - \{v_1, v_2\}) \\ &= Z(P_n \circ G) + Z^2(G)Z(P_{n-2} \circ G) \\ &= Z(G_n) + Z^2(G)Z(G_{n-2}) \\ &= \frac{k_1(k_1 - r_2) + k_2}{\sqrt{k_1^2 + 4k_2}} \left(\frac{k_1 + \sqrt{k_1^2 + 4k_2}}{2}\right)^{n-1} \\ &+ \frac{k_1(r_1 - k_1) - k_2}{\sqrt{k_1^2 + 4k_2}} \left(\frac{k_1 - \sqrt{k_1^2 + 4k_2}}{2}\right)^{n-1} \\ &+ \frac{k_1k_2(k_1 - r_2) + k_2^2}{\sqrt{k_1^2 + 4k_2}} \left(\frac{k_1 + \sqrt{k_1^2 + 4k_2}}{2}\right)^{n-3} \\ &+ \frac{k_1k_2(r_1 - k_1) - k_2^2}{\sqrt{k_1^2 + 4k_2}} \left(\frac{k_1 - \sqrt{k_1^2 + 4k_2}}{2}\right)^{n-3}. \end{aligned}$$

□

The Hosoya index of $C_n \circ K_2$ was computed in [3; Theorem 2]. Now we use from Theorem 2.6 as a corollary to find a formula for the Hosoya index of $C_n \circ K_2$.

Corollary 2.7.

$$Z(C_n \circ K_2) = 2^n [(1 + \sqrt{2})^n + (1 - \sqrt{2})^n].$$

Proof. By Theorem 2.6, we have

$$\begin{aligned}
Z(C_n \circ K_2) &= \frac{2 + \sqrt{2}}{4}(2 + 2\sqrt{2})^n + \frac{2 - \sqrt{2}}{4}(2 - 2\sqrt{2})^n \\
&+ 4\left[\frac{2 + \sqrt{2}}{4}(2 + 2\sqrt{2})^{n-2} + \frac{2 - \sqrt{2}}{4}(2 - 2\sqrt{2})^{n-2}\right] \\
&= 2^n\left[\frac{2 + \sqrt{2}}{4}(1 + \sqrt{2})^n + \frac{2 - \sqrt{2}}{4}(1 - \sqrt{2})^n\right] \\
&+ \frac{2 + \sqrt{2}}{4}(1 + \sqrt{2})^{n-2} + \frac{2 - \sqrt{2}}{4}(1 - \sqrt{2})^{n-2}] \\
&= 2^n[(1 + \sqrt{2})^n + (1 - \sqrt{2})^n].
\end{aligned}$$

□

In continue we state the Hosoya index of the link of two graphs G_1 and G_2 by terms of Hosoya index of G_1 and Hosoya index of G_2 .

Theorem 2.8. *Let G_1 and G_2 be two graphs and $G = (G_1 \sim G_2)(u_1, v_1)$. Then*

$$Z(G) = Z(G_1)Z(G_2) + Z(G_1 - \{u_1\})Z(G_2 - \{v_1\}).$$

Proof. By Lemma 2.1, part (i) and (ii), we have:

$$\begin{aligned}
Z(G) &= Z(G - u_1v_1) + Z(G - \{u_1, v_1\}) \\
&= Z(G_1)Z(G_2) + Z(G_1 - \{u_1\} \cup G_2 - \{v_1\}) \\
&= Z(G_1)Z(G_2) + Z(G_1 - \{u_1\})Z(G_2 - \{v_1\}).
\end{aligned}$$

□

Corollary 2.9. *Let $G = C_{n,m,1}$ be the link of two cycles C_n and C_m . Then*

$$\begin{aligned}
Z(G) &= F_{n-1}F_{m-1} + F_{n-1}F_{m+1} + F_{n+1}F_{m-1} \\
&+ F_{n+1}F_{m+1} + F_{n-2}F_{m-2}.
\end{aligned}$$

Proof. By Theorem 2.8 and Lemma 2.1(iv), we have

$$\begin{aligned}
Z(G) &= Z(C_n)Z(C_m) + Z(P_{n-1})Z(P_{m-1}) \\
&= (F_{n-1} + F_{n+1})(F_{m-1} + F_{m+1}) + F_{n-2}F_{m-2} \\
&= F_{n-1}F_{m-1} + F_{n-1}F_{m+1} + F_{n+1}F_{m-1} \\
&+ F_{n+1}F_{m+1} + F_{n-2}F_{m-2}.
\end{aligned}$$

□

In the next theorem, we use from Theorem 2.8 to determine the Hosoya index of double star graph $S_{n,m}$.

Corollary 2.10.

$$Z(S_{n,m}) = nm + 1.$$

Proof. The proof is straightforward from Theorem 2.8. □

3. Merrifield-Simmons Index

In this section, we obtain some results for Merrifield-Simmons index similar to the Hosoya index.

Theorem 3.1. *Let G be a graph. Then*

$$i(G_n) = \frac{k(k+2-r)}{\sqrt{k^2+4k}} \left(\frac{k+\sqrt{k^2+4k}}{2}\right)^{n-1} + \frac{k(r-k-2)}{\sqrt{k^2+4k}} \left(\frac{k-\sqrt{k^2+4k}}{2}\right)^{n-1},$$

where $k = i(G)$ and $r = \frac{k+\sqrt{k^2+4k}}{2}$.

Proof. By Lemma 2.2, part (iii), we have

$$\begin{aligned} i(G_n) &= i(G_n - \{v_1\}) + i(G_n - N_G[v_1]) \\ &= i(G)i(G_{n-1}) + i(G)i(G_{n-2}) \\ &= i(G)[i(G_{n-1}) + i(G_{n-2})]. \end{aligned}$$

In order to calculate $i(G_n)$, we give $k = i(G)$. The characteristic equation is $r^2 - kr - k = 0$. The roots of this equation are $r_1 = \frac{k+\sqrt{k^2+4k}}{2}$ and $r_2 = \frac{k-\sqrt{k^2+4k}}{2}$. We know that the general solution of this equation is $i(G_n) = c_1r_1^n + c_2r_2^n$ ($n \geq 3$). By Lemma 2.2, parts (ii) and (iii), one can see $i(G_1) = k$ and $i(G_2) = k^2 + 2k$. Thus

$$\begin{cases} i(G_n) = c_1r_1^n + c_2r_2^n \\ i(G_1) = k \\ i(G_2) = k^2 + 2k \end{cases} .$$

Now by substituting the initial conditions in the equation $i(G_n) = c_1r_1^n + c_2r_2^n$, it is easy to see that $c_1 = \frac{k(r_1-k-2)}{r_1(r_2-r_1)}$ and $c_2 = \frac{k(k+2-r_1)}{r_2(r_2-r_1)}$. So we have $i(G_n) = \frac{k(k+2-r_1)}{\sqrt{k^2+4k}} \left(\frac{k+\sqrt{k^2+4k}}{2}\right)^{n-1} + \frac{k(r_1-k-2)}{\sqrt{k^2+4k}} \left(\frac{k-\sqrt{k^2+4k}}{2}\right)^{n-1}$. □

We can see that if in Theorem 3.1, we substitute the graph G by K_2 , we obtain to $i(P_n \circ K_2)$ which was computed in [19] as a theorem.

Corollary 3.2.

$$i(P_n \circ K_2) = \frac{21 + 5\sqrt{21}}{42} \left(\frac{3 + \sqrt{21}}{2}\right)^n + \frac{21 - 5\sqrt{21}}{42} \left(\frac{3 - \sqrt{21}}{2}\right)^n.$$

Also if we give $G = \bar{K}_p$ in Theorem 3.1, we have the following corollary.

Corollary 3.3. For the caterpillar $ca(n, p)$, we have:

$$\begin{aligned}
 i(ca(n, p)) &= \left(\frac{2^{p+1}(2^{p-1} - 2^{p-2} + 1)}{\sqrt{2^{2p} + 2^{p+2}}} - 2^{p-1} \right) \left(\frac{2^p + \sqrt{2^{2p} + 2^{p+2}}}{2} \right)^{n-1} \\
 &+ \left(\frac{2^{p+1}(2^{p-2} - 2^{p-1} - 1)}{\sqrt{2^{2p} + 2^{p+2}}} + 2^{p-1} \right) \left(\frac{2^p - \sqrt{2^{2p} + 2^{p+2}}}{2} \right)^{n-1}.
 \end{aligned}$$

Theorem 3.4. Let G be a graph. Then

$$\begin{aligned}
 i(G'_n) &= \frac{k^2(k + 2 - r)}{\sqrt{k^2 + 4k}} \left(\frac{k + \sqrt{k^2 + 4k}}{2} \right)^{n-2} \\
 &+ \frac{k^2(r - k - 2)}{\sqrt{k^2 + 4k}} \left(\frac{k - \sqrt{k^2 + 4k}}{2} \right)^{n-2} \\
 &+ \frac{k^3(k + 2 - r)}{\sqrt{k^2 + 4k}} \left(\frac{k + \sqrt{k^2 + 4k}}{2} \right)^{n-4} \\
 &+ \frac{k^3(r - k - 2)}{\sqrt{k^2 + 4k}} \left(\frac{k - \sqrt{k^2 + 4k}}{2} \right)^{n-4},
 \end{aligned}$$

where $k = i(G)$ and $r = \frac{k + \sqrt{k^2 + 4k}}{2}$.

Proof. By Lemma 2.2, part (iii), we have

$$\begin{aligned}
 i(G'_n) &= i(G'_n - \{v_1\}) + i(G'_n - N_G[v_1]) \\
 &= i(G)i(P_{n-1} \circ G) + i^2(G)i(P_{n-3} \circ G) \\
 &= \frac{k^2(k + 2 - r_1)}{\sqrt{k^2 + 4k}} \left(\frac{k + \sqrt{k^2 + 4k}}{2} \right)^{n-2} \\
 &+ \frac{k^2(r_1 - k - 2)}{\sqrt{k^2 + 4k}} \left(\frac{k - \sqrt{k^2 + 4k}}{2} \right)^{n-2} \\
 &+ \frac{k^3(k + 2 - r_1)}{\sqrt{k^2 + 4k}} \left(\frac{k + \sqrt{k^2 + 4k}}{2} \right)^{n-4} \\
 &+ \frac{k^3(r_1 - k - 2)}{\sqrt{k^2 + 4k}} \left(\frac{k - \sqrt{k^2 + 4k}}{2} \right)^{n-4}.
 \end{aligned}$$

□

The Merrifield-Simmons index of $C_n \circ K_2$ was computed in [19] as a theorem. Now we use from Theorem 3.4 as a corollary to find a formula for the Merrifield-Simmons index of $C_n \circ K_2$.

Corollary 3.5.

$$\begin{aligned}
 i(C_n \circ K_2) &= \frac{21 + 5\sqrt{21}}{14} \left(\frac{3 + \sqrt{21}}{2} \right)^{n-1} + \frac{21 - 5\sqrt{21}}{14} \left(\frac{3 - \sqrt{21}}{2} \right)^{n-1} \\
 &+ \frac{63 + 15\sqrt{21}}{14} \left(\frac{3 + \sqrt{21}}{2} \right)^{n-3} + \frac{63 - 15\sqrt{21}}{14} \left(\frac{3 - \sqrt{21}}{2} \right)^{n-3}.
 \end{aligned}$$

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