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The conjugated circuits model*

On the geometries of annelated [*n*]annulenes

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Several annelated [*n*]annulenes are examined from a graph-theoretical point of view. It is shown how a new interpretation of the conjugated circuit model can be used in order to study the geometries of such compounds. The work illustrates which energetical factors determine whether a structure with alternating bond lengths, or with reduced symmetry is more stable than one with full double bond delocalization or full symmetry.

Key words: Annelted [*n*]annulenes — Chemical graph theory — Conjugated circuits model — Kekulé structures

1. Introduction

In our recent work [1] on annelated [*n*]annulenes with $n =$ even we have found that two types can be distinguished. Type I compounds have either only one annelated group or there is to be an even number of sites along the portion of the perimeter between the (nearest lying) annelation sites. They are characterized by at least one Kekulé-Robinson-Clar formula [2] (which represents the superposition of Kekulé valence structures) where none of the annelated groups is quinoid. In type II compounds an odd number of carbon atoms are present in the perimeter between two annelated units so that all Kekulé-Robinson-Clar formulae contain at least one quinoid annelated group.

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* Dedicated to Professor J. Koutecký on the occasion of his 65th birthday. He taught us that the progress of chemical science is related to the development of conceptual models with wide ranges of applicability and portability

With more than two annelated groups a further discrimination of type II compounds into types IIa and IIb is possible depending on the number of quinoid and non-quinoid annelated groups. Type IIa compounds possess the same number of quinoid and non-quinoid annelated groups, whilst in type IIb compounds the number of quinoid and non-quinoid groups differ.

In Fig. 1 we give examples of type I and type II annelated [*n*]annulenes. Recently [3] the term phenanth-fused for type I and anth-fused for type II dibenzannelated [4m+2]annulenes has been introduced.

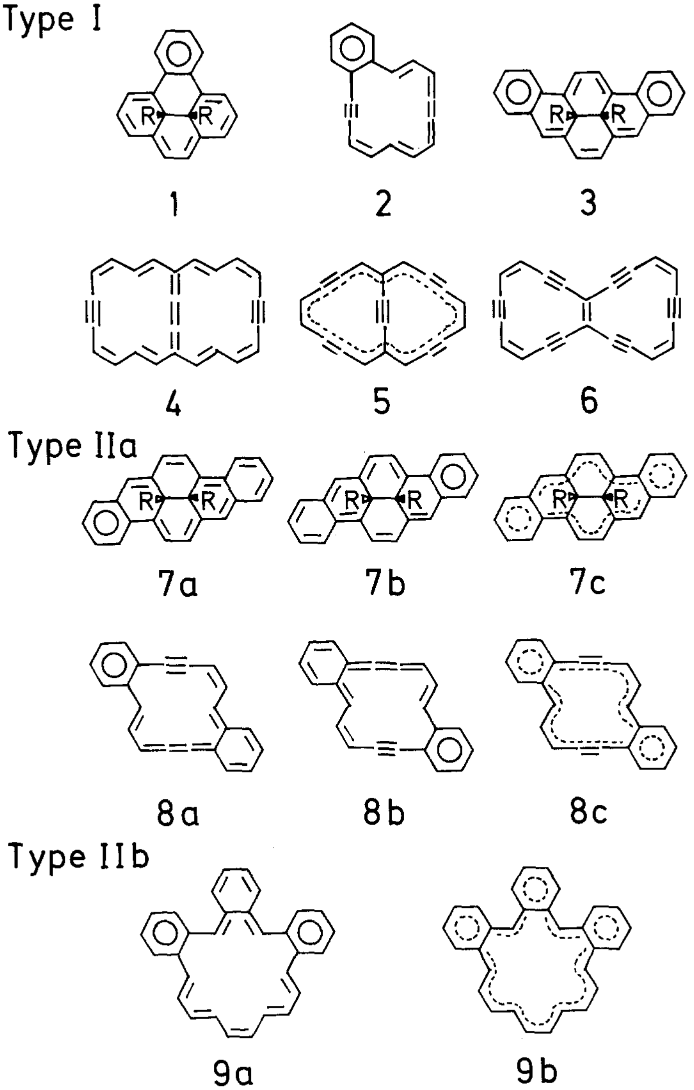


Fig. 1. Illustrative examples of type I and II annelated [*n*]annulenes

The number and mutual arrangements of the annelated groups determines the geometry of the perimeter and the extent of double bond fixation and hence the physical properties such as, for example, ^{1}H NMR shifts [4]. Special interest is drawn to type IIa compounds where two equivalent sets of Kekulé–Robinson–Clar formulae occur, see 7a, b and 8a, b in Fig. 1. The combination of both sets yields a fully symmetric structure. However, we can anticipate that a symmetry reduced structure corresponding to just one of the two equivalent Kekulé–Robinson–Clar formulae could represent a more stable structure with one quinoid benzene ring instead of the fully symmetric one, as in 7c and 8c.

In order to investigate, quantum chemically, whether a type IIa annulene prefers the fully symmetric or a symmetry reduced geometry one could do highly sophisticated calculations with full geometry optimization [4] or study the Hartree–Fock instabilities [5, 6]. Such calculations are very elaborate due to the size of these molecules. There exist several simple pencil-and-paper methods such as the PMO-method [7], Szentpaly's free-electron PMO approach [8], Herndon's structure-resonance theory [9] or the conjugated circuits model [10, 11]. In this paper we will demonstrate how the latter approach can be used for the study of the geometry of annelated annulenes.

2. The conjugated circuits model

The model has been described in detail elsewhere [10–12]. The resonance energy RE^{cc} is given by the formula

$$RE^{cc} = K^{-1} \sum_{i=1}^{K} \sum_{j=1}^{\infty} (a_{ij} R_j + b_{ij} Q_j), \tag{1}$$

where K is the total number of Kekulé structures, whilst the sum runs over all K Kekulé valence structures K_i. a_{ij} (b_{ij}) is the number of conjugated circuits with $4j+2$ ($4j$) carbon atoms in the corresponding Kekulé valence structure K_i. A conjugated circuit is defined as that circuit which exhibits a regular alternation of formal double and single bonds. In Eq. (1) we have neglected contributions from disjoint circuits within a Kekulé valence structure. R_i and Q_i are parameters which have been determined as follows [10–12] (all values in eV):

$R_1 = 0.869$ $\qquad Q_1 = -1.600$

$R_2 = 0.246$ $\qquad Q_2 = -0.450$

$R_3 = 0.100$ $\qquad Q_3 = -0.150$

$R_4 = 0.046$ $\qquad Q_4 = -0.006$

$R_i = 0\ (i > 4)$ $\qquad Q_i = 0\ (i > 4)$.

The total number of conjugated circuits, including disjoint ones, is $K - 1$ per Kekulé valence structure.

The geometry of a molecule is determined by its total energy E_t which can be written as follows:

$$E_t = E_\pi + E_\sigma.$$

The resonance energy is defined as [13]

$$RE^{\mathrm{cc}} = E_t - E_R,$$

where E_R is the energy of a polyene reference structure. Since E_R is constant for a given molecule it should be possible to use resonance energies in order to derive the most stable geometry of a conjugated molecule.

3. Application of the conjugated circuit model

Dibenzo[14]annulene 7 possesses four Kekulé valence structures which can be grouped into two sets A_i and B_i ($i = 1, 2$), see Fig. 2. A_i and B_i are symmetry related with respect to the C_2 axis of this molecule. None of the four Kekulé valence structures transforms according to the fully symmetric representation of the point group of 7 [14].

The geometry of a molecule which is described by a set of Kekulé valence structures can be estimated by means of the Pauling bond characters [15] B_s. These are given as the number of formal double bonds for a given bond s in all Kekulé valence structures K_i in the chosen set $\{K_i\}$ divided by K. $B_s = 0$ corresponds to a quasi single bond (C—C), $B_s = \frac{1}{2}$ to the "aromatic" bond in benzene (C$\overset{...}{-}$C), and $B_s = 1$ to a quasi double bond (C=C). Bond lengths can be calculated [15] from B_s.

Taking into account all Kekulé valence structures for 7 we arrive at geometry 7c with resonance energy

$$RE^{\mathrm{cc}}(A_1 + A_2 + B_1 + B_2) = (1/2)(2R_1 + R_3 + 2R_4 + R_5) = 0.965 \text{ eV}.$$

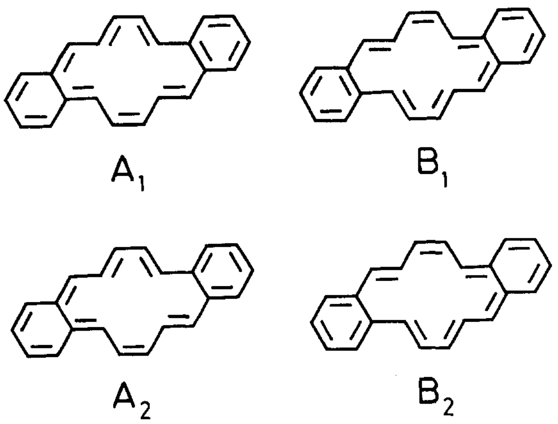


Fig. 2. Kekulé valence structures of dibenzo[14]annulene 7 (only the conjugated carbon skeleton has been given)

Using only one of the sets $\{A_1, A_2\}$ or $\{B_1, B_2\}$ we obtain either quinoid structure 7a or 7b whose resonance energy is given as follows

$$RE^{cc}(A_1+A_2) = RE^{cc}(B_1+B_2) = (1/2)(2R_1+R_3+2R_4+R_5).$$

Thus we have

$$RE^{cc}(A_1+A_2+B_1+B_2) = RE^{cc}(A_1+A_2) = RE^{cc}(B_1+B_2).$$

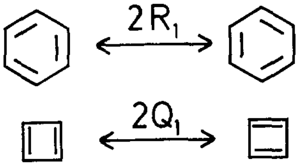
This result holds for all dibenzannelated type II annulenes, as can be verified by inspection of Eq. (1) due to the fact that such compounds always possess two equivalent sets of Kekulé valence structures. Consequently the straightforward application of the conjugated circuit model to subsets of all Kekulé valence structures does not tell us which geometry is preferred.

A closer inspection of all subsets of the four Kekulé valence structures of 7 shows that the resonance energy RE^{cc} for the single Kekulé valence structure A_1 and B_1 is given as $RE^{cc}(A_1) = RE^{cc}(B_1) = R_1+R_3+R_4 = 1.015$ eV, being larger than that for the sets $\{A_1, A_2, B_1, B_2\}$, $\{A_1, A_2\}$ or $\{B_1, B_2\}$. Obviously the application of the conjugated circuit model to arbitrary subsets of the Kekulé valence structures is not justified since it attributes erroneously a non-vanishing resonance energy to a polyene structure. This can also be demonstrated with $[n]$annulenes $\underset{\sim}{X}$, where $n = 4m+2$ or $4m$. Both types of annulenes possess just two Kekulé valence structures A and B which are related by a double bond shift along the perimeter. The full set $\{A, B\}$ leads to a fully delocalized geometry $\underset{\sim}{X}'$ with $B_s = \frac{1}{2}$ for all bonds and a resonance energy $RE^{cc}(A+B) = (R/Q)_m$. Here $(R/Q)_m = R_m$ if $n = 4m+2$ and $(R/Q)_m = Q_m$ if $n = 4m$. As for type IIa annulenes, we obtain $RE^{cc}(A+B) = RE^{cc}(A) = RE^{cc}(B)$ where the sets $\{A\}$ or $\{B\}$ lead to a geometry $\underset{\sim}{X}''$ with alternating quasi single ($B_s = 0$) and double ($B_s = 1$) bonds. Thus $[4m+2]$- and $[4m]$annulenes are not discriminated with respect to their geometry and a non-vanishing resonance energy is erroneously attributed to the reference polyene structure. This indicates that Eq. (1) cannot reasonably be applied to any set of Kekulé valence structures of such a molecule.

4. Modification of the conjugated circuit model

The failure of the conjugated circuit model described in the last chapter can be avoided if we interpret the conjugated circuit approach in terms of Herndon's structure resonance theory [9]. At first sight it might appear that the conjugated circuit model, in which one counts conjugated circuits within each Kekulé valence structure, and the structure resonance theory, which involves resonance integrals between Kekulé structures, are unrelated. However, comparison of the two models in an actual application contradicts this [16]. It was shown that they become identical if the linearly dependent conjugated circuits are retained in the conjugated circuit model and if all resonance integrals are kept in the structure resonance theory [17]. Therefore we may use the concepts from the latter within the conjugated circuit approach. Actually the equivalence of these two models causes each model to constitute a further justification of the other.

Let us interpret $2R_i(2Q_i)$ as the interaction energy between two conjugated circuits with $4i+2(4i)$ carbon atoms which are related by a permutation of the double bonds, i.e. a shift of the double bonds along the circuit, e.g.



The resonance energy in the modified conjugated circuit model is calculated according to the formula

$$RE = (2/K) \sum_{i=1}^{P} \sum_{j=1}^{\infty}{}' (c_{ij}R_j + d_{ij}Q_j), \tag{2}$$

where the first sum runs over all $P = K(K-1)/2$ pairs of Kekulé valence structures. $c_{ij}(d_{ij})$ is the number of conjugated circuits with $4j+2(4j)$ carbon atoms which are related by a double bond shift along the circuit with respect to the chosen pair of Kekulé valence structures. In Eq. (2) any pair of disjoint conjugated circuits which are simultaneously related by a double bond shift in two different Kekulé valence structures are not taken into account. This is signified by a prime in Eq. (2). The omission of such contributions can easily be demonstrated for biphenyl which possesses four Kekulé valence structures which are displayed in Fig. 3. together with all conjugated circuits. The following circuits are related by a double bond shift: a_1–b_1, a_1–d_1, a_2–b_2, a_2–c_2, b_1–c_1, b_2–d_2, c_1–d_1, c_2–d_2, a_3–b_3,

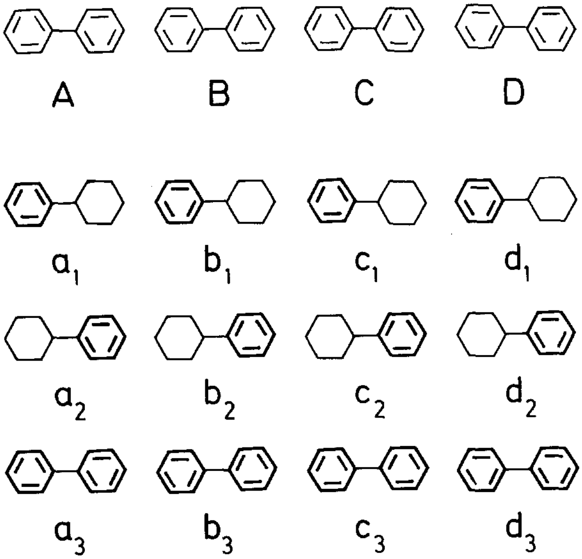


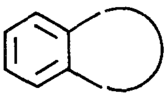
Fig. 3. Kekulé valence structures *A*, *B*, *C*, and *D* and conjugated circuits of biphenyl a_i, b_i, c_i and d_i ($i = 1$-3)

and c_3-d_3. However, the last two interactions are neglected since they are derived from disjoint circuits and a_1-b_1, a_2-b_2, c_1-d_1, and c_2-d_2 are not taken into account, since a_1-b_1 and a_2-b_2 are simultaneously related by a double shift as are c_1-d_1 and c_2-d_2.

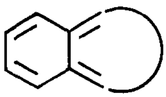
It is obvious that $RE^{cc} = RE$ if the set of all Kekulé valence structures is considered. However, Eq. (2) generally leads to different results with respect to Eq. (1) if subsets are used. This is evident in the case of $[n]$annulenes $\underset{\sim}{X}$. Eq. (2) now correctly yields $RE(A) = RE(B) = 0$ since there are no pairs of Kekulé valence structures. Furthermore we obtain $RE(A+B) = (R/Q)_m$ and so the modified conjugated circuit method attributes the fully delocalized geometry $\underset{\sim}{X}'$ to $[4m+2]$ - and the olefinic $\underset{\sim}{X}''$ to $[4m]$annulenes due to the different signs of R_m and Q_m. This result is in agreement with experimental and other theoretical findings [5, 18, 19] if $m \leq 4$. For larger m our approach does not allow conclusions on the geometry of $[n]$annulenes since then R_m, $Q_m = 0$ according to Eq. (2). Furthermore it does not predict bond length alternation for $[4m+2]$annulenes with sufficiently large m as expected due to more sophisticated quantum chemical studies [20]. This is mainly due to two factors: (i) the Pauling bond character B_s is too crude a description of geometries for large annulenes since B_s can only take the values 0, $\frac{1}{2}$, and 1 whereas the Coulson bond order varies with ring size [20], (ii) the parameters $(R/Q)_i$ have been derived from benzenoid hydrocarbons where bond lengths are scattered around the aromatic bond length value and so σ-compression energies are not properly treated for very short and long bonds. However, there are reports in the literature [21] which suggest that bond-alternation can be predicted for large annulenes in terms of a Kekulé-structure based *ansatz* for the Pauling-Wheland VB model [22].

5. Application of the modified conjugated circuit model

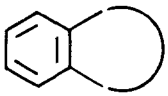
We consider first monobenzannelated $[n]$annulenes. They possess three Kekulé valence structures:



A



B.



C

The resonance energies are given as follows:

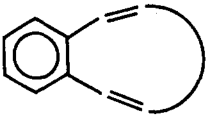
$$RE(A+C) = R_1$$

$$RE(B+C) = (R/Q)_m$$

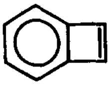
$$RE(A+B) = (R/Q)_{m+1}$$

$$RE(A+B+C) = (2/3)(R_1 + (R/Q)_m + (R/Q)_{m+1}).$$

For $n=4m+2$, $RE(A+B+C)>RE(A+C)=RE(B+C)>RE(A+B)$ if $m=1$ (i.e. for naphthalene) but $RE(A+C)>RE(A+B+C)>RE(B+C)$, $RE(A+B)$ if $m>1$. Consequently, monobenzannelated $[4m+2]$annulenes (except naphthalene) should exhibit a geometry which can be represented by the Kekulé-Robinson-Clar formula

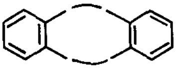


with bond length alternation in the annulenoid perimeter. This agrees with results of experimental [23-25] and quantum chemical [4, 25] studies of ^{1}H NMR shifts in the corresponding benzannelated annulenes (e.g. 1 or 2) which demonstrate that the ring current effect is considerably reduced for the annulenoid protons. For $n=4m$ $RE(A+C)>RE(A+B+C)>RE(A+B)>RE(B+C)$ always. An example is benzocyclobutadiene which is best represented by the Kekulé-Robinson-Clar formula



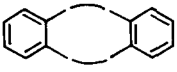
according to more sophisticated calculations and experiment [26] in agreement with our qualitative results.

In case of dibenzannelated $[n]$annulenes we distinguish type I (e.g. 3) and type IIa (e.g. 7, 8) compounds. Type I dibenzo$[n]$annulenes possess five Kekulé valence structures



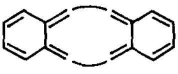
A

B



C

D



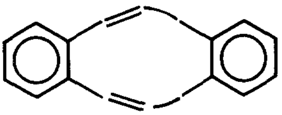
E

which yield the following resonance energies:

$$RE(A+B+C+D+E)=(2/5)(4R_1+(R/Q)_m+2(R/Q)_{m+1}+(R/Q)_{m+2})$$

$$RE(A+B+C+D)=2R_1.$$

All other sets of Kekulé valence structures lead to smaller resonance energies and are not given here. Except for $n=6$ (i.e. phenanthrene) $RE(A+B+C+D)>RE(A+B+C+D+E)$ and so a geometry is expected which can be represented by one Kekulé-Robinson-Clar formula



with bond length alternation in the annulene part. This agrees with experimental [23, 27] and quantum chemical [4, 25] studies for type I dibenzo[$4m+2$]annulenes (e.g. 3) where the ring current effect on ^{1}H NMR is strongly reduced for protons at the annulene perimeter.

Biphenylene is an example of a type I dibenzannelated [$4m$]annulene with $m = 1$. In agreement with our qualitative considerations it is characterized by quasi single bonds (length 151 pm [28]) connecting the benzene ring units. Other examples have been studied elsewhere [29].

Type II dibenzannelated [n]annulenes possess only four Kekulé valence structures A_1, A_2, B_1, and B_2 which are displayed in Fig. 2 for 7. The following resonance energies are derived for a type II dibenzo[n]annulene:

$$RE(A_1+A_2+B_1+B_2) = R_1+(1/2)((R/Q)_{m+1}+(R/Q)_{m+2})$$

$$RE(A_1+A_2) = RE(B_1+B_2) = R_1$$

$$RE(A_1+A_2+B_1) = RE(A_1+B_1+B_2) = (2/3)(R_1+(R/Q)_m+(R/Q)_{m+1})$$

$$RE(A_1+A_2+B_2) = RE(A_2+B_1+B_2) = (2/3)(R_1+(R/Q)_{m+1}+(R/Q)_{m+2})$$

$$RE(A_1+B_1) = (R/Q)_m$$

$$RE(A_1+B_2) = RE(A_2+B_1) = (R/Q)_{m+1}$$

$$RE(A_2+B_2) = (R/Q)_{m+2}.$$

For $n = 4m+2$ we have $RE(A_1+A_2+B_1+B_2) > RE(A_1+A_2) = RE(B_1+B_2)$. Except for $m = 1$ (i.e. anthracene) $RE(A_1+A_2) = RE(B_1+B_2)$ is also larger than any other resonance energy given above. Consequently our modified conjugated circuit approach predicts a fully symmetric geometry such as 7c and 8c for 7 and 8 instead of quinoid structures such as 7a, b, 8a or b. Only for $m > 4$ does our model fail to discriminate between the fully symmetric and the quinoid species. Our result is correct for anthracene ($m = 1$) and agrees with experimental [23, 25, 27] and quantum chemical [4, 25] results for some dibenzannelated [$4m+2$]annulenes such as 7 and 8.

In the case of dibenzannelated type II [$4m$]annulenes, $RE(A_1+A_2) = RE(B_1+B_2)$ is larger than all resonance energies for any other set of Kekulé valence structures. Thus our model predicts a quinoid geometry for such compounds. To the best of our knowledge, examples with a planar geometry of the conjugated system are not known yet.

For type IIb benzannelated [n]annulenes it is impossible to derive general formulae for the resonance energies. Therefore we take 9 as an example. Its six Kekulé valence structures are displayed in Fig. 4.

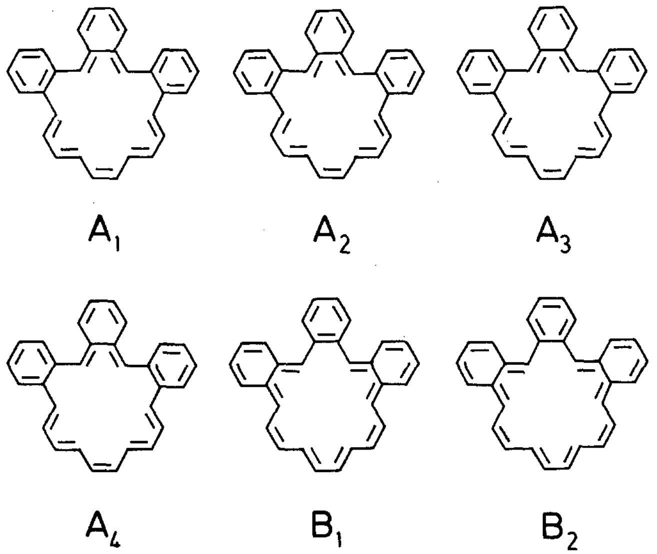


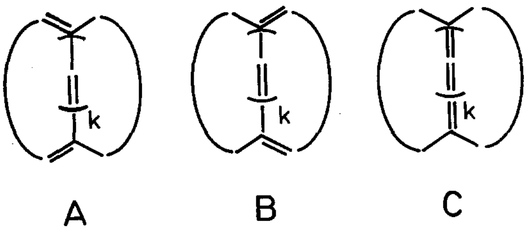
Fig. 4. Kekulé valence structures of tribenzo[18]annulene 9

The two largest resonance energies read as follows:

$$RE(A_1+A_2+A_3+A_4)=2R_1=1.738\text{ eV}>RE(A_1+A_2+A_3+A_4+B_1+B_2)$$
$$=(1/3)(5R_1+R_4+3R_5+3R_6+R_7)=1.464\text{ eV}.$$

Consequently, geometry 9a with one quinoid benzene ring is favoured over the fully delocalized structure 9b which should be reflected in physical properties such as ^{1}H NMR shifts.

Finally we will consider [*n*]annuleno[*n*]annulenes, see for example 4–6 in Fig. 1, which constitute type I systems. We can distinguish three Kekulé valence structures:



Here k can take values ≥ 0. Sets $\{A, B\}$ and $\{A, B, C\}$ lead to fully symmetric geometries where $\{A, B\}$ is characterized by multiple bond delocalization along the outer perimeter and multiple bond localization in the bridge (if $k>0$). Symmetry reduced geometries are derived from sets $\{A, C\}$ and $\{B, C\}$ with one annulene part fully delocalized and the other one with bond length alternation. The occurrence of pairs of adjacent *sp*-hybridized carbon atoms will necessarily lead to shorter bond lengths between such atoms with respect to the CC bond length in benzene even in the case of multiple bond length delocalization. The resonance energies for $[n]$annuleno$[n]$annulenes are given as follows:

$$
\begin{aligned}
n=4m+2: \quad & RE(A+B+C)=(4R_m+2R_{2m-k})/3 \\
& RE(A+C)=RE(B+C)=R_m \\
& RE(A+B)=R_{2m-k} \\
n=4m: \quad & RE(A+B+C)=(4Q_m+2R_{2m-k-1})/3 \\
& RE(A+C)=RE(B+C)=Q_m \\
& RE(A+B)=R_{2m-k-1}.
\end{aligned}
$$

For $n=4m+2$ it follows that $RE(A+B+C)>RE(A+C)=RE(B+C)>RE(A+B)$ and so a fully symmetric geometry derived from $\{A, B, C\}$ should be realized. This agrees with experimental and quantum chemical studies [19] of geometries and ^{1}H NMR shifts for several dehydro$[n]$annuleno$[n]$annulenes with $n=14$, 18 and $k=0$, 1. An example is provided by 4 where the formula given in Fig. 1 only roughly describes the actual bond lengths pattern.

For $n=4m$ the set $\{A, B\}$ exhibits a larger resonance energy than all other sets. For example we obtain $RE(A+B)=0.046$ eV, $RE(A+C)=RE(B+C)=-0.150$ eV, and $RE(A+B+C)=-0.136$ eV for 5 with $n=12$ and $k=1$.

This is in agreement with the results of our earlier work [19] which demonstrated that 5 is well represented by the formula given in Fig. 1. Contrary to 5 we obtain $RE(A+B)=0$ eV in the case of 6 with the same n but $k=0$. Thus the sets $\{A, B\}$, $\{A\}$, $\{B\}$, and $\{C\}$ are degenerate with respect to their resonance energies and the modified conjugated circuit approach only allows the exclusion of the geometries with reduced symmetry which are derived from sets $\{A, C\}$ and $\{B, C\}$. Actually more sophisticated calculations [19] yield a geometry corresponding to Kekulé valence structure C which has been displayed in Fig. 1 for 6.

6. Conclusion

In this paper we have applied the conjugated circuits model as a pencil-and-paper method in order to study the geometries of annelated $[n]$annulenes. This has been achieved by considering all possible sets $\{K_i, K_j, \ldots\}$ of Kekulé valence structures $\{K_i \mid i=1, \ldots, K\}$ of a given molecule. Since each set defines a geometry or a certain bond length pattern we have used the resonance energy obtained within the conjugated circuits model in order to determine the most stable structure. Using this concept it proved necessary to modify the conjugated circuits approach by means of a different interpretation of the terms R_i and Q_i. This modified model, which yields the same results as the original one if all Kekulé valence structures are utilized, has been successfully applied to different types of annelated annulenes.

We want to stress that our results are mainly of a qualitative nature. In order to obtain quantitative results for annulenoid systems with large perimeters one needs a better topological bond order than that provided by the Pauling bond character. Furthermore, part of the σ-compression energy would have to be included explicitly since the R_i, Q_i parameters have been fixed at their values obtained for benzenoid hydrocarbons where there is no strong bond length alternation. Investigations following these lines are under way [30].

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