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Relating Total π-Electron Energy and Resonance Energy of Benzenoid Molecules with *Kekulé*- and *Clar*-Structure-Based Parameters

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Summary. Within classes of isomeric benzenoid hydrocarbons various *Kekulé*- and *Clar*-structure-based parameters (*Kekulé* structure count, *Clar* cover count, *Herndon* number, *Zhang–Zhang* polynomial) are all mutually correlated. This explains why both the total π-electron energy (E), the *Dewar* resonance energy (*DRE*), and the topological resonance energy (*TRE*) are well correlated with all these parameters. Nevertheless, there exists an optimal value of the variable of the *Zhang–Zhang* polynomial for which it yields the best results. This optimal value is negative-valued for E, around zero for *TRE*, and positive-valued for *DRE*. A somewhat surprising result is that *TRE* and *DRE* considerably differ in their dependence on *Kekulé*- and *Clar*-structure-based parameters.

Keywords. *Kekulé* structures; *Clar* theory; *Zhang–Zhang* polynomial; Total π-electron energy; Resonance energy; Benzenoid hydrocarbons.

Introduction

In the theory of benzenoid hydrocarbons [1–5] *Kekulé* and *Clar* structural formulas are often used for rationalizing the π-electron structure, and for predicting physical properties and chemical behavior thereof. For quantitative purposes the *Kekulé structure count* (K) is most frequently employed [2, 5, 6]. In *Herndon's* structure-resonance theory [2, 6–9] the most significant quantity is the number of pairs of *Kekulé* structures that differ in positions of three double bonds; in what follows we refer to it as to the *Herndon number* and denote it by H. The *Herndon* number is equal to the number of edges of the so-called *resonance graph* [10–12]. An example illustrating the numbers K and H as well as the resonance graph is given in Fig. 1.

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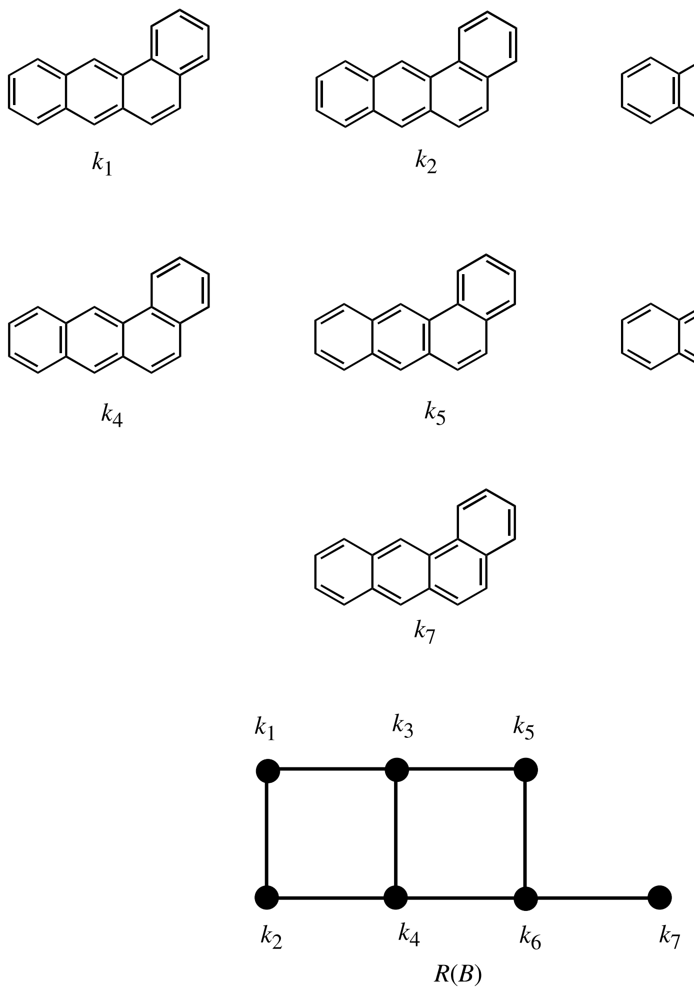

Fig. 1. Benzoanthracene (B) has seven *Kekulé* structural formulas, $k_1, k_2, \ldots, k_7$, and therefore $K(B) = 7$; eight pairs thereof differ in the position of exactly three double bonds; these pairs are (k_1, k_2), (k_1, k_3), (k_2, k_4), (k_3, k_4), (k_3, k_5), (k_4, k_6), (k_5, k_6), and (k_6, k_7), and therefore the *Herndon* number of benzoanthracene is $H(B) = 8$; the edges of the resonance graph $R(B)$ correspond to the above specified pairs of *Kekulé* structures; therefore the number of edges of the resonance graph coincides with the *Herndon* number

In its original formulation [2], the *Clar* aromatic sextet theory was a non-quantitative approach. Eventually, there were several attempts to overcome this limitation [5, 13–15]. Especially far-reaching is the *Hosoya-Yamaguchi* concept of *generalized Clar formulas*, whose number is, for the vast majority of benzenoids, equal to the number of *Kekulé* structures. Each *Clar* formula has a maximum number of aromatic sextets and pertains to a single *Kekulé* structure. The generalized *Clar* formulas (which may possess any number of aromatic sextets) may be compatible with several *Kekulé* structures. An illustrative example is given in Fig. 2. There s_1 and s_2 are the ordinary *Clar* structures of benzoanthracene, because these structures – in contrast to s_3–s_7 – possess a maximum number (in this case: 2)

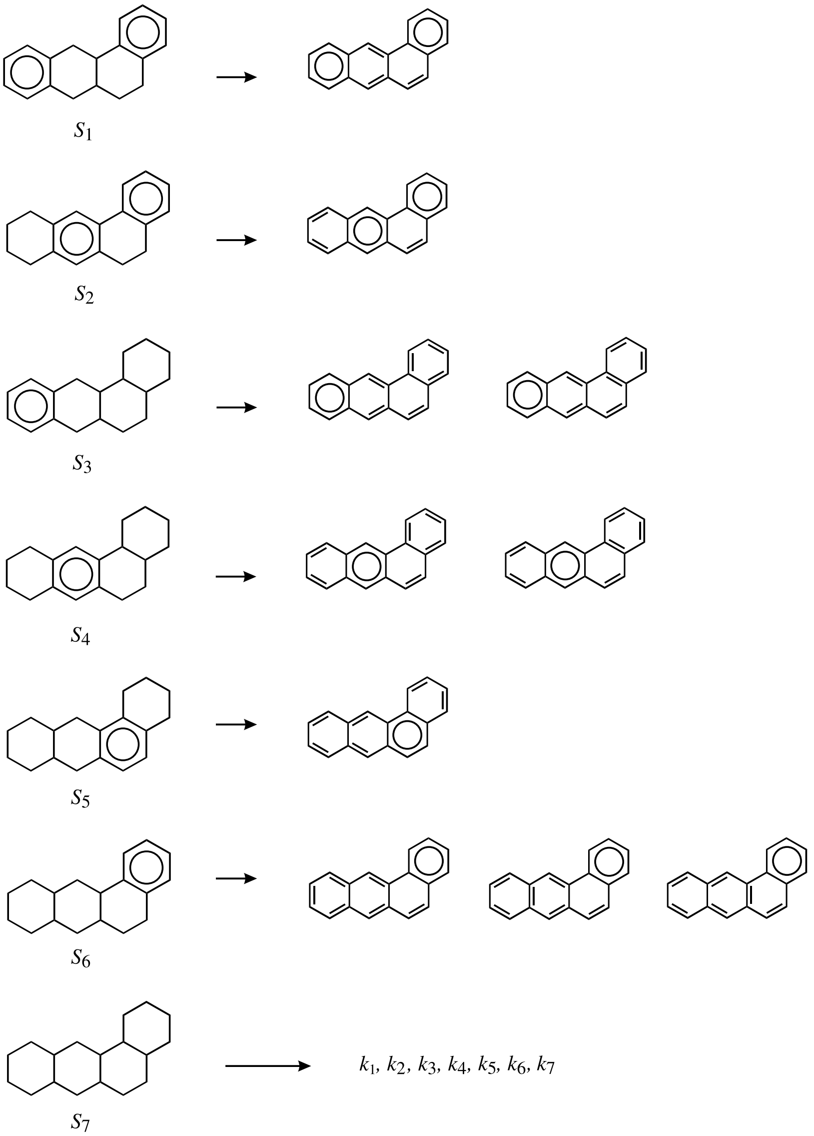

Fig. 2. Benzoanthracene (B) has two *Clar* aromatic sextet formulas (s_1 and s_2), each with two aromatic sextets (symbolized by circles); it has a total of seven generalized *Clar* formulas, $s_1, s_2, \ldots, s_7$, of which s_3, s_4, s_5, and s_6 have a single aromatic sextet, whereas s_7 has none; each generalized *Clar* formula s corresponds to $K(s)$ *Kekulé* structures, referred to as *Clar* covers; in particular, $K(s_1) = 1$, $K(s_2) = 1$, $K(s_3) = 2$, $K(s_4) = 2$, $K(s_5) = 1$, $K(s_6) = 3$, $K(s_7) = 7$, and thus the *Clar* cover count of benzoanthracene is $CCC(B) = 1 + 1 + 2 + 2 + 1 + 3 + 7 = 17$; counting the *Clar* covers with exactly k aromatic sextets, we get $z(B, 2) = 2$, $z(B, 1) = 8$, and $z(B, 0) = 7$, implying that the *Zhang–Zhang* polynomial is $\zeta(B, x) = 2x^2 + 8x + 7$; using the data given from Fig. 1 one can check that $z(B, 0)$ and $z(B, 1)$ are equal to the *Kekulé* structure count and *Herndon* number of B, respectively; both equalities are valid for all benzenoid systems

aromatic sextets. In *Clar* theory [1], it is postulated that exactly these diagrams (namely s_1 and s_2) reflect the main π-electron-based chemical and physical properties of the respective benzenoid molecule.

The structures consisting of aromatic sextets and/or double bonds are called *Clar covers* [16–18]. The Chinese mathematicians *Heping Zhang* and *Fuji Zhang* defined the quantities $z(B,k)$, equal to the number of *Clar* covers of the benzenoid system B, containing exactly k aromatic sextets, $k = 0, 1, 2, \ldots$, and conceived a pertinent counting polynomial [16–18]

$$\zeta(x) = \zeta(B,x) = z(B,0) + z(B,1)\,x + z(B,2)\,x^2 + \cdots .$$

In what follows $\zeta(x)$ will be referred to as the *Zhang–Zhang polynomial*. In Fig. 2 the definition of the *Zhang–Zhang* polynomial is explained in due detail on the example of benzoanthracene.

The *Zhang–Zhang* polynomial can be viewed as a mathematical object that includes and unifies the basic *Kekulé*- and *Clar*-structure-based parameters, encountered in the theory of benzenoid hydrocarbons. In particular, $z(B,0) = K(B)$ (*i.e.*, $\zeta(B,0) = K(B)$) and $z(B,1) = H(B)$.

The main papers on the *Zhang–Zhang* polynomial were published in mathematical journals [16–18]. As a consequence, chemical applications of $\zeta(x)$ started with a considerable delay [19, 20] (but one should mention the work [21], published in a Chinese chemical journal). A review on the *Zhang–Zhang* polynomial, aimed at organic chemists, has recently been prepared [22].

The total number of *Clar* covers will be referred to as the *Clar cover count* and denoted by *CCC*. Clearly, $CCC = \zeta(1)$. Our investigations [19] revealed that *CCC* is a structure-descriptor that deserves particular attention, being related with the topological resonance energy.

In this paper we report our studies of three quantum-chemical characteristics of the energetics of benzenoid molecules, and their relation with the above mentioned *Kekulé*- and *Clar*-structure-based parameters. We examined the total π-electron energy E, as computed within the simple HMO approximation (for a recent review see Ref. [23]), the *Dewar* resonance energy *DRE* [24], as computed by means of the *Hess-Schaad* parametrization scheme (for a recent review see Ref. [25]), and the topological resonance energy *TRE* [26, 27]. At this point it is worth recalling that E is proportional also to the σ-electron energy of benzenoid hydrocarbons [28], and thus E is simply related with their (measurable) enthalpies and other thermodynamic functions [28–30].

In earlier times the following main results along these lines were reported.

- Within classes of isomeric benzenoid molecules, E and K are linearly correlated (the *Hall* rule) [2, 31, 32].
- Within classes of benzenoid molecules of various size, *DRE* and $\log K$ are linearly correlated [33].
- *TRE* and *DRE* are linearly correlated [27]. In fact, in Ref. [27] a rather weak linear correlation between *TREPE* (= *TRE* per π-electron) and *DREPE* (= *DRE* per π-electron) was shown to exist, employing a sample consisting of conjugated molecules of various size, both benzenoid and non-benzenoid, aromatic, nonaromatic, and antiaromatic. Correlation between *TRE* and *DRE* within classes of isomeric benzenoid molecules seems to have not been studied so far.
- Within classes of isomeric benzenoid molecules, *TRE* and log *CCC* are linearly correlated [19].

Because both E, *DRE*, and *TRE*, as well as K, H, *CCC*, and $\zeta(x)$ depend on the size (number of carbon atoms and number of carbon–carbon bonds) of the benzenoid molecules examined, it is purposeful to restrict the considerations to classes of benzenoid isomers. In what follows we present the results obtained for the set consisting of 118 (= all possible) isomers of heptacyclic catacondensed benzenoids, $C_{30}H_{18}$. Analogous results have been obtained for several other sets of both cata- and pericondensed benzenoids; these may be obtained from the authors upon request.

Within sets of benzenoid isomers, many linear or slightly curvilinear correlations exist between the *Kekulé*- and *Clar*-structure-based parameters. In fact, all such parameters mentioned above (K, H, *CCC*, and $\zeta(x)$ for various values of the variable x) occur to be mutually correlated. This, in turn, provides a rationale for the observed linear dependence of E and *TRE*, and logarithmic dependence of *DRE* on any of these parameters. Because these relations are not exact, but only correlations, by means of a detailed analysis some (perhaps important) differences in the structure-dependence of E and the two resonance energies could be envisaged.

In the subsequent section we describe the correlations between the quantities investigated. In the next section we focus our attention to differences in the structure-dependence of E, *DRE*, and *TRE*. In the last section we state some concluding remarks. In the Appendix a mathematical relation between $\zeta(0) = K$ and $\zeta(1) = CCC$ is deduced.

Results and Discussion

Correlations between Kekulé-Structure-Based, Clar-Structure-Based, and Energetic Parameters of Benzenoid Molecules

As already mentioned, in the 1970s, when the two resonance energies *DRE* and *TRE* were introduced (and when numerous papers were published on their chemical applications and mathematical properties), their mutual relation attracted very little attention [27]. In the decades that followed, this problem was not considered at all. In particular, the question of how *TRE* and *DRE* are correlated within sets of benzenoid isomers seems to be first time addressed only quite recently [20].

In Fig. 3 are plotted the *TRE*-values of isomeric catacondensed heptacyclic-benzenoid hydrocarbons *versus* the respective *DRE*-values. The linearity of this correlation is something what one would expect, knowing that both the *Dewar* [24, 25] and the topological resonance energy [26, 27] were aimed at quantifying one and the same π-electron characteristics of polycyclic conjugated molecules [34].

At the first glance, the slight curvilinearity of the correlation shown in Fig. 3 seems to be negligible. If so, then one would expect that the form of the dependence of *TRE* and *DRE* on various structure-descriptors is identical. That this is not the case is shown in Fig. 4.

Figure 4 reveals the very good linear correlation between E and K (previously known [2, 31, 32]) and between *TRE* and K (hitherto not reported). In both cases

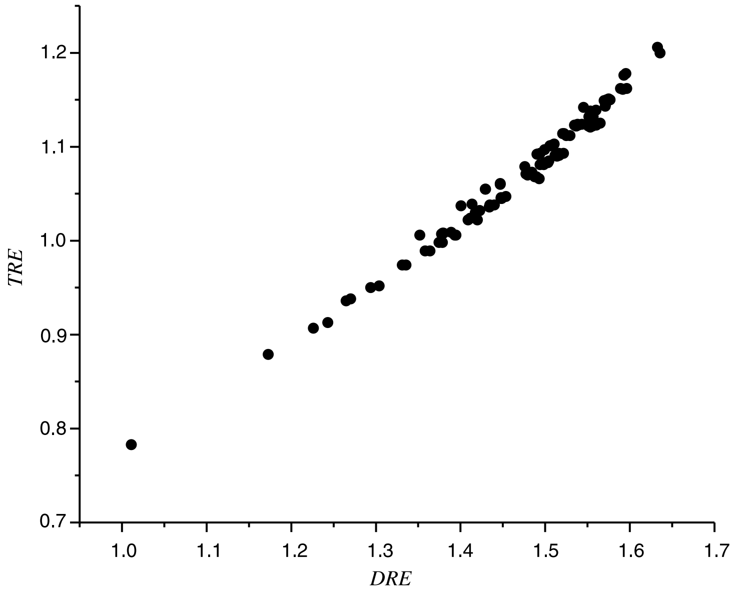

Fig. 3. Correlation between *TRE* and *DRE* for the (complete) set of 118 isomeric heptacyclic catacondensed benzenoid hydrocarbons $C_{30}H_{18}$; the correlation is linear; by a careful inspection a slight curvilinearity can be observed; however, by means of *F*-test, this curvilinearity is found to be statistically not significant at a 90% (or higher) confidence level

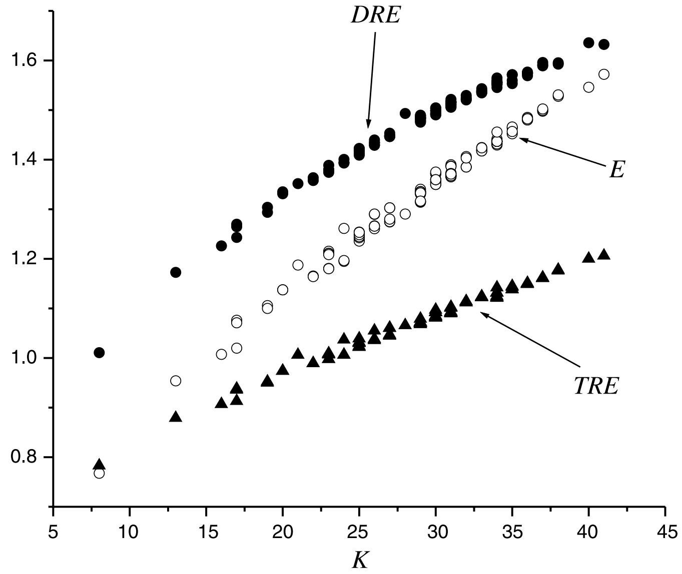

Fig. 4. Dependence of *TRE*, *DRE*, and *E* on the number of *Kekulé* structures ($= \zeta(0)$) for the same data set as in Fig. 3; for technical reasons, the *E*-values are shifted downwards by 41 units. The *TRE*/*K* and *E*/*K* correlations are linear; their curvilinearity is statistically not significant at 90% (or higher) confidence level; the curvilinearity of the *DRE*/*K* correlation is statistically significant at a confidence level greater than 99%

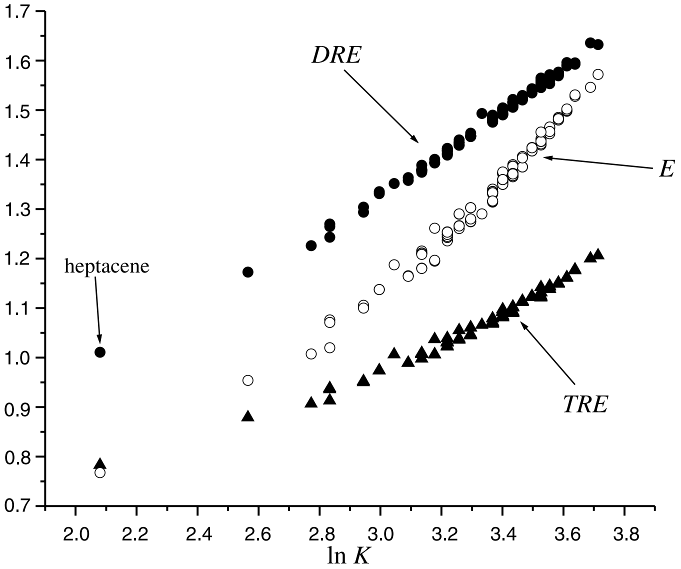

Fig. 5. Dependence of *TRE*, *DRE*, and *E* on the logarithm of the number of *Kekulé* structures ($= \ln\zeta(0)$) for the same data set as in Fig. 3; the *TRE*/ln *K* and *E*/ln *K* correlations are evidently curvilinear, whereas the *DRE*/ln *K* correlation is linear (with correlation coefficient 0.996); the curvilinearity of the latter correlation is not statistically significant at a confidence level 90% or greater, provided the outlier – the data point pertaining to heptacene – is not taken into account

the correlation coefficient is 0.993. The dependence of *DRE* on *K* is essentially logarithmic, as anticipated in Ref. [33], and as shown in Fig. 5.

After establishing the way in which the total π-electron energy and the resonance energies depend on the number of *Kekulé* structures, one may ask about their dependence on other *Kekulé*- and *Clar*-structure-based parameters. The answer to these questions is found by observing that (within sets of benzenoid isomers) various *Kekulé*- and *Clar*-structure-based parameters are all mutually correlated, and that these correlations are essentially linear. In Fig. 6 we show how H and $\zeta(x)$ are correlated with the *Kekulé* structure count $K = \zeta(0)$. We see that there is a linear correlation between K and the *Herndon* number (a feature that also seems to be not recognized until now). In addition, for near-zero values of the variable x, the correlations between $\zeta(0)$ and $\zeta(x)$ is also linear. A slight deviation from linearity takes place only for larger values of x, in particular for $x \approx 1$.

We thus arrive at the previously not fully recognized conclusion that the main *Kekulé*- and *Clar*-structure-based parameters of benzenoid molecules carry essentially one and the same structural information, same as what is provided by the simple *Kekulé* structure count. This implies that if in quantitative theoretical considerations we use the *Herndon* number and/or the *Zhang–Zhang* polynomial instead of (or together with) the *Kekulé* structure count, the gain will not be great.

On the other hand, none of the above described relations is exact and the deviations of the data points from the regression lines must not be disregarded. Therefore,

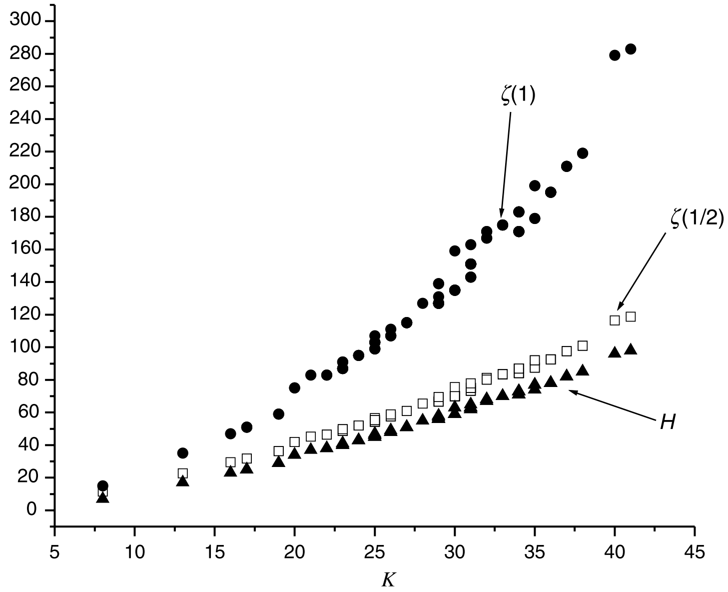

Fig. 6. The dependence of the *Herndon* number (H) and the *Zhang–Zhang* polynomial $\zeta(x)$ for various values of the variable x on the *Kekulé* structure count $K = \zeta(0)$, for the $C_{30}H_{18}$ benzenoid isomers specified in Fig. 3; all these correlations are essentially linear; the correlation coefficients are 0.9946 for H, 0.9986 for $\zeta(0.2)$, 0.9950 for $\zeta(0.4)$, 0.9899 for $\zeta(0.6)$, 0.9840 for $\zeta(0.8)$, and 0.9776 for $\zeta(1.0)$

there still may be some improvement if the *Zhang–Zhang* polynomial $\zeta(x)$ is used instead of $K = \zeta(0)$. The results obtained along these lines are outlined in the subsequent section.

Further Differences in the Structure-Dependence of the Energetic Parameters of Benzenoid Molecules

In order to shed some more light on the role of the *Clar*-structure-based parameters, and in view of the results presented in the previous section, we have examined how E and TRE are correlated with $\zeta(x)$, as well as DRE with $\ln\zeta(x)$. The variable x has been varied in order to find its value for which the approximations (Eqs. (1)–(3)) become optimal.

$$E(B) \approx a\,\zeta(B,x) + b \tag{1}$$

$$TRE(B) \approx a'\,\zeta(B,x) + b' \tag{2}$$

$$DRE(B) \approx a''\ln\zeta(B,x) + b'' \tag{3}$$

For each value of x the coefficients a, b, a', b', a'', b'' were determined by least-squares fitting, and the average relative error (*ARE*) was taken as the criterion of the precision of the respective approximation. The results obtained for the $C_{30}H_{18}$ isomers are shown in Fig. 7.

Analogous results (that can be obtained from the authors upon request) have been found for other classes of benzenoid isomers, but the values of x for which

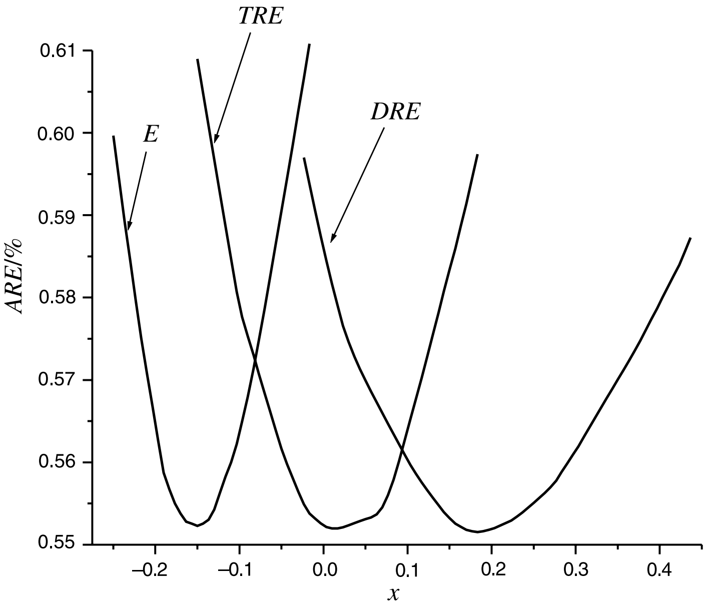

Fig. 7. Dependence of the average relative error (*ARE*) of Eqs. (1)–(3) on the variable x, computed for the $C_{30}H_{18}$ benzenoid isomers specified in Fig. 3; the minima are attained for $x = -0.15$, $x = 0.01$, and $x = +0.19$, respectively, and are equal to 0.022, 0.55, and 0.41%, respectively; in order to present all the three curves on one diagram, the *ARE* values pertaining to Eqs. (1) and (3) were multiplied by 25 and 1.3, respectively

ARE becomes minimal were not the same. Anyway, the general regularity that emerged is the following:

- Equation (1) is optimal for some negative-valued x, $x_{optimal} \in \{-0.2, -0.1\}$. In the case of the $C_{30}H_{18}$ isomers, $x_{optimal} = -0.15$ and $ARE_{min} = 0.022\%$.
- Equation (2) is optimal for some near-zero x, $|x_{optimal}| \leq 0.03$. In the case of the $C_{30}H_{18}$ isomers, $x_{optimal} = 0.01$ and $ARE_{min} = 0.55\%$.
- Equation (3) is optimal for some positive-valued x, $x_{optimal} \in \{0.1, 0.2\}$. In the case of the $C_{30}H_{18}$ isomers, $x_{optimal} = 0.19$ and $ARE_{min} = 0.41\%$.

We mention in passing that in Refs. [19, 20] also the approximation (4) was examined (for which $x_{optimal} \approx 0.7$).

$$TRE(B) \approx a^* \ln \zeta(B, x) + b^* \tag{4}$$

As explained above, the dependence between *TRE* and $\zeta(0)$ is not logarithmic. Therefore we now realize that the usage of the expression occurring on the right-hand side of Eq. (4) was not legitimate.

Concluding Remarks

Our studies revealed certain hitherto concealed properties of the resonance energies of benzenoid molecules, and their dependence on *Kekulé*- and *Clar*-structure-based parameters.

For a usually educated chemist, the meaning of our findings is that the two resonance energies encountered in the chemical literature (*DRE* and *TRE*) differ more than it previously was expected. Therefore, when "aromaticity" of conjugated molecules is rationalized and predicted by means of resonance energies [25, 35], one should be careful which of them to apply.

For chemists familiar with the details of *Kekulé*- and *Clar*-structure-based theories, we could say more:

First of all, in spite of the apparent linear correlation between the two resonance energies (*cf.* Fig. 3), the topological resonance energy (*TRE*) is a linear function of the *Kekulé* structure count K (*cf.* Fig. 4), whereas the analogous dependence of the *Dewar* resonance energy (*DRE*) is logarithmic (*cf.* Fig. 5).

All *Kekulé*- and *Clar*-structure-based parameters investigated in this work (*Kekulé* structure count, *Herndon* number, *Clar* cover count, and the *Zhang–Zhang* polynomial for various values of the variable x) are mutually correlated, and these correlations are essentially linear, *cf.* Fig. 6. Therefore, E, *TRE*, and *DRE* depend on the mentioned parameters in the essentially same manner as on K.

By using the *Zhang–Zhang* polynomial instead of K, it is possible to somewhat improve the precision of the approximations for E and *DRE*, Eqs. (1) and (3), but not for *TRE*, Eq. (2). An interesting finding, that is not fully understood, is that in the case of total π-electron energy, Eq. (1), the *Zhang–Zhang* polynomial with a negative-valued variable $x_{optimal}$ needs to be used, whereas in the case of the *Dewar* resonance energy, Eq. (3), the corresponding $x_{optimal}$ is positive-valued, *cf.* Fig. 7. Equally interesting is the finding that for the topological resonance energy, Eq. (2), $x_{optimal} \approx 0$. This means that *TRE* depends only on K (which is equal to the *Zhang–Zhang* polynomial at $x = 0$), and is thus insensitive to other structure-descriptors originating from *Herndon's* structure-resonance theory [2, 6–9] and/or from the quantitative versions of *Clar's* aromatic sextet theory [1, 13, 14, 16–19].

Appendix: Relations between ζ (0) and ζ (1)

As already explained, the *Zhang–Zhang* polynomial at $x = 0$ and $x = 1$ is equal to the *Kekulé* structure count K and the *Clar* cover count *CCC*, respectively. We now show that $\zeta(1)$ is bounded from both below and above by linear functions of $\zeta(0)$.

Consider a benzenoid system B whose *Clar* formulas contain $Cl = Cl(B)$ aromatic sextets; Cl is called the *Clar number* of the respective benzenoid molecule [22]. (In the example shown in Fig. 2, $Cl = 2$.)

The *Zhang–Zhang* polynomial of B can be written as Eq. (5).

$$\zeta(B, x) = \sum_{k=0}^{Cl} z(B, k)\, x^k \tag{5}$$

The sextet polynomial of a benzenoid system B is defined as Eq. (6) [13] where $s(B, k)$ is the number of generalized *Clar* formulas of B with k aromatic sextets. (In the example shown in Fig. 2, $s(B, 0) = 1$, $s(B, 1) = 4$, and $s(B, 2) = 2$.) By definition, $s(B, 0) = 1$ for all benzenoid systems. It is known that Eqs. (7) [13] and (8) [18] are true.

$$\sigma(B, x) = \sum_{k=0}^{Cl} s(B, k)\, x^k \tag{6}$$

$$\sigma(B, 1) = \sum_{k=0}^{Cl} s(B, k) = K(B) = \zeta(0) \tag{7}$$

$$\zeta(B, x) = \sigma(B, x + 1) \tag{8}$$

Bearing these relations in mind, we have Eqs. (9) and (10).

$$\begin{aligned}\zeta(B,1) &= \sigma(B,2)\\ &= \sum_{k=0}^{Cl} s(B,k)\,2^k = s(B,0) + \sum_{k=1}^{Cl} s(B,k)\,2^k\\ &\geq s(B,0) + 2\sum_{k=1}^{Cl} s(B,k) = s(B,0) + 2\left[\sum_{k=0}^{Cl} s(B,k)\ - s(B,0)\right]\\ &= 1 + 2\,[K(B)-1] = 2\,\zeta(B,0) - 1\end{aligned} \tag{9}$$

$$\begin{aligned}\zeta(B,1) &= \sigma(B,2)\\ &= \sum_{k=0}^{Cl} s(B,k)\,2^k = s(B,0) + \sum_{k=1}^{Cl} s(B,k)\,2^k\\ &\leq s(B,0) + 2^{Cl}\sum_{k=1}^{Cl} s(B,k) = s(B,0) + 2^{Cl}\left[\sum_{k=0}^{Cl} s(B,k)\ - s(B,0)\right]\\ &= 1 + 2^{Cl}\,[K(B)-1] = 2^{Cl}\,\zeta(B,0) - [2^{Cl}-1]\end{aligned} \tag{10}$$

Thus we arrived at the inequalities (Eq. (11)) or, what is the same Eq. (12).

$$2\,\zeta(B,0) - 1 \;\leq\; \zeta(B,1) \;\leq\; 2^{Cl(B)}\,\zeta(B,0) - \left[2^{Cl(B)} - 1\right] \tag{11}$$

$$2\,K(B) - 1 \;\leq\; CCC(B) \;\leq\; 2^{Cl(B)}\,K(B) - \left[2^{Cl(B)} - 1\right] \tag{12}$$

Equality on both sides is attained if and only if the *Clar* number is equal to unity, which happens if *B* is a linear polyacene and only then.

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