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A CONJECTURE IN THE THEORY OF CYCLIC CONJUGATION AND AN EXAMPLE SUPPORTING ITS VALIDITY

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Abstract. For the success of Aihara's theory of cyclic conjugation it is essential that the zeros of the graph polynomial $\beta(G,C,x)$ are real-valued numbers. It has been conjectured that, indeed, for all graphs G and all circuits C contained in G, all the zeros of $\beta(G,C,x)$ are real. In this paper we show that the conjecture is true for the graphs of the type $G(p_1,p_2,p_3,q_1,q_2,q_3,r)$.

Introduction

In 1977 two closely similar, but not equivalent theories of cyclic conjugation have been independently put forward by Aihara [1] and Bosanac and Gutman [2,3]. Both were aimed to express the contribution of an individual ring to the resonance energy or total π-electron energy of a polycyclic conjugated molecule. Both employed the mathematical apparatus of graph theory and both utilised a reasoning based on the Sachs-graph formalism [4-6].

In order to describe the basic features of these two theories denote by G the molecular graph of a polycyclic conjugated π-electron system and by $C_1, C_2, \ldots, C_r$ its circuits. Then in Aihara's approach the energy-effect of the i-th circuit is measured by the difference

$$ef_A(G,C_i) = E(0,0,\ldots,0,1,0,\ldots,0) - E(0,0,\ldots,0,0,0,\ldots,0) \qquad (1)$$

whereas in the Bosanac-Gutman approach the respective effect is

$$ef_{BG}(G,C_i) = E(1,1,\ldots,1,1,1,\ldots,1) - E(1,1,\ldots,1,0,1,\ldots,1) \ . \qquad (2)$$

In the above formulas $E(t_1,t_2,\ldots,t_{i-1},t_i,t_{i+1},\ldots,t_r)$ is a total-π-electron-energy-like quantity in which the parameter t_j is the extent by which the effect of the j-th circuit contributes to total π-electron energy; if $t_j = 1$ then the effect of C_j is completely taken into account; if $t_j = 0$ then the effect of C_j is completely neglected [7,8]. Accordingly, in this notation $E(1,1,\ldots,1,1,1,\ldots,1)$ stands for the actual total π-electron energy of the conjugated molecule considered.

We note in passing that the difference

$$E(1,1,\ldots,1,1,1,\ldots,1) - E(0,0,\ldots,0,0,0,\ldots,0)$$

measures the overall energy-effect of all cycles in a conjugated molecule;

this quantity is found very suitable to serve as a resonance energy [9,10].

The terms occurring on the right-hand sides of eqs. (1) and (2) are computed as follows:

$$E(0,0,\ldots,0,0,0,\ldots,0) = \sum_{j=1}^{n} g_j \, x_j(\alpha) \tag{3}$$

$$E(0,0,\ldots,0,1,0,\ldots,0) = \sum_{j=1}^{n} g_j \, x_j(\beta) \tag{4}$$

$$E(1,1,\ldots,1,1,1,\ldots,1) = \sum_{j=1}^{n} g_j \, x_j(\phi) \tag{5}$$

$$E(1,1,\ldots,1,0,1,\ldots,1) = \sum_{j=1}^{n} g_j \, x_j(\psi) \quad . \tag{6}$$

In eqs. (3)-(6) g_j is the occupation number of the j-th molecular orbital, corrseponding to the graph eigenvalue $x_j(\phi)$ [5,11]. Further, $x_j(\alpha)$, $x_j(\beta)$, $x_j(\phi)$ and $x_j(\psi)$, $j=1,2,\ldots,n$, are the zeros of the polynomials

$\alpha(G, x)$ = the matching polynomial [12,13]

$$\beta(G,C,x) = \alpha(G, x) - 2\,\alpha(G-C, x) \tag{7}$$

$\phi(G, x)$ = the characteristic polynomial [11,14]

$$\psi(G,C,x) = \phi(G, x) + 2\,\phi(G-C, x)$$

respectively.

For the success of the theory of cyclic conjugation it is essential that the quantities ef_A and ef_{BC} are real-valued. This, of course, will be the case if the zeros of the polynomials α, β, ϕ and ψ are real. The reality of the zeros of the characteristic polynomial $\phi(G,\ x)$ is an elementary and well-known result [14]. The reality of the zeros of the matching polynomial $\alpha(G,\ x)$ has been proved some time ago [13,15]. Herndon discovered cases in which the polynomial $\psi(G,C,x)$ has complex-valued zeros [16]. This observation eventually required a slight reformulation of the ef_{BG}-concept [17].

The only polynomial in the above list for which the problem of the reality of the zeros is not resolved in $\beta(G,C,x)$. In spite of the fact that the reality of the zeros of the β-polynomial has been verified for several classes of graphs [18-20] (among which are all unicyclic and all bicyclic graphs), a general proof of this property has still not been found. Nevertheless, it has been conjectured that [19]

for all graphs G and all circuits C contained in G, all the zeros of the polynomial $\beta(G,C,x) = \alpha(G,x) - 2\,\alpha(G-C,x)$ are real-valued numbers. (*)

In the present paper we show that the above conjecture is true for one more general (infinite) class of graphs, namely for the six-membered circuit of the graph $G(p_1,p_2,p_3,q_1,q_2,q_3,r)$ with arbitrary values of the parameters p_1, p_2, p_3, q_1, q_2, q_3 and r.

The Graph $G(p_1, p_2, p_3, q_1, q_2, q_3, r)$ and Its β-Polynomial

The matching polynomial of a graph G is defined as [12,13]

$$\alpha(G,\ x) = \sum_{k=0}^{n/2} (-1)^k \ m(G,\ k) \ x^{n-2k}$$

where m(G, k) is the number of ways in which k independent (i.e. mutually non-incident) edges can be selected in G.

For the β-polynomial, eq. (7), we need both the matching polynomial of the graph G and of its subgraph G-C. Here G-C denotes the graph obtained by deleting from G the vertices belonging to the circuit C. Whence the degree of α(G-C, x) is $n-|C|$, where n is the number of vertices of G and $|C|$ is the size of the circuit C.

Suppose that the size of the circuit C is an even number and that in the graph G it is not possible to select more than $\nu = |C|/2$ independent edges. Then the conditions $m(G,\ \nu) \neq 0$, $m(G,\ \nu+1) = 0$ are obeyed and

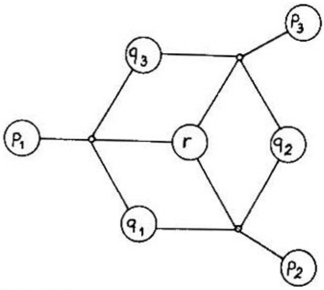
$$\beta(G,C,x) = x^{n-|C|} \left[\sum_{k=0}^{\nu} (-1)^k \ m(G,\ k) \ x^{2(\nu-k)} - 2 \right] . \qquad (8)$$

From (8) is immediately seen that β(G,C,x) has real-valued zeros if and only if the polynomial

$$\beta_0(G,C,x) = \sum_{k=0}^{\nu} (-1)^k \ m(G,\ k) \ x^{\nu-k} - 2$$

has real-valued zeros.

In this paper we consider the class of graphs possessing three independent edges ($\nu = 3$) and six-membered circuits C^*. A diagram indicating the structure of such graphs is depicted in Fig. 1. We show that the statement of the conjecture (*) is true for the circuits C^* and for all graphs from the class examined.



$G = G(p_1, p_2, p_3, q_1, q_2, q_3, r)$

Fig. 1

In Fig. 1 the large circles represent sets of mutually disconnected vertices. The number of vertices in such a set is indicated by the inscribed symbol. Each small circle represents an individual vertex. Hence, the graph displayed in Fig. 1 and denoted by $G(p_1, p_2, p_3, q_1, q_2, q_3, r)$ is assumed to possesses $p_1 + p_2 + p_3 + q_1 + q_2 + q_3 + r + 3$ vertices. For example, the graph for which $p_1 = p_2 = p_3 = 3$, $q_1 = q_2 = q_3 = 2$ and $r = 1$ is presented in Fig. 2.

$G(3,3,3,2,2,2,1)$ =

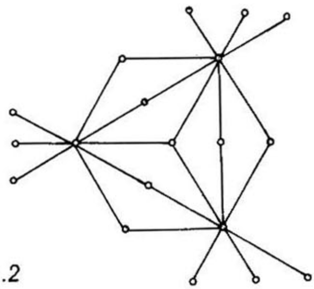


Fig.2

In particular, in this paper we prove that for an arbitrary six-membered circuit C^* of $G = G(p_1,p_2,p_3,q_1,q_2,q_3,r)$ the zeros of the polynomial $\beta(G,C^*,x)$ are real for any choice of the parameters p_i, q_i, r $(i = 1,2,3)$, such that $p_i \geq 0$, $q_i \geq 1$, $r \geq 0$. By this we generalize a previous result, reported in [20], establishing the validity of the conjecture (*) in the case of the graphs $G(p,p,p,q,q,q,r)$, $p \geq 0$, $q \geq 1$, $r = 0$.

In the sequel we will use the following shorthand notation:

(p_i,q_i,r) instead of $(p_1,p_2,p_3,q_1,q_2,q_3,r)$

$\alpha(x)$ or $\alpha(p_i,q_i,r)(x)$ instead of $\alpha(G(p_1,p_2,p_3,q_1,q_2,q_3,r),\ x)$

$\beta(x)$ or $\beta(p_i,q_i,r)(x)$ instead of $\beta(G(p_1,p_2,p_3,q_1,q_2,q_3,r),C^*,x)$

m_k or $m_k(p_i,q_i,r)$ instead of $m(G(p_1,p_2,p_3,q_1,q_2,q_3,r)\ ,k)$.

Using the above introduced notation, the matching polynomial of the graph $G(p_1, p_2, p_3, q_1, q_2, q_3, r)$ is of the form

$$\alpha(x) = x^n - m_1 x^{n-2} + m_2 x^{n-4} - m_3 x^{n-6}$$

where

$$m_1 = p_1 + p_2 + p_3 + 2q_1 + 2q_2 + 2q_3 + 3r \tag{9}$$

$$\begin{aligned} m_2 = {} & p_1p_2 + p_1p_3 + p_1q_1 + 2p_1q_2 + p_1q_3 + 2p_1r + p_2p_3 + p_2q_1 + \\ & p_2q_2 + 2p_2q_3 + 2p_2r + 2p_3q_1 + p_3q_2 + p_3q_3 + 2p_3r + q_1^2 - q_1 + \\ & 3q_1q_2 + 3q_1q_3 + 4q_1r + q_2^2 - q_2 + 3q_2q_3 + 4q_2r + q_3^2 - q_3 + \\ & 4q_3r + 3r^2 - 3r \end{aligned} \tag{10}$$

$$\begin{aligned} m_3 = {} & p_1p_2p_3 + p_1p_2q_2 + p_1p_2q_3 + p_1p_2r + p_1p_3q_1 + p_1p_3q_2 + \\ & p_1p_3r + p_1q_1q_2 + p_1q_1q_3 + p_1q_1r + p_1q_2(q_2 - 1) + p_1q_2q_3 + \\ & 2p_1q_2r + p_1q_3r + p_1r(r - 1) + p_2p_3q_1 + p_2p_3q_3 + p_2p_3r + \\ & p_2q_1q_2 + p_2q_1q_3 + p_2q_1r + p_2q_2q_3 + p_2q_2r + p_2q_3(q_3 - 1) + \\ & 2p_2q_3r + p_2r(r - 1) + p_3q_1(q_1 - 1) + p_3q_1q_2 + p_3q_1q_3 + \\ & 2p_3q_1r + p_3q_2q_3 + p_3q_2r + p_3q_3r + p_3r(r - 1) + q_1(q_1 - 1)q_2 \\ & + q_1(q_1 - 1)q_3 + q_1(q_1 - 1)r + q_1q_2(q_2 - 1) + 2q_1q_2q_3 + \\ & 3q_1q_2r + q_1q_3(q_3 - 1) + 3q_1q_3r + 2q_1r(r - 1) + q_2(q_2 - 1)q_3 \\ & + q_2(q_2 - 1)r + q_2q_3(q_3 - 1) + 3q_2q_3r + 2q_2r(r - 1) + \\ & q_3(q_3 - 1)r + 2q_3r(r - 1) + r(r - 1)(r - 2) \end{aligned} \tag{11}$$

and $m_k = 0$ for $k \geq 4$. The matching polynomial of the subgraph $G-C^*$ is equal to x^{n-6} because $G-C^*$ is a graph with n-6 vertices and with no edges. Consequently, the corresponding β-polynomial is of the form

$$\beta(x) = x^{n-6} \, (x^6 - m_1 x^4 + m_2 x^2 - m_3 - 2) \quad .$$

Whence the question of the reality of the zeros of $\beta(x)$ is reduced to the finding the roots of the polynomial

$$\beta_0(x) = \alpha_0(x) - 2$$

where

$$\alpha_0(x) = x^3 - m_1 x^2 + m_2 x - m_3 \quad .$$

Note that by the Descartes sign-rule if the zeros of $\beta_0(x)$ are real, then they are necessarily positive.

An Auxiliary Result

Proposition 1. For any real numbers x and s and for any value of the parameters p_i, q_i, r $(i = 1,2,3)$, the following relations are obeyed

(i) $\quad \alpha_0(p_i+s, q_i, r)(x+s) = \alpha_0(p_i, q_i, r)(x)$

(ii) $\quad \beta_0(p_i+s, q_i, r)(x+s) = \beta_0(p_i, q_i, r)(x)$.

Proof. From the definition of the polynomial $\alpha_0(x)$ we have

$$\alpha_0(p_1+s,q_1,r)(x) = x^3 - m_1^s x^2 + m_2^s x - m_3^s \tag{12}$$

where $m_k^s = m_k(p_1+s,q_1,r)$. Bearing in mind the relations (9)-(11) it is easy to see that

$$m_1^s = 3\,s + m_1 \tag{13}$$

$$m_2^s = 3\,s^2 + 2\,m_1\,s + m_2 \tag{14}$$

$$m_3^s = s^3 + m_1\,s^2 + m_2\,s + m_3 \quad . \tag{15}$$

By substituting m_k^s $(k = 1,2,3)$ back into (12) we immediately arrive at the statement (i). Relation (ii) is proved in a fully analogous manner. □

Denote by x_1, x_2, x_3 and y_1, y_2, y_3 the zeros of the polynomials $\alpha_0(p_1,q_1,r)(x)$ and $\beta_0(p_1,q_1,r)(x)$, respectively. Then by using the relations (i) and (ii) in Proposition 1, we immediately have that $x_j + s$ and $y_j + s$, $j = 1,2,3$, are the zeros of the polynomials $\alpha_0(p_1+s,q_1,r)(x)$ and $\beta_0(p_1+s,q_1,r)(x)$, respectively.

We are now prepared to prove the main result of this paper. It is based on Proposition 1 and the fact that the polynomial $\alpha(G,x)$ has real roots for any graph G [13,15].

The Main Result

Theorem 1. For any choice of the parameters p_1, q_1, r the zeros of the polynomial $\beta_0(x) = \alpha_0(x) - 2$ are real and nonnegative.

Proof. Let G be an arbitrary graph from the class $G(p_1, q_1, r)$, and let s be any real-valued constant. Then the polynomial $\alpha_0(p_1+s, q_1, r)(x)$ satisfies the relation (12). By taking into account eq. (13) we choose s_0 such that $m_1^{s_0} = 0$. Relations (14) and (15) now reduce to

$$m_2^{s_0} = -(m_1)^2/3 + m_2 \tag{16}$$

$$m_3^{s_0} = 2\,(m_1)^3/27 - m_1 m_2/3 + m_3 \quad . \tag{17}$$

By means of the condition $m_1^{s_0} = 0$ the polynomials $\alpha_0(x)$ and $\beta_0(x)$ are transformed into their respective canonical forms $\alpha^0(x)$ and $\beta^0(x)$ where $\alpha^0(x) = \alpha^0(p_1, q_1 r)(x)$, $\beta^0(x) = \beta^0(p_1, q_1, r)(x)$. Consequently, the problem of the reality of the zeros of $\alpha_0(x)$, $\beta_0(x)$ is reduced to the determining the zeros of the corresponding canonical polynomials. From (12) it immediately follows that these canonical polynomials are represented as

$$\alpha^0(p_1, q_1, r)(x) = x^3 + m_2^{s_0}\, x - m_3^{s_0}$$

$$\beta^0(p_i,q_i,r)(x) = \alpha^0(p_i,q_i,r)(x) - 2 \quad .$$

Now, if we define $A(p_i,q_i,r) = m_2^{s_0}$ and $B(p_i,q_i,r) = m_3^{s_0}$ then by (16), (17), (9), (10) and (11) the following two relations are deduced:

$$\begin{aligned} -3\,A(p_i,q_i,r) = {} & p_1^2 + p_2^2 + p_3^2 - p_1p_2 - p_1p_3 - p_2p_3 + p_1q_1 - 2p_1q_2 + \\ & p_1q_3 + p_2q_1 + p_2q_2 - 2p_2q_3 - 2p_3q_1 + p_3q_2 + p_3q_3 + \\ & q_1^2 + q_2^2 + q_3^2 - q_1q_2 - q_1q_3 - q_2q_3 + 3q_1 + 3q_2 + 3q_3 \\ & + 9r \end{aligned}$$

$$\begin{aligned} 27\,B(p_i,q_i,r) = {} & 2p_1^3 - 3p_1^2p_2 - 3p_1^2p_3 + 3p_1^2q_1 - 6p_1^2q_2 + 3p_1^2q_3 - 3p_1p_2^2 \\ & + 12p_1p_2p_3 - 12p_1p_2q_1 + 6p_1p_2q_2 + 6p_1p_2q_3 - 3p_1p_3^2 + \\ & 6p_1p_3q_1 + 6p_1p_3q_2 - 12p_1p_3q_3 - 3p_1q_1^2 - 6p_1q_1q_2 + \\ & 12p_1q_1q_3 + 9p_1q_1 + 6p_1q_2^2 - 6p_1q_2q_3 - 18p_1q_2 - \\ & 3p_1q_3^2 + 9p_1q_3 + 2p_2^3 - 3p_2^2p_3 + 3p_2^2q_1 + 3p_2^2q_2 - 6p_2^2q_3 \\ & - 3p_2p_3^2 + 6p_2p_3q_1 - 12p_2p_3q_2 + 6p_2p_3q_3 - 3p_2q_1^2 + \\ & 12p_2q_1q_2 - 6p_2q_1q_3 + 9p_2q_1 - 3p_2q_2^2 - 6p_2q_2q_3 + \\ & 9p_2q_2 + 6p_2q_3^2 - 18p_2q_3 + 2p_3^3 - 6p_3^2q_1 + 3p_3^2q_2 + \\ & 3p_3^2q_3 + 6p_3q_1^2 - 6p_3q_1q_2 - 6p_3q_1q_3 - 18p_3q_1 - 3p_3q_2^2 \\ & + 12p_3q_2q_3 + 9p_3q_2 - 3p_3q_3^2 + 9p_3q_3 - 2q_1^3 + 3q_1^2q_2 + \\ & 3q_1^2q_3 + 18q_1^2 + 3q_1q_2^2 - 12q_1q_2q_3 - 18q_1q_2 + 3q_1q_3^2 - \\ & 18q_1q_3 - 2q_2^3 + 3q_2^2q_3 + 18q_2^2 + 3q_2q_3^2 - 18q_2q_3 - 2q_3^3 \\ & + 18q_3^2 + 54r. \end{aligned}$$

The latter two relations imply

$$A(p_i+s, q_i+t, r+u) = A(p_i, q_i, r) - 3(t + u) \tag{18}$$

$$B(p_i+s, q_i+t, r+u) = B(p_i, q_i, r) + 2u \quad . \tag{19}$$

Consider now the polynomial $\alpha_0(p_i, q_i-1, r+1)(x)$. Its corresponding canonical polynomial is

$$\alpha^0(p_i, q_i-1, r+1)(x) = x^3 + \bar{m}_2^{s\,0}\, x - \bar{m}_3^{s\,0}$$

where $\bar{m}_2^{s\,0} = A(p_i, q_i-1, r+1)$ and $\bar{m}_3^{s\,0} = B(p_i, q_i-1, r+1)$. From (18) and (19) we now immediately get $\bar{m}_2^{s\,0} = m_2^{s\,0}$ and $\bar{m}_3^{s\,0} = m_3^{s\,0} + 2$. From these conditions it follows

$$\alpha^0(p_i, q_i-1, r+1)(x) = \beta^0(p_i, q_i, r)(x) \quad . \tag{20}$$

Since the zeros of the polynomial $\alpha^0(p_i, q_i, r)(x)$ are necessarily real for all values of the parameters $p_i \geq 0$, $q_i \geq 0$, $r \geq 0$, the relation (20) implies that also the zeros of the polynomial $\beta^0(p_i, q_i, r)(x)$ must be real for all $p_i \geq 0$, $q_i \geq 1$, $r \geq 0$, $i = 1,2,3$. Proposition 1 (ii) leads now to the conclusion that the zeros of the polynomial $\beta_0(p_i, q_i, r)(x)$ are real for any choice of parameters p_i, q_i, r.

This completes the proof of Theorem 1. $\square$

Let, as before, $\phi(G)$ stand for the characteristic polynomial of a graph G. If $\phi(G_1) = \phi(G_2)$ for two nonisomorphic graphs G_1 and G_2, then we say that G_1 and G_2 are cospectral [14]. Let further O_s denote the graph with s vertices and without edges.

Proposition 2. Let $q = \min\{q_1, q_2, q_3\}$. Then for any choice of the parameters p_i, q_i, r $(i = 1,2,3)$ and any $s \in \{1,2,\dots,q\}$, the graph $G(p_i, q_i, r) \cup O_s$ is cospectral with the graph $G(p_1+s, q_1-s, r+s)$.

Proof. It is easy to see that the characteristic polynomial of the graph $G(p_i, q_i, r)$ has the form

$$\phi(G(p_i, q_i, r), x) = x^{n-6}\,(x^6 - a_1\, x^4 + a_2\, x^2 - a_3) \quad .$$

A straightforward, yet somewhat tedious calculation yields:

$$a_1 = p_1 + p_2 + p_3 + 2q_1 + 2q_2 + 2q_3 + 3r$$

$$\begin{aligned} a_2 = {} & p_1p_2 + p_1p_3 + p_1q_1 + 2p_1q_2 + p_1q_3 + 2p_1r + p_2p_3 + p_2q_1 + p_2q_2 + \\ & 2p_2q_3 + 2p_2r + 2p_3q_1 + p_3q_2 + p_3q_3 + 2p_3r + 3q_1q_2 + 3q_1q_3 + \\ & 2q_1r + 3q_2q_3 + 2q_2r + 2q_3r \end{aligned}$$

$$\begin{aligned} a_3 = {} & p_1p_2p_3 + p_1p_2q_2 + p_1p_2q_3 + p_1p_2r + p_1p_3q_1 + p_1p_3q_2 + p_1p_3r + \\ & p_1q_1q_2 + p_1q_1q_3 + p_1q_1r + p_1q_2q_3 + p_1q_3r + p_2p_3q_1 + p_2p_3q_3 + \\ & p_2p_3r + p_2q_1q_2 + p_2q_1q_3 + p_2q_1r + p_2q_2q_3 + p_2q_2r + p_3q_1q_2 + \\ & p_3q_1q_3 + p_3q_2q_3 + p_3q_2r + p_3q_3r + 4q_1q_2q_3 + q_1q_2r + q_1q_3r + \\ & q_2q_3r\ . \end{aligned}$$

If we consider a_k as a function $a_k(p_1,q_1,r)$ of the parameters p_1,q_1,r, then it is simple to check that for k=1,2,3,

$$a_k(p_1+s,q_1-s,r+s) = a_k(p_1,q_1,r) \quad .$$

Proposition 2 follows now from the well known facts [14] that $\phi(O_s) = x^s$ and $\phi(G_a \cup G_b) = \phi(G_a)\ \phi(G_b)$. □

References

[1] J.Aihara, J.Amer.Chem.Soc. **99**, 2048 (1977).

[2] S.Bosanac and I.Gutman, Z.Naturforsch. **32a**, 10 (1977).

[3] I.Gutman and S.Bosanac, Tetrahedron **33**, 1809 (1977).

[4] H.Sachs, Publ.Math.Debrecen **11**, 119 (1964).

[5] A.Graovac, I.Gutman and N.Trinajstić, Theor.Chim.Acta **26**, 67 (1972).

[6] J.Aihara, J.Amer.Chem.Soc. **98**, 6840 (1976).

[7] I.Gutman and O.E.Polansky, Theor.Chim.Acta **60**, 203 (1981).

[8] I.Gutman, Theor.Chim.Acta **66**, 43 (1984).

[9] J.Aihara, J.Amer.Chem.Soc. **98**, 2750 (1976).

[10] I.Gutman, M.Milun and N.Trinajstić, J.Amer.Chem.Soc. **99**, 1692 (1977).

[11] A.Graovac, I.Gutman and N.Trinajstić, Topological Approach to the Chemistry of Conjugated Molecules, Springer-Verlag, Berlin 1977.

[12] I.Gutman, Match **6**, 75 (1979).

[13] C.D.Godsil and I.Gutman, J.Graph Theory **5**, 137 (1981).

[14] I.Gutman and O.E.Polansky, Mathematical Concepts in Organic Chemistry, Springer-Verlag, Berlin 1986.

[15] C.D.Godsil and I.Gutman, Z.Naturforsch. **34a**, 776 (1979).

[16] W.C.Herndon, J.Amer.Chem.Soc. **104**, 3541 (1982).

[17] I.Gutman and W.C.Herndon, Chem.Phys.Letters **105**, 281 (1984).

[18] N.Mizoguchi, Bull.Chem.Soc.Japan **63**, 765 (1990).

[19] I.Gutman and N.Mizoguchi, J.Math.Chem. **5**, 81 (1990).

[20] M.Lepović, I.Gutman, M.Petrović and N.Mizoguchi, J.Serb.Chem.Soc. **55**, 193 (1990).