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THE MERRIFIELD-SIMMONS INDICES OF 2-METHYL ALKANES AND 1-METHYL BICYCLO [X.1.0] ALKANES

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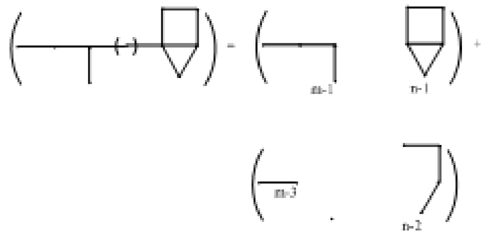
In this paper the Merrifield-Simmons indices of the 2-methyl alkanes and the 1-methyl bicyclo [X.1.0] alkanes are obtained. After that, the Merrifield-Simmons index of the binary compositions of these molecules which are connected with a single carbon atom are obtained.



INTRODUCTION

The Merrifield-Simmons (or σ-index) index was introduced by Richard Merrifield and Howard Simmons in a series of articles[1-5] and this theory was outlined in the book.[6]

The name "Merrifield-Simmons index" for the graph invariant σ was first time used by Ivan Gutman.[7] Today, in mathematical chemistry this name is commonly accepted. For details of the theory of the Merrifield-Simmons index see the review.[8]

Let $G = (V, E)$ be a simple connected graph whose vertex set V and the edge set E. A set X of the vertices of the graph G is called independent if no two distinct vertices of X are adjacent.[9] A k-independent set of G is as set of k-mutually independent vertices. The number of k-independent sets of G is denoted by $\sigma(G, k)$. By definition $\sigma(G, 0) = 1$ for any graph G. Furthermore the Merrifield-Simmons index of a graph G, denoted by $\sigma(G)$, is defined as

$$\sigma(G) = \sum_{k=0}^{n} \sigma(G,k)$$

in other words, $\sigma(G)$ is equal to the total number of independent sets of G.[10]

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 vertices of W, respectively. For the neighborhood of a vertex υ in a graph G, the notation $N_G(\upsilon)$ is used which is defined as $N_G(\upsilon) = \{u \mid (u, v) \in E(G)\}$ and $N_G[\upsilon] = N_G(\upsilon) \cup \{\upsilon\}$.

The path graphs and the cycle graphs are denoted by P_n and C_n which has n vertices respectively.

Lemma 1. Let $G = (V(G), E(G))$ be a graph. Then[9]
i) If $G_1, G_2, ..., G_m$ are the components of the graph G, then $\sigma(G) = \prod_{k=1}^{m} \sigma(G_k)$.

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ii) If $e = xy \in E(G)$, then

$$\sigma(G) = \sigma(G - \{x, y\}) + \sigma(G - N_G[x]) + \sigma(G - N_G[y])$$

iii) If $x \in V(G)$, then $\sigma(G) = (G - \{x\} + \sigma(G - N_G[x])$.
iv) $\sigma(P_n) = F_{n+2}$ $n \geq 1$ and $\sigma(Cn) = L_n$ for $n \geq 3$.

We use Fibonacci number sequence which is defined with $F_1 = F_2 = 1$, $F_n = F_{n-1} + F_{n-2}$ $n \geq 3$ and Lucas number sequence which is defined with $L_1 = 1, L_2 = 3$, $L_n = L_{n-1} + L_{n-2}$ $(n \geq 3)$.[11]

Example 1. We calculate the Merrifield-Simmons index of the 1-methyl-[3.1.0] bicyclo butane by definition of the Merrifield-Simmons index. The molecular graph and labeled vertices of 1-methyl-[3.1.0] bicyclo butane are showed in Figure 1.

It is clear from the Table 1

$$\sigma(G) = \sum_{k=1}^{3} \sigma(G, k) = 11 = L_5.$$

In this paper we investigate the Merrifield-Simmons indices of 2-methyl alkanes and the 1-methyl bicyclo [X.1.0] alkanes and after that we obtained the Merrifiel-Simmons index of the binary compositions of these molecules which are connected with a C atom. The first molecule has *m* C atoms and the second molecule has *n* C atoms which are connected with a common C atom. In this situation the main molecule has m + n – 1 C atoms and its graph is denoted with $G_{m,n}$.

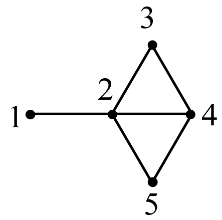


Fig. 1 – Molecular graph of the 1-methyl-[3.1.0] bicyclo butane.

We showed the first four 2-methyl alkanes and the 1-methyl bicyclo [X.1.0] alkanes and their Merrifield-Simmons indices on the below.

Table 1

Number of the *k*-independent sets of 1-methyl-[3.1.0] bicyclo butane

σ(G, 0) = 1	σ(G, 1) = 5	σ(G, 2) = 4	σ(G, 3) = 1
1	1, 2, 3, 4, 5	1-3, 1-4, 1-5, 3-5	1-3-5

Table 2

Merrifield-Simmons indices of the first four 2-Methyl Alkanes

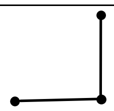
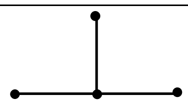
Numbers of points	Moleculer Graph	Name	σ-Index
3		propane	5
4		2-methyl propane	9

Table 2 (continued)

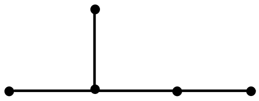
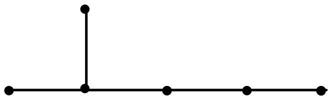
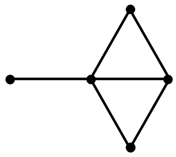
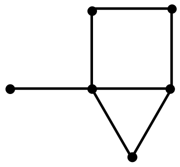
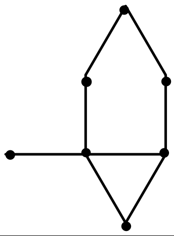
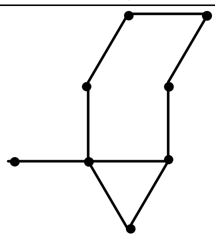
5		2-methyl butane	14
6		2-methyl pentane	23

Table 3

The Merrifield-Simmons indices of the first four 1-Methyl Bicyclo [X.1.0] Alkanes

Numbers of points	Moleculer Graph	Name	σ-Index
5		1-methyl-[3.1.0] bicyclo butane	11
6		1-methyl -[4.1.0] bicyclopentane	18
7		1-methyl-[5.1.0] bicyclohexane	29
8		1-methyl-[6.1.0] bicycloheptane	47

CONCLUSIONS

Theorem 1. If G_n is a graph of a 2-methyl alkane, then

$$\sigma(G_n) = L_n + F_{n-1} \quad (n \geq 3).$$

Proof. We use Lemma 1 (*iii*) in here.

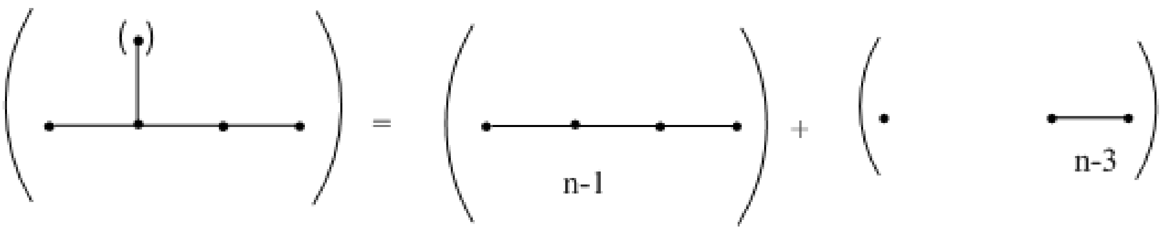


Fig. 2 – Molecular graph of a 2-methyl alkane which has n points needed for the calculation of the σ(G_n).

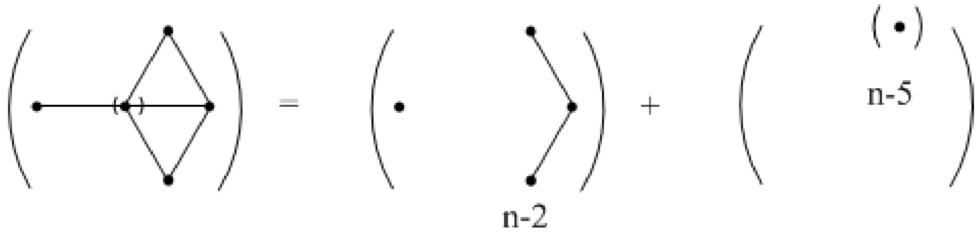


Fig. 3 – Molecular graph of a 1-methyl bicyclo [X.1.0] alkane which has n points needed for the calculation of the $\sigma(G_n)$.

We delete the point on the top of the graph which is showed in small brackets firstly.

$$\begin{aligned}\sigma(G_n) &= \sigma(P_{n-1}) + \sigma(P_1)\,\sigma(P_{n-3})\\ &= F_{n+1} + F_3F_{n-1}\\ &= F_{n+1} + 2F_{n-1}\\ &= F_{n+1} + F_{n-1} + F_{n-1}\\ &= L_n + F_{n-1}.\end{aligned}$$

Theorem 2. If G_n is a graph of a 1-methyl bicyclo [X.1.0] alkane, then

$$\sigma(G_n) = L_n \ (n \geq 5).$$

Proof. We use Lemma 1 (*iii*).

We delete the point which is showed in small brackets.

$$\begin{aligned}\sigma(G_n) &= \sigma(P_1)\sigma(P_{n-2}) + \sigma(P_{n-5})\\ &= F_3F_n + F_{n-3}\\ &= 2F_n + F_{n-3}\\ &= F_n + F_{n-1} + F_{n-2} + F_{n-3}\\ &= F_{n+1} + F_{n-1}\\ &= L_n.\end{aligned}$$

Lemma 2. If G_m is a graph of a 2-methyl alkane, then
$\sigma(G_m) = \sigma(G_{m-1}) + \sigma(G_{m-2})$.

Proof. $$\begin{aligned}\sigma(G_m) &= L_m + F_{m-1}\\ &= L_{m-1} + L_{m-2} + F_{m-2} + F_{m-3}\\ &= L_{m-1} + F_{m-2} + L_{m-2} + F_{m-3}\\ &= \sigma(G_{m-1}) + \sigma(G_{m-2}).\end{aligned}$$

Lemma 3. If G_m is a graph of a 1-methyl bicyclo [X.1.0] alkane, then

$$\sigma(G_m) = \sigma(G_{m-1}) + \sigma(G_{m-2}).$$

Proof. $$\begin{aligned}\sigma(G_m) &= L_m\\ &= L_{m-1} + L_{m-2}\\ &= \sigma(G_{m-1}) + \sigma(G_{m-2})\end{aligned}$$

Theorem 3. If the main molecule is a composition of a 2-methyl alkane and 1-methyl bicyclo [X.1.0] alkane, then

$$\sigma(G_{m,n}) = 2(F_{m+1}F_{n-1} + F_{m-1}F_n)$$

Proof.

We applicate Lemma 1 (*iii*) the point which is showed in small brackets in Figure 4. The σ-index of the first term on the right hand is a pruduct of σ-index of a path graph and σ-index of the remaining part of a 1-methyl bicyclo alkane which has $m - 1$ and $n-1$ points respectively.

The σ-index of the second term on the right side is a product of the σ -indices of three paths graphs which has 1, $m - 3$ and $n - 2$ points respectively.

Now we obtain the Merrifield-Simmons of the remaining part of the 1-methyl bicyclo alkane which has $n - 1$ points which is shown in Fig. 5.

We apply Lemma 1 (iii) the point which is at the bottom in Fig. 5. The σ-index of the remaining part of the 1-methyl bicyclo alkane is a product of a cycle graph and a path graph which has $n - 2$ and $n - 4$ points respectively. Therefore σ-index of the remaining part of the 1-methyl bicyclo alkane is

$$\begin{aligned}\sigma(G_{n-1}) &= \sigma(G_{n-2}) + \sigma(P_{m-4})\\ &= F_{n-1} + F_{n-3} + F_{n-2} = 2F_{n-1}.\end{aligned}$$

Finally we calculate the σ-index of the main molecule

$$\begin{aligned}\sigma(G_{m,n}) &= \sigma(P_{m-1})\sigma(G_{n-1}) + \sigma(P_1)\,\sigma(P_{m-3})\sigma(P_{n-2})\\ &= F_{m+1}2F_{n-1} + F_3F_{m-1}F_n\\ &= 2(F_{m+1}F_{n-1} + F_{m-1}F_n).\end{aligned}$$

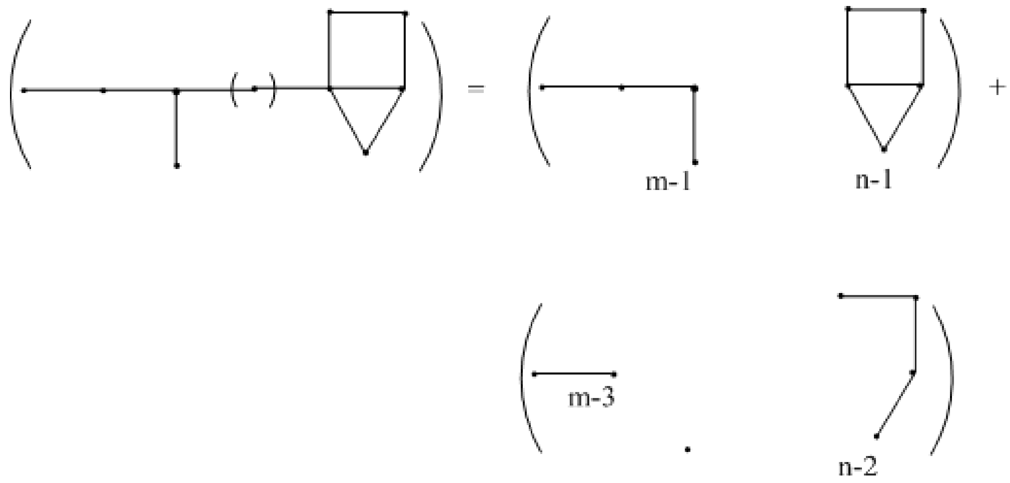


Fig. 4 – Molecular graph of the composition of a 2-methyl alkane and 1-methyl bicyclo alkane which has *m* and *n* points respectively.

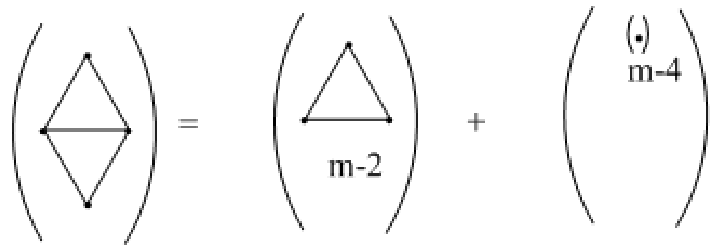


Fig. 5 – Molecular graph of the remaining of a 1-methyl bicyclo [X.1.0] alkane which has *n* – **1** points.

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