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Investigation of Some Molecular Graphs Whose Topological Indices Are Equal to Lucas Numbers

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Abstract

The Hosoya index is equal to total number of matchings and the Merrifield-Simmons index is equal to total number of independent sets. The Hosoya index of cyclic alkanes, the Hosoya index and the Merrifield-Simmons index of 1-methyl bicyclo [X.1.0] alkanes are possess same value which is represented by Lucas sequence. In this paper we investigate these molecular graphs in terms of matchings and independent sets.

Keywords. Hosoya Index, Merrifield-Simmons Index, Molecular Graphs
MSC: 05C09

Introduction

Let G be a graph which contains the vertex set $V(G)$ and the edge set $E(G)$. For a vertex v in a graph G, the notation $N_G(v) = \{u | uv \in E(G)\}$ denotes the vertices which are adjacent to v and $N_G[v] = \{v\} \cup N_G(v)$.

The degree of a vertex u is cardinality of $N_G(u)$ and it is denoted with the notation $deg_G(u)$The paths and cycles are denoted by P_n and C_n. If $A \subset E(G)$, then $G - A$ denotes the subgraph of G obtained by removing the edges of A. By a similar definition if $B \subset V(G)$, then $G - B$ denotes the subgraph of G obtained by removing vertices of B.

The Hosoya index (or Z-index) was defined by Hosoya in 1971 [6] and the Hosoya index of a graph G is denoted by $Z(G)$. A matching of the graph G is a subset of $E(G)$ such that no two edges share a common vertex. The number of matchings which have k edges is denoted by $m(G,k)$ and the Hosoya index of a graph G is defined such that in the following expression

$$Z(G) = \sum_{k\geq 0} m(G,k)$$

with empty set $m(G,0) = 1$.

The Merrifield-Simmons index (or σ-index) was introduced by Merrifield and Simmons ([10]). A subset $W \subseteq V(G)$ is called independent, if the vertices of W are not neighbor in it. The number of independent sets with cardinality k is showed by $\sigma(G,k)$. The number of independent set for empty graph is one by the definition. The Merrifield-Simmons index of a graph G is denoted by $\sigma(G)$ and it is computed by

$$\sigma(G) = \sum_{k\geq 0} \sigma(G,k).$$

This two topolgical indices are well known molecular descriptors in mathematical chemistry. More details can be found about these topological indices in [14]. These two topological indices are studied for trees [1,5,6,9,13,16], for unicyclic graphs [8,11]. A different characterization of graphs with respect to σ-index is obtained for the number of recurrence relations [3]. Moreover the most private features of the Hosoya index is showed by Hosoya[7].

The following lemmas are essential for our investigations.

Lemma 1. Let H be a graph. Then ([2])

$i)$ If $H_1, H_2, \dots, H_m$ are the subgraphs of the graph G, then $Z(H) = \prod_{k=1}^{m} Z(H_k)$,

$ii)$ If $e = uv \in E(H)$, then $Z(H) = Z(H - uv) + Z(H - \{u,v\})$,

$iii)$ If $u \in V(H)$, then $Z(H) = Z(H - u) + \sum_{u\sim v} Z(H - \{u,v\})$

for the vertices v adjacent to u.

$iv)$ $Z(C_n) = L_n$.

Lemma 2. Let H be a graph. Then ([10])

$i)$ If $H_1, H_2, \ldots, H_m$ are the subgraphs of the graph H, then $\sigma(H) = \prod_{k=1}^{m} \sigma(H_k)$,

$ii)$ If $e = uv \in E(H)$, then $\sigma(H) = \sigma(H - uv) - \sigma\big(H - (N_H[u] \cup N_H[v])\big)$,

$iii)$ If $u \in V(H)$, then $\sigma(H) = \sigma(H - u) + \sigma(H - N_H[u])$.

$iv)$ $\sigma(C_n) = L_n$.

The Lucas numbers are defined with initial numbers $L_1 = 1, L_2 = 3$ and the following terms are calculated by the equation $L_n = L_{n-1} + L_{n-2}$ ($n \geq 3$).

We know that Hosoya index and Merrifield-Simmons index of cycles is equal to Lucas numbers. By the summation of the matchings or independent sets the Lucas numbers are partitioned. Moreover Randic et al. obained high order Lucas numbers using the Hosoya index of cycles [12].

In this paper we use 1-methyl bicyclo [X.1.0] alkanes. Westerberg et al. [15] showed that the Hosoya index of these molecular graphs is equal to Lucas numbers and Güntekin et al. [4] showed that the Merrifield-Simmons index of these molecular graphs is also equal to Lucas numbers for same order. We obtained two different partitions of Lucas numbers by using the matchings and independent sets of the 1-methyl bicyclo [X.1.0] alkanes.

2. Main Results

The cycles are regular graphs. Thus the number of vertices of cycles is equal to the number of edges. Therefore the Hosoya index or the Merrifield-Simmons index of cycles is equal to Lucas numbers such that

$$Z(C_n) = \sigma(C_n) = L_n \ (n \geq 3)$$

The numbers of matchings of cycles are showed in Table 1.

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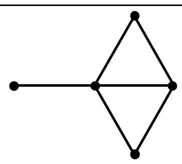
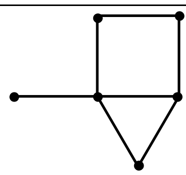
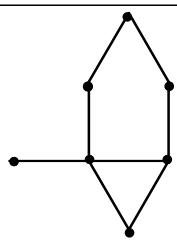
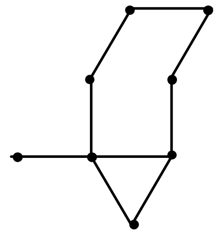
Table 1. k-matchings of Cycles

Graphs	$m(G,0)$	$m(G,1)$	$m(G,2)$	$m(G,3)$	$m(G,4)$	$m(G,5)$	Z-index or σ-index
C_3	1	3					4
C_4	1	4	2				7
C_5	1	5	5				11
C_6	1	6	9	2			18
C_7	1	7	14	7			29
C_8	1	8	20	16	2		47
C_9	1	9	27	30	9		76
C_{10}	1	10	35	50	25	2	123

The first four members of 1-methyl bicyclo [X.1.0] alkanes are showed in Table 2.

Table 2. Topological indices of the first four1-methyl bicyclo [X.1.0] alkanes

Graphs	Number of Vertices	Molecular Graph	Name	σ-Index or Z-Index
G_5	5		1-methyl-[3.1.0] bicyclo butane	11
G_6	6		1-methyl -[4.1.0] bicyclopentane	18
G_7	7		1-methyl-[5.1.0] bicyclohexane	29

G_8	8		1-methyl-[6.1.0] bicycloheptane	47

In order to obtain the matchings and independent sets of these graphs, we compute the k-matchings and k-independent sets of G_5, G_6, G_7, G_8.

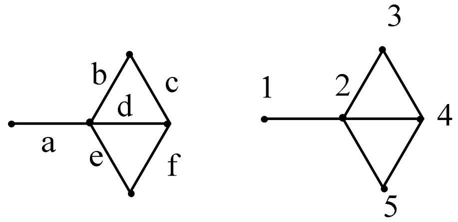


Figure 1. The graph G_5 is labeled with edges and vertices

The set of matchings with cardinality two is $\{\{a,c\},\{a,f\},\{b,f\},\{c,e\}\}$. It means that $m(G_5\,,2) = 4$.

The set of independent sets with cardinality two is $\{\{1,3\},\{1,4\},\{1,5\},\{3,5\}\}$. Thus $\sigma(G_5\,,2) = 4$

The set of independent sets with cardinality three is $\{1,3,5\}$ and $\sigma(G_5\,,3) = 1$.

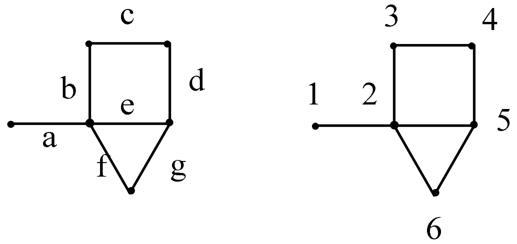


Figure 2. The graph G_6 is labeled with edges and vertices

The set of matchings with cardinality two is
$\{\{a,c\},\{a,d\},\{a,g\},\{b,d\},\{b,g\},\{c,f\},\{c,g\},\{d,f\}\}$ and $m(G_6\,,2) = 8$

The set of matchings with cardinality three is $\{a,c,g\}$ and $m(G_6\,,3) = 1$

The set of independent sets with cardinality two is

$\{\{1,3\},\{1,4\},\{1,5\},\{1,6\},\{2,4\},\{3,5\},\{3,6\},\{4,6\}\}$ and $\sigma(G_6,2) = 8$

The set of independent sets with cardinality three is $\{\{1,3,5\},\{1,3,6\},\{1,4,6\}\}$ and $\sigma(G_6,3) = 3$.

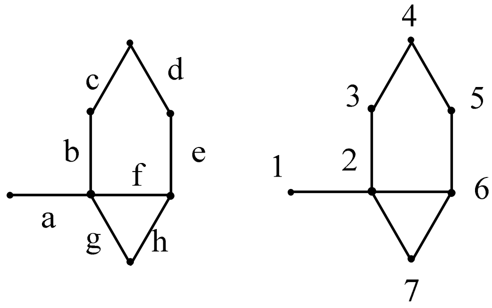


Figure 3. The graph G_7 is labeled with edges and vertices

The set of matchings with cardinality two is

$\{\{a,c\},\{a,d\},\{a,e\},\{a,h\},\{b,d\},\{b,e\},\{b,h\},\{c,e\},\{c,f\},\{c,g\},\{c,h\},\{d,f\},\{d,g\},\{d,h\}\{e,g\}\}$.

Thus we obtain that $m(G_7,2) = 15$.

The set of matchings with cardinality three is $\{\{a,c,e\},\{a,c,h\},\{a,d,h\},\{b,d,h\},\{c,e,g\}\}$ and $m(G_7,3) = 5$.

The set of independent sets with cardinality two is

$\{\{1,3\},\{1,4\},\{1,5\},\{1,6\},\{1,7\},\{2,4\},\{2,5\},\{3,5\},\{3,6\},\{3,7\},\{4,6\},\{4,7\},\{5,7\}\}$ and $\sigma(G_7,2) = 13$

The set of independent sets with cardinality three is

$\{\{1,3,5\},\{1,3,6\},\{1,3,7\},\{1,4,6\},\{1,4,7\},\{1,5,7\},\{3,5,7\}\}$ and $\sigma(G_7,3) = 7$.

The set of independent sets with cardinality four is $\{1,3,5,7\}$ and $\sigma(G_7,4) = 1$.

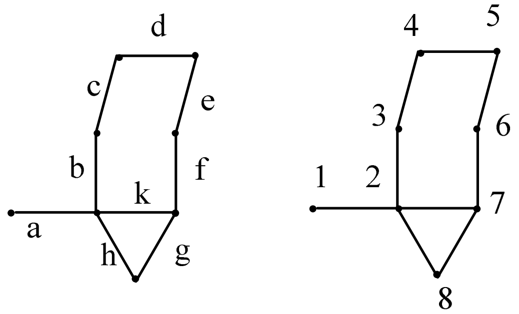


Figure 4. The graph G_8 is labeled with edges and vertices

The set of matchings with cardinality two is

$$\left\{ \begin{matrix} \{a,c\},\{a,d\},\{a,e\},\{a,f\},\{a,g\},\{b,d\},\{b,e\},\{b,f\},\{b,g\},\{c,e\}, \\ \{c,f\},\{c,g\},\{c,h\},\{c,k\},\{d,f\},\{d,g\},\{d,h\},\{d,k\},\{e,g\},\{e,h\},\{e,k\},\{f,h\} \end{matrix} \right\}.$$

Therefore $m(G_8\,,2) = 22$.

The set of matchings with cardinality three is

$$\left\{ \begin{matrix} \{a,c,e\},\{a,c,f\},\{a,c,g\},\{a,d,f\},\{a,d,g\},\{a,e,g\},\{b,d,e\},\{b,d,f\},\{b,d,g\},\{b,e,g\}, \\ \{c,e,g\},\{c,e,k\},\{c,e,h\},\{d,f,h\} \end{matrix} \right\}$$

Therefore $m(G_8\,,3) = 14$.

The set of matchings with cardinality four is $\{a,c,e,g\}$ and $m(G_8\,,4) = 1$.

The set of independent sets with cardinality two is

$$\left\{ \begin{matrix} \{1,3\},\{1,4\},\{1,5\},\{1,6\},\{1,7\},\{1,8\},\{2,4\},\{2,5\},\{2,6\},\{3,5\}, \\ \{3,6\},\{3,7\},\{3,8\},\{4,6\},\{4,7\},\{4,8\},\{5,7\},\{5,8\},\{6,8\} \end{matrix} \right\}.$$

Thus we obtain that $\sigma(G_8\,,3) = 19$.

The set of independent sets with cardinality three is

$$\left\{ \begin{matrix} \{1,3,5\},\{1,3,6\},\{1,3,7\},\{1,3,8\},\{1,4,6\},\{1,4,7\},\{1,4,8\},\{1,5,7\}, \\ \{1,5,8\},\{1,6,8\},\{2,4,6\},\{3,5,7\},\{3,5,8\},\{3,6,8\},\{4,6,8\} \end{matrix} \right\}.$$

It implies that $\sigma(G_8\,,3) = 15$.

The set of independent sets with cardinality four is $\{\{1,3,5,7\},\{1,3,5,8\},\{1,3,6,8\},\{1,4,6,8\}\}$.

$$\sigma(G_8\,,4) = 4.$$

Now we can prepare two tables which shows the matchings and independent sets of 1-methyl bicyclo [X.1.0] alkanes. Moreover we obtain some relations from these tables.

Table 3. k-matchings of 1-methyl bicyclo [X.1.0] alkanes

Graphs	$m(G,0)$	$m(G,1)$	$m(G,2)$	$m(G,3)$	$m(G,4)$	$m(G,5)$	$m(G,6)$	Z-index
G_5	1	6	4					11
G_6	1	7	9	1				18
G_7	1	8	15	5				29
G_8	1	9	22	14	1			47
G_9	1	10	30	29	6			76
G_{10}	1	11	39	51	20	1		123
G_{11}	1	12	49	81	49	7		199
G_{12}	1	13	60	120	100	27	1	322

Table 4. k-independent Sets of 1-methyl bicyclo [X.1.0] alkanes

Graphs	$\sigma(G,0)$	$\sigma(G,1)$	$\sigma(G,2)$	$\sigma(G,3)$	$\sigma(G,4)$	$\sigma(G,5)$	$\sigma(G,6)$	σ-index
G_5	1	5	4	1				11
G_6	1	6	8	3				18
G_7	1	7	13	7	1			29
G_8	1	8	19	15	4			47
G_9	1	9	26	28	11	1		76
G_{10}	1	10	34	47	26	5		123
G_{11}	1	11	43	73	54	16	1	199
G_{12}	1	12	53	107	101	42	6	322

Results 3. It is seen from the Table 3 and Table 4 that with order of n,

$i)$ $m(G_i,0) = 1$ and $\sigma(G_i,0) = 1$ by definition.

$ii)$ $m(G_i,1) = n+1$ and $\sigma(G_i,1) = n$ $(i \geq 5)$.

$iii)$ $m(G_i,2) = m(G_{i-1},2) + m(G_{i-1},1) - 1$, and

$\sigma(G_i, 2) = \sigma(G_{i-1}, 2) + \sigma(G_{i-1}, 1) - 1\ (i \geq 6).$

$iv)$ $m(G_i, k) = m(G_{i-1}, k) + m(G_{i-2}, k-1)$, and

$\sigma(G_i, k) = \sigma(G_{i-1}, k) + \sigma(G_{i-2}, k-1)\ \left(i \geq 6,\ 1 \leq k < \left\lceil \frac{n}{2} \right\rceil\right).$

$v)$ If n is even, the number of the last matching is equal to $m\left(G_i, \frac{n}{2}\right) = 1\ (i \geq 6)$,

If n is odd, the number of the last matching is equal to $m\left(G_i, \left\lfloor \frac{n}{2} \right\rfloor\right) = \left\lceil \frac{n}{2} \right\rceil + 1\ (i \geq 5)$.

$vi)$ If n is odd, the number of the last independent set is equal to $\sigma\left(G_i, \left\lceil \frac{n}{2} \right\rceil\right) = 1\ (i \geq 5)$,

If n is even, the number of the last independent set is equal to $\sigma\left(G_i, \frac{n}{2}\right) = \frac{n}{2}\ (i \geq 6)$.

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