MATCH
Communications in Mathematical and in Computer Chemistry

MATCH Commun. Math. Comput. Chem. **59** (2008) 257-268

ISSN 0340 - 6253

NOTE ON THE COULSON AND COULSON–JACOBS INTEGRAL FORMULAS

Miodrag Mateljević[a] and Ivan Gutman[b]

[a] *Faculty of Mathematics, University of Belgrade, Studentski Trg 16, 11000 Belgrade, Serbia*

[b] *Faculty of Science, University of Kragujevac, P. O. Box 60, 34000 Kragujevac, Serbia*

(Received May 18, 2007)

Abstract

Appropriate corrections and generalizations of the Coulson–Jacobs formula are reported. We also extend the Coulson integral formula to the case when not all the zeros of the underlying polynomial are real and simple.

INTRODUCTION: THE COULSON AND COULSON–JACOBS FORMULAS

In quantum chemistry the energies of the electrons in organic molecules are usually computed by solving a pertinent approximate Schrödinger equation [1, 2]. The sum of the electron energies, referred to as the total electron energy, is an important characteristic of the underlying molecule, from which chemists are able to draw far-reaching conclusions on its chemical and physical properties. Within the so-called Hückel molecular orbital approximation, the total electron energy is found to be equal to two times the sum of the positive zeros of a particular polynomial, the so-called characteristic polynomial. In the early days of molecular orbital theory, Coulson [3] discovered a formula that makes it possible to compute the total energy E (i. e., the sum of the positive zeros of the characteristic polynomial, times two) without actually knowing these zeros. The expression, that in what follows we refer to as the *Coulson formula*, reads [3]:

$$E = \frac{1}{\pi} \int_{-\infty}^{+\infty} \left[n - ix \, \frac{P'(ix)}{P(x)} \right] dx \tag{1}$$

where $P(x)$ is the characteristic polynomial, $P'(x)$ is its first derivative, n the degree of $P(x)$, and $i = \sqrt{-1}$. More details on the Coulson formula and its numerous applications can be found in [4–10], and in the references cited therein. For some of its most recent applications see [11–14].

All the zeros of the characteristic polynomial are real–valued numbers, and their sum is equal to zero. Therefore, the quantity E on the left–hand side of Eq. (1) is equal to the sum of the absolute values of all zeros of $P(x)$. This observation led to the introduction of the concept of the energy of graphs [15].

In another early paper, Coulson and Jacobs [16] reported an elegant expression for the difference of the E-values, pertaining to characteristic polynomials $P_1(x)$ and $P_2(x)$ whose degrees are equal. This expression, that in what follows we refer to as the *Coulson–Jacobs formula*, reads:

$$E_1 - E_2 = \frac{1}{\pi} \int_{-\infty}^{+\infty} \ln \left[\frac{P_1(ix)}{P_2(ix)} \right] dx \; . \tag{2}$$

Formula (2) found remarkably many applications in theoretical chemistry; for details see the review [17], the papers [18–24], and the references cited therein.

In the recent work [10], published more than half a century after Coulson's [3], we showed that the integral formula (1) holds if and only if the sum of zeros of the underlying polynomial is equal to zero. We also showed how this formula has to be modified, so that it be applicable in the case when this sum is not zero. In the present paper we extend this result to the case when not all zeros of the polynomial are real and simple.

In many of the reported applications of (2), the zeros of the polynomials P_1 and/or P_2 may be complex–valued, and their sums need not be equal to zero. Therefore it seems to be of interest to precisely determine the conditions under which (2) is valid, and to establish the corrections that need to be done when it fails to be valid. The main purpose of the present paper is to show how the Coulson–Jacobs theorem [16] has to be modified, so that it can be applicable in the general case.

More precisely, we define the branch of LnR, where R is the corresponding rational function, and introduce a new term in the original Coulson–Jacobs formula.

In order to achieve our goals we need some preparations.

2. PRELIMINARIES

Let P be a polynomial of degree n, and let $a_1, a_2, \ldots, a_h$ be its mutually distinct zeros. Define:

$$\Phi(z) = \Phi_P(z) = z\,\frac{P'}{P} - n \quad ; \quad \Pi^+ = \{z : Re\, z > 0\} \quad ; \quad \Pi^- = \{z : Re\, z < 0\}\ .$$

If all zeros of P are simple (i. e., $h = n$), then

$$\Phi(z) = \sum \frac{a_\nu}{z - a_\nu} = \sum a_\nu\, K_{a_\nu}(z)$$

where

$$K_a(z) = \frac{1}{z - a}\ . \tag{3}$$

Let s, s^+, and s^- denote the sum of zeros of P in $\mathbf{C}$, Π^+, and Π^-, respectively, counting multiplicities. If n_ν is the multiplicity of a_ν, then $s = \sum n_\nu\, a_\nu$ and

$$\Phi(z) = \sum n_\nu\, \frac{a_\nu}{z - a_\nu} = \sum n_\nu\, a_\nu K_{a_\nu}(z)\ .$$

By $v.p.$ we denote the principal value of the Cauchy integral (cf. [25–27] and the Appendix).

Let $a \in \Pi^+$, and let arg be the branch of the argument of a, whose values belong to $(0,\, 2\pi)$. Let further $\varphi(z) = \varphi_a(z) = \ln(z - a)$ be the corresponding branch of the logarithm defined by $\ln(z - a) = \ln|z - a| + i\arg(z - a)$. Then φ_a is a primitive function of K_a in the half plane Π^- (see e. g. [25–27]).

Since, $\varphi(+\infty\, i) - \varphi(-\infty\, i) = i\pi/2 - i3\pi/2 = -i\pi$, we arrive at:

Claim 1. If $a = a_\nu \in \Pi^+$, then

$$v.p. \int_{-\infty}^{+\infty} K_a(iy)\, dy = -\pi \ .$$

In a similar way, using the branch arg of the argument by values in $(-\pi,\, +\pi)$ and the corresponding branch of the logarithm, we get:

Claim 2. If $a = a_\nu \in \Pi^-$, then

$$v.p. \int_{-\infty}^{+\infty} K_a(iy)\, dy = \pi \ .$$

Noting that $v.p. \int\limits_{-\infty}^{+\infty} (1/y)\, dy = 0$, in a similar way we deduce:

Claim 3. If $a = a_\nu$ is purely imaginary, then

$$v.p. \int_{-\infty}^{+\infty} K_a(iy)\, dy = 0 \ .$$

Define $K(a) = v.p. \int\limits_{-\infty}^{+\infty} K_a(iy)\, i\, dy$, where $K_a(z)$ is as in Eq. (3). Then

$$K(a) = \begin{cases} -i\pi & \text{if } a \in \Pi^+ \\ 0 & \text{if } a \text{ is purely imaginary} \\ i\pi & \text{if } a \in \Pi^- \end{cases} \ .$$

In what follows we are concerned with the Coulson–type integrals (cf. Eq. (1)):

$$J = J(P) = v.p. \int_{-\infty}^{+\infty} \Phi(iy)\, dy, \quad ; \quad I = i\, J \quad ; \quad I_0 = \frac{I}{2\pi\, i} = \frac{J}{2\pi} \ .$$

Let $Z_0 = \{b_k\}$ be the set of all zeros of the polynomial P , such that $\mathrm{Re}\, \mathrm{b_k} = 0$ and let $s_0 = \sum n_k\, b_k$, where n_k is the multiplicity of b_k .

Since $\Phi = \sum n_\nu\, a_\nu\, K_\nu$, from Claims 1–3 it follows that

$$I = -i\, \pi\, s^+ + i\, \pi\, s^-$$

and

$$J = \pi\, s^- - \pi\, s^+ = (s^- - s^+)\pi \tag{4}$$

i. e., $J = (s - s_0 - 2s^+)\pi$ and thus $I_0 = (s - s_0)/2\, - s^+$.

3. ON THE COULSON–JACOBS FORMULA

Let P_1 and P_2 be two polynomials and let s_k be the sum of zeros of P_k in $\mathbf{C}$, $k = 1, 2$. By (4),

$$J^* = J(P_1) - J(P_2) = J_1 - J_2 = \pi(s_1^- - s_1^+ + s_2^+ - s_2^-) .$$

Thus we proved:

Theorem 1. *In the above specified notation,* $J = (s^- - s^+)\,\pi$ *and* $J_1 - J_2 = \pi\,(s_1^- - s_1^+ + s_2^+ - s_2^-)$.

The Coulson–Jacobs formula (2) is a corollary of the Coulson integral formula (1). It is convenient to state it in the form:

Theorem 2. *Let* P_1 *and* P_2 *be two polynomials of the same degree,* $R = P_1/P_2$ *,* $R(\infty) = 1$ *, and* $J^* = J(P_1) - J(P_2)$ *. Suppose in addition that* P_1 *and* P_2 *do not have purely imaginary zeros. Then*

$$J^* = -v.p. \int_{-\infty}^{+\infty} [\ln R(iy)]\, dy .$$

First, we observe that we need to define the branch of LnR, where R is the corresponding rational function, for which the original Coulson–Jacobs formula is valid. It turns out that we can do this only under very restrictive conditions. In order to overcome these difficulties we introduce a new term, concerning the variation of the argument of R along the y-axis, in the original Coulson–Jacobs formula, and we prove a new version.

Let P_1 and P_2 be two polynomials, $R = P_1/P_2$ and

$$\Psi(z) = z\,\frac{P_1'}{P_1} - z\,\frac{P_2'}{P_2} .$$

Suppose that $degP_1 = degP_2 = n$, $n \geq 1$, and that P_1 and P_2 do not have purely imaginary zeros. Then $\lim R(z) = c \neq 0$ when z tends to ∞ . It is convenient to suppose that $c = 1$, that is $R(\infty) = 1$.

Then there is an $\varepsilon > 0$ such that $P_1\,P_2$ has no zeros in $V = V_\varepsilon = \{z : |\mathrm{Re}\, \mathrm{z}| < \varepsilon\}$. Hence, since V is simply connected, there is a branch $\mathcal{S} = lnR$ of LnR in V , such that

$$\Psi(z) = z\,[(\ln P_1)' - (\ln P_2)'] = z\,(\ln P_1/P_2)' = z\,(\ln R)'\ .$$

Let for $k = 1, 2$, n_k and n_k^+ be the number of zeros of P_k in $\mathbf{C}$ and in Π^+, respectively, counting multiplicities, and let $m = n_1^+ - n_2^+$.

Let s_k be the sum of zeros of P_k in $\mathbf{C}$, $k = 1, 2$, and let $a = s_2 - s_1$. Then $P_1/P_2 = 1 + a/z + 0(1/z)$ and $R(iy) = 1 - i\,a/y + 0(1/y)$, when y tends to ∞. We can choose the branch such that $\mathcal{S}(iy) = lnR(iy) = -ia/y + 0(1/y)$, when y tends to $+\infty$.

For $y \in \mathbf{R}$, let $\varphi(iy) = \operatorname{Im}\ln R(iy)$, $f(y) = y\,[\ln R(iy) - i\,\pi\,m]$, and $\Upsilon(y) = f(y) - f(-y)$. It is clear that $\Upsilon(y) = -\Upsilon(-y)$ and

$$\begin{aligned} \Upsilon(y) &= y\,[\ln R(iy) - i\,\pi\,m] + y\,[\ln R(-iy) - i\,\pi\,m] \\ &= y\,[\ln R(iy) + \ln R(-iy) - i\,2\pi\,m]\ . \end{aligned}$$

It is also convenient to use the notation $\arg R(iy)$ instead of $\varphi(iy)$.

The proof of Theorem 2 is based on the following:

Lemma 3. *There exists a constant $c \in \mathbf{C}$, such that for $y \to \infty$,*

$$\ln R(iy) + \ln R(-iy) = 2\,\frac{c}{y^2} + 0\left(\frac{1}{y^{2+\epsilon}}\right) + i\,2\pi\,m\ . \tag{5}$$

As immediate corollaries of Lemma 3 we have:

1. $\Upsilon(y) \to 0$ when $y \to \infty$.
2. The integral *v.p.* $\int\limits_{-\infty}^{+\infty} [\ln R(iy) - i\,\pi\,m]\,dy$ is finite.

Proof of Lemma 3. We first demonstrate that

$$\varphi(iy) - \varphi(-iy) \to -2\pi\,m \quad \text{for } y \to +\infty\,. \tag{6}$$

Let the curve $C_r = C_r^+$ be defined by $C_r(\theta) = C_r^+(\theta) = r\,e^{i\,\theta}$ $(-\pi/2 \le \theta \le \pi/2)$. For $r > 0$, let Λ and Λ_r, be defined by $\Lambda(t) = i\,t$, $-\infty < t < +\infty$, and $\Lambda_r(t) = i\,t$, $-r < t < +r$, respectively. Let Γ_r be the curve consisting of C_r^+ and $-\Lambda_r$.

Since $R(z) \to 1$ when z tends to ∞, by the basic formula for $Var\arg$, we have

$$\lim_{r \to +\infty} Var \arg_{C_r^+} R = 0\ .$$

Choose r_0 such that all zeros of $P_1\,P_2$ are in the disk $\{z : |z| < r_0\}$. For $r > r_0$, by the Argument Principle (see e. g. [25–27]), we conclude

$$Var\,\arg_{\Gamma_r} R = 2\pi(n_1^+ - n_2^+) = 2\pi\, m$$

and therefore

$$Var\,\arg_{\Lambda_r} R \to -2\pi\, m \qquad r \to +\infty\ .$$

Hence

$$Var\,\arg_{\Lambda} R = -2\pi(n_1^+ - n_2^+) = -2\pi\, m\ .$$

Since $\varphi(iy) - \varphi(-iy) = \arg R(iy) - \arg R(-iy) = Var\,\arg_{\Lambda_y} R$, we find that

$$\varphi(iy) - \varphi(-iy) \to -2\pi\, m \qquad \text{for } y \to +\infty\ .$$

By this we prove (6).

In order to complete the proof of Lemma 3, note that there exists an $\epsilon > 0$ and $b \in \mathbf{C}$, such that

$$R(iy) = 1 - i\,\frac{a}{y} + \frac{b}{y^2} + 0\left(\frac{1}{y^{2+\epsilon}}\right)$$

for $y \to \infty$.

Let $\ln_0$ be a branch of Log in a neighborhood of the point 1, defined by $\ln_0(1) = 0$. When $y \to +\infty$, we have

$$\ln R(iy) = \ln_0[R(iy)] = -i\,\frac{a}{y} + \frac{c}{y^2} + 0\left(\frac{1}{y^{2+\epsilon}}\right) \qquad ; \qquad c \in \mathbf{C}\ .$$

There exists a $y_0 > 0$, such that $\ln R(-iy)$ and $\ln_0[R(-iy)]$ are two branches of $LnR(-iy)$ in $L_{y_0} = \{y : y > y_0\}$. Hence there is a $k \in \mathbf{Z}$ (actually, we are going to show that $m = k$) such that

$$\ln R(-iy) = \ln_0[R(-iy)] + i\,2\pi\, k = i\,\frac{a}{y} + \frac{c}{y^2} + 0\left(\frac{1}{y^{2+\epsilon}}\right) + i\,2\pi\, k\ .$$

Hence

$$\ln R(iy) + \ln R(-iy) = 2\,\frac{c}{y^2} + 0\left(\frac{1}{y^{2+\epsilon}}\right) + i\,2\pi\, k \tag{7}$$

$$\varphi(iy) = -\frac{\alpha}{y} + \frac{\beta}{y^2} + 0\left(\frac{1}{y^{2+\epsilon}}\right) \qquad ; \qquad \alpha, \beta \in \mathbf{R}$$

and

$$\varphi(-iy) = \frac{\alpha}{y} + \frac{\beta}{y^2} + 0\left(\frac{1}{y^{2+\epsilon}}\right) + 2\pi\, k$$

and therefore,

$$\varphi(iy) - \varphi(-iy) = -2\,\frac{\alpha}{y} + 0\left(\frac{1}{y^{2+\epsilon}}\right) - 2\pi\, k\ . \tag{8}$$

If $y \to +\infty$, then, by (6), $\varphi(iy) - \varphi(-iy) \to -2\pi\, m$ and, then by (8),

$$\varphi(iy) - \varphi(-iy) = +\varepsilon(y) - 2\pi\, k$$

for $\varepsilon(y) \to 0$. It follows that $m = k$, and by (7) we obtain (5), i. e., we proved Lemma 3.

Theorem 4. *Let P_1 and P_2 be two polynomials of the same degree. Let for $k = 1, 2$, n_k^+ be the number of zeros of P_k in Π^+, counting multiplicities, and $m = n_1^+ - n_2^+$. Let $R = P_1/P_2$, $R(\infty) = 1$, and $J^* = J(P_1) - J(P_2)$. Suppose, in addition, that P_1 and P_2 do not have purely imaginary zeros. Then*

$$J^* = -v.p. \int_{-\infty}^{+\infty} [\ln R(iy) - i\,\pi\, m]\, dy$$

and

$$J^* = \pi\,(s_1^- - s_1^+ + s_2^+ - s_2^-) = -v.p. \int_{-\infty}^{+\infty} [\ln R(iy) - i\,\pi\, m]\, dy\ . \tag{9}$$

Proof. Recall that

$$f(y) = y\,[\ln R(iy) - i\,\pi\, m]$$

and

$$\Upsilon(y) = f(y) - f(-y) = y\,[\ln R(iy) + \ln R(-iy) - i\, 2\pi\, m]\ .$$

Since $k = m$, by (5),

$$\Upsilon(y) = y\,\left[2\,\frac{c}{y^2} + 0\left(\frac{1}{y^{2+\epsilon}}\right)\right]\ .$$

Thus $\Upsilon(y) \to 0$ when $y \to \infty$ and $y\,[\ln R(iy) - i\,\pi\, m]\,\Big|_{-\infty}^{+\infty} = 0$.

By partial integration and Lemma 3,

$$J^* = v.p. \int_{-\infty}^{+\infty} \Psi(iy)\, dy = y\,[\ln R(iy) - i\,\pi\, m]\,\Big|_{-\infty}^{+\infty} - v.p. \int_{-\infty}^{+\infty} [\ln R(iy) - i\,\pi\, m]\, dy$$

from which Theorem 4 immediately follows.

Note that it is convenient to use the formula (9) for computations of certain integrals.

4. APPENDIX

In this section we re-state some facts from the theory of functions with complex variables [25–27], that were explicitly or implicitly utilized in our considerations.

The Cauchy theorem. Recall that K_a is defined via Eq. (3).

Let γ be a closed simple piecewise continuously differentiable curve and $G = Int(\gamma)$. If f is a holomorphic function on $\overline{G}$, then

$$f(z) = \frac{1}{2\,\pi\,i} \int_\gamma \frac{f(\zeta)}{\zeta - z}\, d\zeta \qquad z \in G\ .$$

In particular,

$$C(a) = \int_\gamma K_a\, dz = \begin{cases} 2\pi i & \text{if } a \in Int(\gamma) \\ 0 & \text{if } a \in Ext(\gamma) \end{cases} \quad .$$

The Jordan lemma. *a*) Let the curve $C_r = C_r^+$ be defined by $C_r(\theta) = C_r^+(\theta) = r\, e^{i\,\theta}$ $(-\pi/2 \leq \theta \leq \pi/2)$. If f is a continuous function on Π^+ and $z f(z) \to A$ when $\Pi^+ \ni z \to \infty$, then

$$\lim_{r \to +\infty} \int_{C_r} f(z)\, dz = i\,\pi\, A\ .$$

b) In particular, if f is holomorphic in a neighborhood of ∞ and has a zero of order at least 2 at ∞, then

$$\lim_{r \to +\infty} \int_{C_r} f(z)\, dz = 0\ .$$

We may use *b*) to prove the Coulson formula if $s = 0$.

Branches of Ln. For $z \neq 0$, we define $Arg\, z = \{\varphi \in \mathbf{R} : z = |z|\, e^{i\varphi}\}$ and $Ln\, z = \ln|z| + i\, Arg\, z$.

Let P_1 and P_2 be two polynomials of the same degree, $R = P_1/P_2$. Suppose, in addition, that P_1 and P_2 do not have purely imaginary zeros. For $s \in \mathbf{R}$, let $l_s = [0, is]$ be an oriented segment.

Put $R(0) = |R(0)|\, e^{i\,\varphi_0}$ (note that $R(0) \neq 0$). Let further, $\theta(iy) = Var \arg_{l_y} R$ and $\varphi(iy) = \arg R(iy) = \theta(iy) + \varphi_0$. Then $R(iy) = |R(iy)|\, e^{\varphi(iy)}$ and therefore $\ln R(iy) = \ln|R(iy)| + i\, \arg R(iy)$ is a branch of $Ln R$.

Example 1. Let $R(z) = (z-1)/(z+1)$. Then $m = 1$, $a = 2$, $R(0) = -1$, and we can choose $\varphi_0 = \pi$. For $y \to +\infty$, we have $\varphi(iy) \to 0$, $\varphi(-iy) \to 2\pi$, $\ln R(iy) = -i\,2/y + c/y^2 + 0(1/y^{2+\epsilon})$, and $\ln R(-iy) = \ln R(iy) + i\,2\pi$. Hence, since $s_1^- - s_1^+ = 0 - 1 = -1$ and $s_2^+ - s_2^- = 0 - (-1) = 1$, it follows that

$$J^* = -v.p. \int_{-\infty}^{+\infty} [\ln R(iy) - i\,\pi]\, dy = 0\ .$$

It can be shown that for $y \to \infty$,

$$\ln|R(iy)| = 1 \qquad \text{and} \qquad \varphi(iy) + \varphi(-iy) = 2\pi\ . \tag{10}$$

From (10) it also follows that $J^* = 0$.

Example 2. If $\overline{R(z)} = R(\bar{z})$ and $R(0) > 0$, then we can choose $\varphi_0 = 0$ and therefore $\varphi(-iy) = -\varphi(iy)$, i. e., $\varphi(iy) + \varphi(-iy) = 0$. In this case, $\varphi(iy) \to -m\pi$, $\varphi(-iy) \to m\pi$ when $y \to +\infty$. Since, $m\pi \in Arg\,1$, then m is even. For instance, this is the case if all zeros of P_1 and P_2 are real, and $R(0) > 0$, e. g., if $R(z) = [(z-1)(z-2)]/[(z+1)(z+2)]$.

References

[1] M. J. S. Dewar, *The Molecular Orbital Theory of Organic Chemistry*, McGraw–Hill, New York, 1969.

[2] C. A. Coulson, B. O'Leary, R. B. Mallion, *Hückel Theory for Organic Chemists*, Academic Press, London, 1978.

[3] C. A. Coulson, On the calculation of the energy in unsaturated hydrocarbon molecules, *Proc. Cambridge Phil. Soc.* **36** (1940) 201–203.

[4] H. Hosoya, K. Hosoi, I. Gutman, A topological index for the total π-electron energy. Proof of a generalised Hückel rule for an arbitrary network, *Theor. Chim. Acta* **38** (1975) 37–47.

[5] I. Gutman, N. Trinajstić, Graph theory and molecular orbitals. XV. The Hückel rule, *J. Chem. Phys.* **64** (1976) 4921–4925.

[6] I. Gutman, A class of approximate topological formulas for total π-electron energy, *J. Chem. Phys.* **66** (1977) 1652–1655.

[7] I. Gutman, Acyclic systems with extremal Hückel π-electron energy, *Theor. Chim. Acta* **45** (1977) 79–87.

[8] I. Gutman, O. E. Polansky, Cyclic conjugation and the Hückel molecular orbital model, *Theor. Chim. Acta* **60** (1981) 203–226.

[9] B. O'Leary, R. B. Mallion, C. A. Coulson's work on a contour–integral approach to the London theory of magnetic susceptibility of conjugated molecules, *J. Math. Chem.* **3** (1989) 323–342.

[10] I. Gutman, M. Mateljević, Note on the Coulson integral formula, *J. Math. Chem.* **39** (2006) 259–266.

[11] A. Chen, A. Chang, W. C. Shiu, Energy ordering of unicyclic graphs, *MATCH Commun. Math. Comput. Chem.* **55** (2006) 95–102.

[12] L. Ye, X. Yuan, On the minimal energy of trees with a given number of pendent vertices, *MATCH Commun. Math. Comput. Chem.* **57** (2007) 193–201.

[13] H. Hua, On minimal energy of unicyclic graphs with prescribed girth and pendent vertices, *MATCH Commun. Math. Comput. Chem.* **57** (2007) 351–361.

[14] H. Hua, Bipartite unicyclic graphs with large energy, MATCH Commun. Math. Comput. Chem. **58** (2007) 57–83.

[15] I. Gutman, The energy of a graph: Old and new results, in: A. Betten, A. Kohnert, R. Laue, A. Wassermann (Eds.), *Algebraic Combinatorics and Applications*, Springer–Verlag, Berlin, 2001, pp. 196–211.

[16] C. A. Coulson, J. Jacobs, Conjugation across a single bond, *J. Chem. Soc.* **36** (1949) 2805–2812.

[17] I. Gutman, Cyclic conjugation energy effects in polycyclic π-electron systems, *Monatsh. Chem.* **136** (2005) 1055–1069.

[18] I. Gutman, M. Milun, N. Trinajstić, Graph theory and molecular orbitals. 19. Nonparametric resonance energies of arbitrary conjugated systems, *J. Am. Chem. Soc.* **99** (1977) 1692–1704.

[19] S. Bosanac, I. Gutman, Effect of a ring on the stability of polycyclic conjugated molecules, *Z. Naturforsch.* **32a** (1977) 10–12.

[20] I. Gutman, Proof of the Hückel rule, *Chem. Phys. Lett.* **46** (1977) 169–171.

[21] I. Gutman, S. Bosanac, Quantitative approach to Hückel rule. The relations between the cycles of a molecular graph and the thermodynamic stability of a conjugated molecule, *Tetrahedron* **33** (1977) 1809–1812.

[22] I. Gutman, M. Stanković, On the Hückel $(4m + 2)$ rule in polycyclic alternant hydrocarbons, *J. Mol. Struct. (Theochem)* **309** (1994) 301–304.

[23] I. Gutman, Topological studues on heteroconjugated molecules. VI. Alternant systems with two heteroatoms, *Z. Naturforsch.* **45a** (1990) 1085–1089.

[24] I. Gutman, S. Stanković, J. Đurđević, B. Furtula, On the cycle–dependence of topological resonance energy, *J. Chem. Inf. Model.* **47** (2007) 776–781.

[25] J. Conway, *Functions of One Complex Variable*, Springer-Verlag, Berlin, 1978.

[26] R. Churchill, J. Brown *Complex Variables and Applications*, McGraw–Hill, New York, 1984.

[27] C. A. Berenstein, R. Gay, *Complex Variables*, Springer–Verlag, New York, 1991.