ON THE FIBONACCI NUMBERS OF THE MOLECULAR GRAPHS OF SOME BENT PHENYLENES

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Abstract. The Fibonacci number $f(G)$ of a graph $G = (V, E)$ is defined as the number of all subsets U of V such that no two vertices in U are adjacent. Phenylenes represent a class of condensed polycyclic conjugated compounds which have the molecular graph possessing both six-membered and four-membered circuits. In this paper we are concerned with special types of bent phenylenes expanding our previous results on the linear phenylenes. The explicit formulas for the Fibonacci numbers of the bent phenylenes are found as functions of the number n of hexagons in both mentioned branches of phenylene.

Keywords: Molecular graph, Fibonacci number, bent phenylene.

1. Introduction

A molecular graph in chemical graph theory is a representation of the structural formula of a chemical compound in terms of graph theory. Vertices of it correspond to the atoms of the compound and edges correspond to the chemical bonds. Many chemical structures and compounds are usually modeled by a molecular graph to analyze underlying theoretical properties.

Phenylenes are an important class of conjugated hydrocarbons. Characteristic structural features of the phenylenes are alternating fused benzene and cyclobutadiene rings (circuits) which can be arranged in linear, angular or branched geometries. It means that the six-membered circuits (hexagons) are adjacent only to four-membered circuits, and every four-membered circuit is adjacent to a pair of nonadjacent hexagons. If each six-membered circuit in the molecular graph of a phenylene is adjacent only to two four-membered circuits, we say that it is a $[N]$phenylene chain, where N signifies the number of benzene units. The molecular graphs of several phenylenes are presented in Fig. 1. In

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particular, there are the linear [3]phenylene (a), the angular [3]phenylene (b) and the triangular [4]phenylene (c) as the case of a branched phenylene.

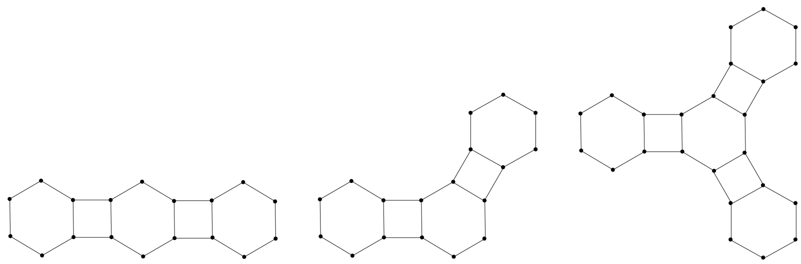

Figure 1:

A topological index of a graph can be viewed as a numerical quantity which is invariant under isomorphism of graphs. Many topological indices are closely correlated with some physico-chemical characteristics of the respective compounds. Hexagonal systems are of the great importance for theoretical chemistry because they are the natural graph representations of the benzenoid hydrocarbons [2]. The structure of these graphs is apparently the simplest among all hexagonal systems [3]. Therefore the first results on topological indices were achieved for hexagonal chains. One of the most famous and interested topological indices is the Fibonacci number of a molecular graph. For the general graph-theoretic terminology we refer the reader to any of standard monographs, e.g. [10].

In the number theory the Fibonacci numbers F_n are defined by the second order recurrence $F_{n+2} = F_{n+1} + F_n$ with $F_0 = 0$, $F_1 = 1$. Similarly, the Lucas numbers L_n satisfy the same recurrence with the initial terms $L_0 = 2$, $L_1 = 1$. The total number of subsets of $\{1, 2, \ldots, n\}$ such that no two elements are adjacent is the Fibonacci number F_{n+2}. In view of this fact Prodinger and Tichy introduced in 1982 the Fibonacci number of a graph [6].

Definition 1. *Let $G - (V, E)$ be a simple graph. The Fibonacci number $f(G)$ of G is defined as the number of all subsets U of V such that no two vertices in U are adjacent.*

The subset U of k mutually independent vertices is called the $k-$independent set of G. We denote $i(G, k)$ the number of the $k-$independent sets of G and $i(G, 0) = 1$ by definition for any graph G. Then, the Fibonacci number of G is given by the relation $f(G) = \sum_k i(G, k)$, where the summation is taken over all nonnegative integers k.

The chemists Merrifield and Simmons [4] elaborated a theory aimed at describing molecular structure by means of finite set topology. As their graph-topological considerations containing independent sets of vertices attracted wide attention there is used the name the Merrifield-Simmons index in chemistry instead of the Fibonacci number of a graph. However, we will use primarily the name the Fibonacci number of a graph in this paper. In recent years, a lot of works have been published on the extremal problem for the Fibonacci number of graphs. Wagner and Gutman gave in [9] a survey which collects and classifies these results, and also provides some useful auxiliary tools and techniques that are used in the study of this type of problems.

Directly from Definition 1 it is easy to find the Fibonacci numbers for paths and circuits (rings).

Theorem 1. *Let P_n be a path with n vertices and C_n a circuit with n vertices. Then $f(P_n) = F_{n+2}$ and $f(C_n) = L_n$.*

The Fibonacci numbers for various classes of graph have been found. For example, Yeh [11] computed algorithmically the Fibonacci numbers of the lattice product graphs, Ren, He and Yang [7] found the Fibonacci number of zig-zag tree-type hexagonal systems and Alameddine [1] found upper and below bounds for the Fibonacci numbers of maximal outerplanar graphs on a given number of vertices.

2. Preliminary results

In this section, we remind some important and useful results for the following calculations.

Theorem 2 ([6])**.** *If G_1, G_2 are disjoint graphs then $f(G_1 \sqcup G_2) = f(G_1)f(G_2)$.*

Theorem 3 ([5])**.** *Let G be a graph with at least two vertices and v be its arbitrary vertex. Then for the Fibonacci number of G the formula $f(G) = f(G - v) + f(G - (v))$ holds, where $G - v$ is the subgraph of G obtained from G by deletion of the vertex v and $G - (v)$ is the subgraph of G obtained by deletion of the vertex v and all the vertices adjacent to v.*

Theorem 4 ([5])**.** *If vertices u, v are adjacent in a graph G then*

a) $f(G) = f(G - \{u, v\}) + f(G - (u)) + f(G - (v))$, where $G - \{u, v\}$ is the subgraph of G obtained by deletion of the vertices u and v of G,

b) $f(G) = f(G - uv) - f(G - (u, v))$, where $G - uv$ is the subgraph of G obtained by deletion of the edge uv of G and $G - (u, v)$ is the subgraph of G obtained by deletion of the vertices u, v and all the vertices adjacent to them.

In [8] we expressed the Fibonacci number of the linear phenylene as a function of the number of its hexagons. We mention the principle of our considerations as it will be used it the next section.

The following formulas were derived from Theorem 3 by suitable choices of the vertex v in the particular cases.

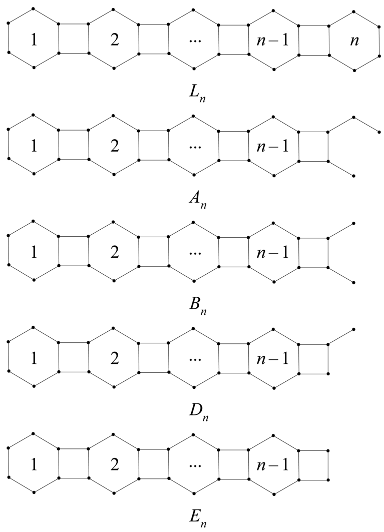

Figure 2:

Lemma 1 ([8])**.** *Let L_n be the linear phenylene with n hexagons and let A_n, B_n, D_n, E_n be graphs as in Fig. 2. Then the following relations hold for any positive integer $n > 1$.*

$$f(L_n) = f(A_n) + f(D_n), \tag{1}$$

$$f(A_n) = f(B_n) + f(D_n), \tag{2}$$

$$f(B_n) = 4f(L_{n-1}) + 4f(A_{n-1}), \tag{3}$$

$$f(D_n) = f(L_{n-1}) + f(A_{n-1}) + f(E_n), \tag{4}$$

$$f(E_n) = f(L_{n-1}) + 2f(A_{n-1}). \tag{5}$$

We denote $f(L_n) = l_n$, $f(A_n) = a_n$, $f(B_n) = b_n$, $f(D_n) = d_n$ and $f(E_n) = e_n$ for short.

Theorem 5. *The values of the Fibonacci numbers for the graphs A_n are $a_n = (1/(\gamma - \delta)) \left[(199 - 13\delta)\gamma^{n-1} - (199 - 13\gamma)\delta^{n-1}\right]$ for any positive integer n, where $\gamma = (15 + \sqrt{241})/2$, $\delta = (15 - \sqrt{241})/2$.*

The proof is based on Lemma 1. After elimination of the remaining variables identities (1)-(5) lead to the homogeneous linear difference equation of the second order with constant coefficients $a_{n+2} - 15a_{n+1} - 4a_n = 0$. The general solution of this equation has the form $a_n = K_1\gamma^n + K_2\delta^n$, where K_1, K_2 are arbitrary real numbers. It is easy to calculate that $a_1 = 13$ and $a_2 = 199$, and therefore $K_1 = \frac{199-13\delta}{\gamma(\gamma-\delta)}$, $K_2 = \frac{199-13\gamma}{\delta(\gamma-\delta)}$, which gives the expression for a_n.

Using the expression for a_n and the relation $l_n = \frac{1}{6}a_{n+1} - \frac{7}{6}a_n$ we have the following result.

Theorem 6. *The Fibonacci number of the linear phenylene with n hexagons can be expressed in the form*

$$f(L_n) = l_n = \frac{1}{\gamma - \delta}\left[(18\gamma + 4)\gamma^{n-1} - (18\delta + 4)\delta^{n-1}\right] \tag{6}$$

for any positive integer n.

Remark. The closed expression for b_n, d_n, e_n are obtained by the similar way. For any positive integer we have

$b_n = \frac{1}{\gamma-\delta}\left[(124\gamma + 32)\gamma^{n-2} - (124\delta + 32)\delta^{n-2}\right]$,

$d_n = \frac{5}{\gamma-\delta}(\gamma^n - \delta^n)$,

$e_n = \frac{1}{\gamma-\delta}\left[(44\gamma + 12)\gamma^{n-2} - (44\delta + 12)\delta^{n-2}\right]$.

3. Main results

Now we consider the molecular graph $L_{n,n}$ of the bent phenylene which consists of two linear phenylenes L_n of the same length of $n \geq 2$. The phenylenes have the common hexagon (Fig.3). It is possible to use the results from the previous section.

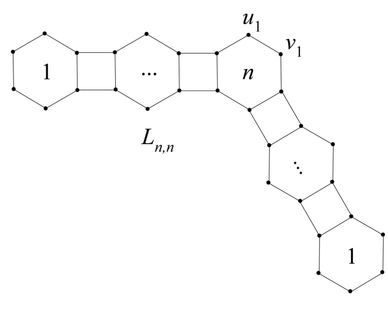

Figure 3:

First, we prove the following Lemma.

Lemma 2. *The terms of the sequence $\{f(L_{n,n})\}$ satisfy the relation*

$$f(L_{n,n}) = d_n^2 - 4a_{n-1}^2 - l_{n-1}^2 - 2l_{n-1}a_{n-1} \tag{7}$$

for any positive integer $n \geq 2$.

Proof. The relation can be derived by repeatedly using Theorem 2 and the both statements of Theorem 4. First, we choose the edge u_1v_1 in $L_{n,n}$ (see Fig. 3) and use statement (b) of Theorem 4. Then we choose the edge u_2v_2 in $L_{n,n} - u_1v_1 = L^{(1)}$ and use the statement (b) of Theorem 4. Finally, we use the vertices u_3, v_3 in $L_{n,n} - (u_1, v_1) = L^{(2)}$ and the statement (a) of Theorem 4 (see Fig.4).

So we have successively

$$\begin{aligned} f(L_{n,n}) &= f(L_{n,n} - u_1v_1) - f(L_{n,n} - (u_1, v_1)) \\ &= f(L^{(1)}) - f(L^{(2)}) \\ &= f(L^{(1)} - u_2v_2) - f(L^{(1)} - (u_2, v_2)) - (f(L^{(2)} - \{u_3, v_3\}) \\ &+ f(L^{(2)} - (u_3)) + f(L^{(2)} - (v_3))) \\ &= d_nd_n - 2a_{n-1}2a_{n-1} - (l_{n-1}l_{n-1} + l_{n-1}a_{n-1} + a_{n-1}l_{n-1}) \end{aligned}$$

which gives the desired expression. □

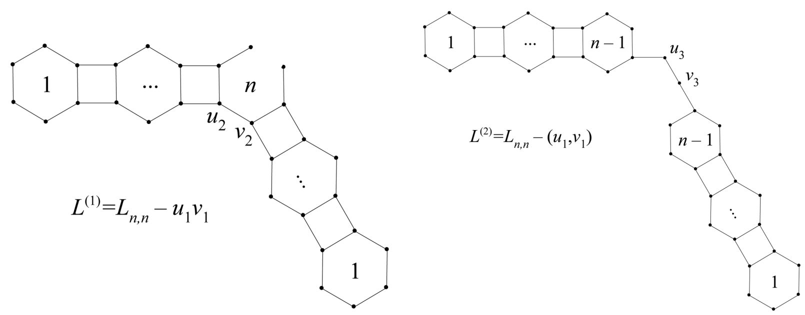

Figure 4:

Lemma 3. *For the roots $\gamma = (15+\sqrt{241})/2$, $\delta = (15-\sqrt{241})/2$ of the equation $x^2 - 15x - 4 = 0$ the following relations hold: $\gamma\delta = -4$, $\gamma^2 = 15\gamma + 4$, $\gamma^4 = 3495\gamma + 916$, $\delta^2 = 15\delta + 4$, $\delta^4 = 3495\delta + 916$.*

Proof. These identities are trivial consequences of roots properties of a quadratic equation. For instance, $\gamma^4 = (15\gamma + 4)^2 = 225(15\gamma + 4) + 120\gamma + 16 = 3495\gamma + 916$. □

Theorem 7. *The Fibonacci number of the graph $L_{n,n}$ for any positive integer n can be written in the form*

$$\begin{aligned} f(L_{n,n}) = &\frac{1}{(\gamma-\delta)^2}[(64547\gamma + 16916)\gamma^{2n-4} \\ &+ (64547\delta + 16916)\delta^{2n-4} - 200(-4)^{n-2}]. \end{aligned} \tag{8}$$

Proof. We will use Lemma 2 and the explicit formulas for l_n, a_n and d_n. Then we can write successively for any positive integer $n \geq 2$

$$\begin{aligned} f(L_{n,n}) = &\frac{1}{(\gamma-\delta)^2}(25(\gamma^n-\delta^n)^2 \\ &-4[(199-13\delta)\gamma^{n-2}-(199-13\gamma)\delta^{n-2}]^2-[(18\gamma+4)\gamma^{n-2}-(18\delta+4)\delta^{n-2}]^2 \\ &-2[(199-13\delta)\gamma^{n-2}-(199-13\gamma)\delta^{n-2}][(18\gamma+4)\gamma^{n-2}-(18\delta+4)\delta^{n-2}]) \\ =&\frac{1}{(\gamma-\delta)^2}([25\gamma^4-4(199-13\delta)^2-(18\gamma+4)^2-2(199-13\delta)(18\gamma+4)]\gamma^{2n-4} \\ &+[25\delta^4-4(199-13\gamma)^2-(18\delta+4)^2-2(199-13\gamma)(18\delta+4)]\delta^{2n-4} \\ &+[-800+8(199-13\delta)(199-13\gamma)+2(18\gamma+4)(18\delta+4) \\ &+2(199-13\delta)(18\delta+4)+2(199-13\gamma)(18\gamma+4)](-4)^{n-2}) \quad \text{as } \gamma\delta=-4. \end{aligned}$$

This expression can be simplified using the identities of Lemma 3. Further details of this part of the proof are left to readers.

Then

$$\begin{aligned} f(L_{n,n}) &= \frac{1}{(\gamma-\delta)^2}[(75207\gamma+10660\delta-142984)\gamma^{2n-4} \\ &+(75207\delta+10660\gamma-142984)\delta^{2n-4} \\ &+(307480-20512\gamma-20512\delta)(-4)^{n-2}] \\ &= \frac{1}{(\gamma-\delta)^2}[(64547\gamma+10660(\gamma+\delta)-142984)\gamma^{2n-4} \\ &+(64547\delta+10660(\gamma+\delta)-142984)\delta^{2n-4} \\ &+(307480-20512(\gamma+\delta))(-4)^{n-2}]. \end{aligned}$$

As $\gamma+\delta=15$ and $\gamma-\delta=\sqrt{241}$, the formula (8) is obtained immediately for $n \geq 2$.

Moreover,

$$\begin{aligned} f(L_{1,1}) &= \frac{1}{(\gamma-\delta)^2}[(64547\gamma+16916)\gamma^{-2}+(64547\delta+16916)\delta^{-2}-200(-4)^{-1}] \\ &= \frac{1}{(\gamma-\delta)^2}\left[(64547\gamma+16916)\frac{\delta^2}{16}+(64547\delta+16916)\frac{\gamma^2}{16}-200\left(-\frac{1}{4}\right)\right] \\ &= \frac{1}{(\gamma-\delta)^2}\left[\left(\frac{64547}{16}\gamma+\frac{4229}{4}\right)(15\delta+4)+\left(\frac{64547}{16}\delta+\frac{4229}{4}\right)(15\gamma+4)+50\right] \\ &= \frac{1}{241}\left[\frac{968205}{8}\gamma\delta+\frac{63991}{2}(\gamma+\delta)+8508\right]=18=f(C_6). \end{aligned}$$

As $L_{1,1}=C_6$, the statement holds also for $n=1$. □

Example. The previous function expression of $f(L_{n,n})$ can be used to find $f(L_{2,2})$ and $f(L_{3,3})$. In this case, $L_{2,2}$ and $L_{3,3}$ represent the molecular graphs of a bent [3]phenylene and of a bent [5]phenylene, respectively.

Thus,

$$f(L_{2,2}) = \frac{1}{(\gamma-\delta)^2}[(64547\gamma+16916)\gamma^0 + (64547\delta+16916)\delta^0 - 200(-4)^0]$$
$$= \frac{1}{241}[64547(\gamma+\delta)+33832-200] = 4157.$$

Similarly,

$$f(L_{3,3}) = \frac{1}{(\gamma-\delta)^2}[(64547\gamma+16916)\gamma^2 + (64547\delta+16916)\delta^2 - 200(-4)]$$
$$= \frac{1}{(\gamma-\delta)^2}[(64547\gamma+16916)(15\gamma+4) + (64547\delta+16916)(15\delta+4)+800]$$
$$= \frac{1}{(\gamma-\delta)^2}[968205(15\gamma+4)+511928\gamma+67664+968205(15\delta+4)+511928\delta$$
$$+67664+800] = \frac{1}{241}[15035003(\gamma+\delta)+7880968+800] = 968493.$$

Further we consider the molecular graph $Z_{n,n}$ of the bent phenylene which consists of two linear phenylenes L_n of the same length of $n \geq 1$. In this case, the linear phenylenes are linked using a square (Fig. 5).

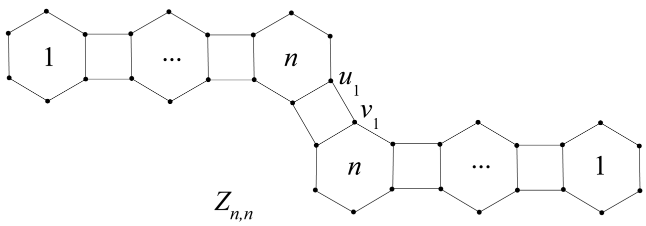

Figure 5:

First, we prove the following Lemma.

Lemma 4. *The terms of the sequence* $\{f(Z_{n,n})\}$ *satisfy the relation*

$$f(Z_{n,n}) = l_n^2 - 2d_n(3l_{n-1} + 2a_{n-1}) \tag{9}$$

for any positive integer $n \geq 2$.

Proof. The relation can be derived by repeatedly using Theorem 2 and the both statements of Theorem 4. First we choose the edge u_1v_1 in $Z_{n,n}$ (see Fig. 5) and use the statement (b) of Theorem 4. Then we choose the edge u_2v_2 in $Z_{n,n} - u_1v_1 = Z^{(1)}$ and use the statement (b) of Theorem 4. Hence $f(Z_{n,n}) = f(Z_{n,n} - u_1v_1) - f(Z_{n,n} - (u_1, v_1)) = f(Z^{(1)}) - f(Z^{(2)})$.

It can be easily seen (Fig. 6) that $f(Z^{(2)}) = f(D_n)f(U_{n-1})$. If we choose the vertices u_3, v_3 in U_{n-1} and use the statement (a) of Theorem 4 (see Fig. 6), we obtain (with the help of Theorem 2) $f(U_{n-1}) = 2l_{n-1} + l_{n-1} + 2a_{n-1}$. Then $f(Z_{n,n}) = l_nl_n - d_nf(U_{n-1}) - d_nf(U_{n-1}) = l_n^2 - 2d_n(3l_{n-1} + 2a_{n-1})$, which was to be shown. □

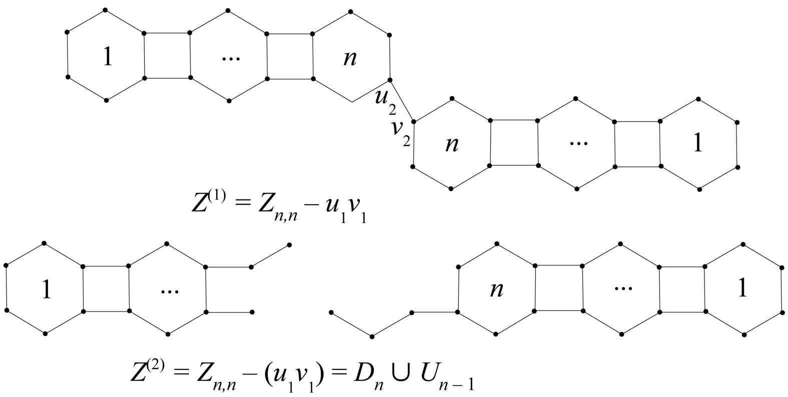

Figure 6:

Theorem 8. *The Fibonacci number of the graph $Z_{n,n}$ has the closed function expression*

$$\begin{aligned} f(Z_{n,n}) = {} & \frac{1}{(\gamma-\delta)^2}\left[(4204\gamma+1112)\gamma^{2n-2}\right. \\ & \left. +(4204\delta+1112)\delta^{2n-2} - 3000(-4)^{n-2}\right] \end{aligned} \tag{10}$$

for any positive integer n.

Proof. Using Lemma 2 and the explicit formulas for l_n, a_n and d_n, we get for $n \geq 2$

$$\begin{aligned} f(Z_{n,n}) = {} & \frac{1}{(\gamma-\delta)^2}\{\left[(18\gamma+4)\gamma^{n-1} - (18\delta+4)\delta^{n-1}\right]^2 \\ & - 10(\gamma^n - \delta^n)(3\left[(18\gamma+4)\gamma^{n-2} - (18\delta+4)\delta^{n-2}\right] \\ & + 2\left[(199-13\delta)\gamma^{n-2} - (199-13\gamma)\delta^{n-2}\right])\} \\ = {} & \frac{1}{(\gamma-\delta)^2}\{\left[(18\gamma+4)^2 - 800\gamma - 200\right]\gamma^{2n-2} \\ & + \left[(18\delta+4)^2 - 800\delta - 200\right]\delta^{2n-2} \\ & + \left[-2(18\gamma+4)(18\delta+4) + 10\delta^2(80\gamma+20) + 10\gamma^2(80\delta+20)\right](-4)^{n-2}\} \\ = {} & \frac{1}{(\gamma-\delta)^2}[(4204\gamma+1112)\gamma^{2n-2} + (4204\delta+1112)\delta^{2n-2} \\ & + (24000\gamma\delta + 6200\gamma + 6200\delta)(-4)^{n-2}]. \end{aligned}$$

Since $\gamma + \delta = 15$ and $\gamma\delta = -4$, we arrive at the expression (10) for $f(Z_{n,n})$, if $n \geq 2$. Moreover, $f(Z_{1,1}) = \frac{1}{(\gamma-\delta)^2}[(4204\gamma+1112)\gamma^0 + (4204\delta+1112)\delta^0 - 3000(-4)^{-1}] = \frac{1}{(\gamma-\delta)^2}[4204(\gamma+\delta) + 2224 - 3000(-\frac{1}{4})] == \frac{1}{241}[63060 + 2224 + 750] = 274 = f(L_2)$ as $Z_{1,1} = L_2$. It completes the proof for all $n \geq 1$. □

4. Conclusion

The total number of independent subsets of graph vertices finds its application mainly in organic chemistry. In particular, there exists the link between the Merrifield-Simmons index and a boiling point of organic compounds. It is the reason why the name "Merrifield-Simmons index" is preferred in the literature to originally pure mathematical "Fibonacci number". In case of molecular graphs, there exists a lot of works devoted to the calculation of the Merrifield-Simmons index for various classes of graphs. The method of calculation used in this paper and the obtained results can be generalized for other classes of molecular graphs.

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