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The Merrifield-Simmons indices and Hosoya indices of some classes of cartesian graph product

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Abstract. The Merrifield-Simmons index of a graph is defined as the total number of the independent sets of the graph and the Hosoya index of a graph is defined as the total number of the matchings of the graph. In this paper, we give formula for Merrifield-Simmons and Hosoya indices of some classes of cartesian product of two graphs $K_2 \times H$, where H is a path graph P_n, cyclic graph C_n, or star graph S_n, with n vertices (These are called: ladder graph, prism graph, and book graph).

Keywords: Merrifield-Simmons index, Hosoya index, cartesian graph product, ladder graph, prism graph
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Introduction

Let G be a graph with vertex set $\mathrm{V}(G)$ and edge set $\mathrm{E}(G)$. A subset $C \subseteq \mathrm{V}(G)$ is a *minimal vertex cover* of G if: (1) every edge of G is incident with one vertex in C, and (2) there is no proper subset of C with the first property. Note that C is a minimal vertex cover if and only if $\mathrm{V}(G) \setminus C$ is a maximal independent set (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

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as the total number of the independent sets of G. The Merrifield-Simmons index was introduced in 1982 in a paper of Prodinger and Tichy [11], although it is called Fibonacci number of a graph there. The Merrifield-Simmons index is one of the most popular topological indices in chemistry, which was extensively studied in a monograph [9]. There have been many papers studying the Merrifield-Simmons index. In [11], it is shown that, for n-vertex trees, the star has the maximal Merrifield-Simmons index and the path has the minimal Merrifield-Simmons index. In [7], Li et al characterized the tree with the maximal Merrifield-Simmons index among the trees with given diameter. In [10], Pedersen and Vestergaard studied the Merrifield-Simmons indices of the unicyclic graphs. In [3], Deng, Chen and Zhang determined the upper bound for the Merrifield-Simmons index in $(n, n+1)$-graphs in terms of the order n (recall that a $(n, n+1)$-graph is a connected simple graph with n vertices and $n+1$ edges). In [14], H. Wang and Hua determined unicycle graphs with the largest and smallest Merrifield-Simmons index. In [15], M. Wang, Hua and D. Wang investigated the Merrifield-Simmons index for a tree with n vertices and with k pendent vertices.

First we having a description of introduction of [13]:

The number of different structures with the formula $C_{64}H_{130}$ is more than one hundred million billion times greater that the number of different molecules of all types (and formulas) cataloged in all of human history. Therefore, it is imperative that theoretical chemists develop methods to predict properties of molecules from their structure so that synthetic chemists can identify on which of the enumerable molecular structures they should expend their finite resources. This is one of the primary reasons for developing quantative structure-property relationships.

The Hosoya index (Z) is an example of a graph invariant, called a topological index, which may be calculated directly from the structure of a molecule [12]. Topological indices have proven to be very useful in QSPR models, especially when a physical property such as the normal boiling point is modeled for a specific family of molecular graphs [8].

Similarly, two edges of G are said to be independent if they are not adjacent in G. A k-matching of G is a set of k mutually independent edges. Denote by $z(G, k)$ the number of the k-matchings of G. For convenience, we regard the empty edge set as a matching. Then $z(G, 0) = 1$ for any graph G. The Hosoya index of G, denoted by $z(G)$, is defined as $z(G) = \sum_{k=0}^{[n/2]} z(G, k)$. Obviously, $z(G)$ is equal to the total number of matchings of G. The Hosoya index of a graph was introduced by Hosoya [6] and was applied to correlations with boiling points, entropies, calculated bond orders, as well as for coding of chemical structures [9]. Since then, many authors have investigated the Hosoya index (e.g., see [1], [2], [4], [5]). In [16], Yu and Lv characterized the trees with maximal Merrifield-Simmons indices and minimal Hosoya indices, respectively, among the trees with k pendant vertices.

In this paper we investigate the Merrifield-Simmons indices and the Hosoya indices for the Cartesian graph product $G = K_2 \times H$ in the following cases:

(1) $H = P_n$, where P_n is a path graph with n vertices (this is called ladder graph of order n).

(2) $H = C_n$, where C_n is a cyclic graph with n vertices (this is called prism graph of order n).

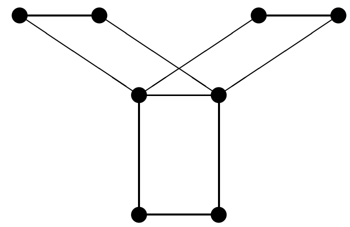
(3) $H = S_n$, where S_n is a star graph with n vertices (this is called book graph of order n).

1. Main results

The Cartesian graph product $G = G_1 \times G_2$, sometimes simply called the graph product of graphs G_1 and G_2 with disjoint point sets V_1 and V_2 and edge sets E_1 and E_2 is the graph with point set $V_1 \times V_2$ and $u = (u_1, u_2)$ adjacent with $v = (v_1, v_2$ whenever ($u_1 = v_1$ and u_2 adjacent v_2) or (u_1 adjacent v_1 and $u_2 = v_2$). The ladder graph of order n is defined as $L_n = K_2 \times P_n$, where P_n is a path graph. The graph obtains via this definition has the advantage of looking like a ladder, having two rails and rungs between them.

A prism graph of order n, Y_n, is the graph Cartesian product $Y_n = K_2 \times C_n$, where K_2 is the complete graph on two vertices and C_n is the cycle graph on n vertices. This graph is corresponding to the skeleton of an n-prism. Prism graphs are therefore both planar and polyhedral. A prism graph of order n has $2n$ vertices and $3n$ edges.

The book graph of order n, B_n, is defined as the graph Cartesian product $B_n = K_2 \times S_n$, where S_n is a star graph and K_2 is the complete graph on two vertices.



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The following theorem is one of the main result of this paper.

Theorem 1.1. *Let L_n be a ladder graph, Y_n prism graph, and B_n book graph of order n. Then*

(a) $i(L_n) = 1/2(1+\sqrt{2})^{n+1} + 1/2(1-\sqrt{2})^{n+1}$.
(b) $i(Y_n) = 3\sqrt{2}/2[(1+\sqrt{2})^{n-1} - (1-\sqrt{2})^{n-1}] + (-1)^{n-1}$.
(c) $i(B_n) = 2^n + 3^{n-1}$.

Proof. (a) Note that L_n has four corner vertices. Let H_n be the graph comes from L_n by removing one of a corner vertex (see Table 1). Let S be an independent set of L_n and let v be the corner vertex of L_n. We consider two cases.

Case 1. Assume that $v \in S$. Clearly $S \setminus v$ is an independent set of H_{n-1}. Thus the number of independent sets of L_n is equal to $i(H_{n-1})$.

Case 2. Assume that $v \notin S$. In this case S is an independent set of H_n and so the number of independent sets of L_n is equal to $i(H_n)$. Thus $i(L_n) = i(H_n) + i(H_{n-1})$ for $n > 1$.

By a same argument we have $i(H_n) = i(H_{n-1}) + i(L_{n-1})$ for $n > 1$. Thus by solving equations system, we have $i(L_n) = 2i(L_{n-1}) + i(L_{n-2})$ with the initial conditions $i(L_1) = 3$ and $i(L_2) = 7$. Now the assertion follows from solving this system of equations.

(b) Set O_n be a graph obtained from L_n by removing two corner vertices of opposite side (for example left below row and right above row) and S_n be a graph obtained from L_n by removing two corner vertices of the same row (for example left and right above row). Then from part (a) we have

$$i(H_n) = 1/2[i(L_n) + i(L_{n-1})] = \sqrt{2}/2[(1+\sqrt{2})^{n+1} - (1-\sqrt{2})^{n+1}].$$

In addition, we have $i(O_n) = i(H_{n-1}) + i(S_{n-1})$ and $i(S_n) = i(H_{n-1}) + i(O_{n-1})$. Thus

$$i(O_n) - i(O_{n-2}) = i(H_{n-1}) + i(H_{n-2}) = (1+\sqrt{2})^n + (1-\sqrt{2})^n = 2i(L_{n-1}).$$

By solving the above non-homogenous linear recursion relation we conclude that $i(O_n) = C_1 + C_2(-1)^n + C_3(1+\sqrt{2})^n + C_4(1-\sqrt{2})^n$.

Now by solving this equation we have

$$i(O_n) = 1/4[(1+\sqrt{2})^{n+1} + (1-\sqrt{2})^{n+1}] + (-1)^n/2.$$

Now clearly $i(Y_n) = i(L_n) - 2i(S_{n-2})$. Thus $i(Y_n) = 3\sqrt{2}/2[(1+\sqrt{2})^{n-1} - (1-\sqrt{2})^{n-1}] + (-1)^{n-1}$.

(c) Suppose that v and v' are center of two copies of stars, and

$$E(B_n) = \{vv', vv_i, v'v'_i, v_iv'_i | 1 \le i \le n-1\}.$$

Suppose that S is an independent set of B_n. If $v \in S$, then $S \setminus v$ is an independent set of $\bar{K}_{n-1}$, which in this case we have 2^{n-1} independent set.

Now suppose that $v \notin S$, then we consider two cases.

Case 1 If $v' \in S$, then again $S \setminus \{v'\}$ is an independent set of $\bar{K}_{n-1}$. Hence we have 2^{n-1} independent set.

Case 2 If $v' \notin S$, then S is an independent set of $n-1$ parallel edges and hence we have 3^{n-1} independent set in this case. This implies, $i(B_n) = 2^n + 3^{n-1}$.

□

The following theorem is the second main result of this paper.

Theorem 1.2. *Let L_n be a ladder graph, Y_n prism graph, and B_n book graph of order n. Then*

(a) $z(L_n) = 3z(L_{n-1}) + z(L_{n-2}) - z(L_{n-3})$
(b) $z(Y_{n+1}) - z(Y_{n-1}) = 3z(H_{n+1}) + z(H_{n-3})$.
(c) $z(B_n) = 2^{n-3}(n^2 + 3n + 4)$.

Proof. (a) Consider one of the right edge of L_n (an edge of L_n with two end of degree 2). Suppose that M is any matching in L_n. If $e \notin M$, then M is a matching in the graph T_n. So in this case the number of matching will be $Z(T_n)$. If $e \in M$, then $M \setminus \{e\}$ is a matching in L_{n-1}, and so in this case the number of matching is $Z(L_{n-1})$. Thus $Z(L_n) = Z(L_{n-1}) + Z(T_n)$.

Now let e be an edge of T_n with an end vertex of degree 1. Suppose that M is a matching in T_n. No matter that e does or does not belong to M we have that $Z(T_n) = Z(C_n) + Z(H_n)$. Therefore

$$Z(L_n) = Z(L_{n-1}) + Z(C_n) + Z(H_n).$$

By a same argument we can show that

$$Z(H_n) = Z(L_{n-1}) + Z(H_{n-1}) \qquad (1)$$
$$Z(C_n) = Z(H_{n-1}) + Z(L_{n-2}) \qquad (2)$$

By considering the above recursive relations, we obtain

$$Z(L_n) = 3Z(L_{n-1}) + Z(L_{n-2}) - Z(L_{n-3}) \qquad (3)$$

This is a recursive relations of order 3 and by solving these equations we have $Z(L_n) = c_1r_1^n + c_2r_2^n + c_3r_3^n$. But $Z(L_1) = 2$, $Z(L_2) = 7$, and $Z(L_3) = 22$. Therefore we can find the coefficient c_i.

(b) Consider two consecutive vertices v_1 and v_2 in the cycle C_n and suppose that v'_1, v'_2 are the corresponding vertices of v_1, v_2 in the copy of C_n, respectively. Set $v_1v_2 = e$ and $v'_1v'_2 = e'$. Suppose that M is a matching of Y_n. Consider the following three cases:

Case 1. Let $e, e' \in M$. Then $M \setminus \{e, e'\}$ is a matching in the ladder L_{n-2}. So the number of matching in this case is equal to $Z(L_{n-2})$.

Case 2. Let $e, e' \notin M$. Then M is a matching in the ladder L_n and so the number of matching is equal to $Z(L_n)$.

Case 3. $e \notin M$ and $e' \in M$. Then $M \setminus \{e'\}$ is a matching of S_n. Thus the number of matching is equal to $z(S_n)$.

Therefore

$$Z(Y_n) = Z(L_n) + Z(L_{n-2}) + 2Z(S_n) \qquad (4)$$

By the same argument we have that

$$\begin{aligned} Z(S_n) &= Z(H_{n-1}) + Z(O_{n-1}) \qquad (5) \\ Z(O_n) &= Z(H_{n-1}) + Z(S_{n-1}) \qquad (6) \end{aligned}$$

By (1) and the recursive relations of $Z(L_n)$, we conclude that

$$Z(H_{n+1}) = 4Z(H_n) - 2Z(H_{n-1}) - 2Z(H_{n-2}) + Z(H_{n-3}) \qquad (7)$$

and hence $Z(H_n) = c'_1r_1 + c'_2r_2 + c'_3r_3 + c'_4$, where r_1, r_2, r_3 are the roots of recursive relation of $Z(L_n)$. Now by considering $Z(H_1) = 1$, $Z(H_2) = 3$, $Z(H_3) = 10$, and $Z(H_4) = 32$, we can find the coefficient c'_i. By combination of recursive relations 4, 5, 6, we conclude that

$$Z(Y_{n+1}) - Z(Y_{n-1}) = 2Z(H_{n-1}) + 2Z(H_n) + Z(L_{n+1}) - Z(L_{n-3}) \qquad (8)$$

Now from 1 and 8 we have

$$Z(Y_{n+1}) - Z(Y_{n-1}) = 3Z(H_{n+1}) + Z(H_{n-3}).$$

(c) Suppose that v and v' are center of two copies of stars, and

$$E(B_n) = \{vv', vv_i, v'v'_i, v_iv'_i | 1 \le i \le n-1\}.$$

Also suppose that M is a matching of B_n. If $e = vv' \in M$, then $M \setminus \{e\}$ is a supset of $\{v_iv'_i | 1 \le i \le n-1\}$. Hence in this case we have 2^{n-1} different matching. If $e = vv' \notin M$, then M is a matching in the edge set $\{vv_i, v'v'_i, v_iv'_i | 1 \le i \le n-1\}$. but $S = |M \cap \{vv_i | 1 \le i \le n-1\}| \le 1$ and $S' = |M \cap \{v'v'_i | 1 \le i \le n-1\}| \le 1$. Now consider the following cases:

Case 1. Let $S = S' = 0$. Then M is a supset of $\{vv_i | 1 \le i \le n-1\}$ and so we have 2^{n-1} different matchings.

Case 2. Let $S = 1$ and $S' = 0$. Assume that $vv_j \in M$. Then $M \setminus \{vv_j\}$ is subset of $\{v_iv'_i | 1 \le i \le n-1, i \ne j\}$. So we have 2^{n-2} different matchings. Since $1 \le j \le n$ we have $(n-1)2^{n-2}$ different matchings.

Case 3. Let $S = 0$ and $S' = 1$. This is the same as Case 2.

Case 4. Let $S = 1$ and $S' = 1$. Assume that $vv_i, v'v'_j \in M$. If $i = j$, then $M \setminus \{vv_i, v'v'_j\} \subseteq \{v_k v'_k | 1 \leq k \leq n-1, k \neq i\}$. Hence we have 2^{n-2} different matchings. In addition, we have $(n-1)$ choice for i, and so we have $(n)2^{n-2}$ different matchings. If $i \neq j$, then $M \setminus \{vv_i, v'v'_j\} \subseteq \{v_k v'_k | 1 \leq k \leq n, k \neq i\}$. Hence we have 2^{n-3} different matchings for a fixed i and j. Since we have $(n-1)(n-2)$ choice for i and j, we have $(n-1)(n-2)2^{n-3}$ different matchings.

Therefore

$$\begin{aligned} Z(B_n) &= 2.2^{n-1} + (n-1)2^{n-2} + (n-1)2^{n-2} + (n-1)2^{n-2} + (n-1)(n-2)2^{n-3} \\ &= 2^{n-3}(n^2 + 3n + 4). \end{aligned}$$

□

Remark 1.3. *Note that in Theorem 1.2, the solving of the recursive relations of $Z(L_n)$ and $Z(H_n)$ deduced that $r_1 = 2r^{1/3}\cos(\varphi/3) + 1$, $r_2 = 2r^{1/3}\cos(\varphi + 2\pi/3) + 1$, and $r_3 = 2r^{1/3}\cos(\varphi + 4\pi/3) + 1$, where $\cos\varphi = 3\sqrt{3}/8$, and $r = 8/3\sqrt{3}$. By applying the primary conditions, we can find the coefficient c_i's. In addition,*

$$Z(Y_n) = d_1 r_1^n + d_2 r_2^n + d_3 r_3^n + d_4 + d_5(-1)^n.$$

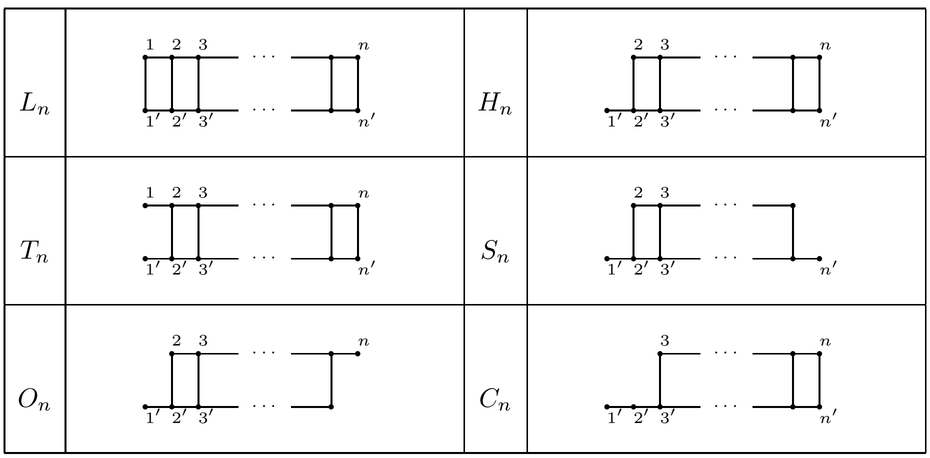

Table 1

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