Number of Kekulé Structures of Systems with Repeated Units

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Z. Naturforsch. **42 a**, 181 – 186 (1987); received November 10, 1986


Combinatorial formulas are derived for the number of Kekulé structures of conjugated (benzenoid) systems composed of repeated, mutually condensed units.

Introduction

Continuing our work on the enumeration of Kekulé structures of aromatic (benzenoid) hydrocarbons, especially of pericondensed systems (see [1−3] and the references cited therein), we have examined the system

$$C_N = A_0 : A_1 : A_2 : \ldots : A_{N-1} : A_N : A_\omega,$$

whose structure is depicted on the following diagram:
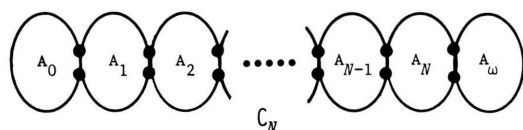
We can describe C_N as being composed of N mutually condensed units $A_1, A_2, \ldots, A_N$, to which two further terminal fragments A_0 and A_ω are attached. Needless to say that a great number of chemically important conjugated (benzenoid) hydrocarbons and/or systems for which the problem of the enumeration of Kekulé structures has been treated previously, are special cases of C_N. Pertinent examples will be given in the last section of this paper.

Although the main applications of our results are certainly to benzenoid molecules, the entire formalism developed in the present paper applies to non-benzenoids as well.

Definitions

Let G be a molecular graph [4]. Let further a_L, b_L, a_R and b_R be distinct vertices of G, such that a_L and b_L are adjacent, and a_R and b_R are adjacent. The edges connecting a_L with b_L and a_R with b_R will be denoted by e_L and e_R, respectively. Conventionally we say that e_L is the left edge and e_R the right edge of G, and we present G as
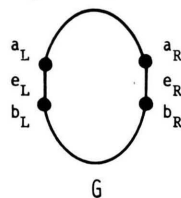
In the following we shall always assume that in the molecular graph considered there are a left and a right edge. This particularly applies to the subgraphs A_i; $i = 1, 2, \ldots, N$, from which C_N is composed. Exceptionally, in the terminal fragment A_0 only a right edge, whereas in the fragment A_ω only a left edge need to be distinguished.

Let P and Q be two arbitrary molecular graphs. In the following the symbol P:Q will stand for the graph obtained by identifying the right edge of P with the left edge of Q, so that the vertices a_R and b_R of P are identified with the vertices a_L and b_L of Q:
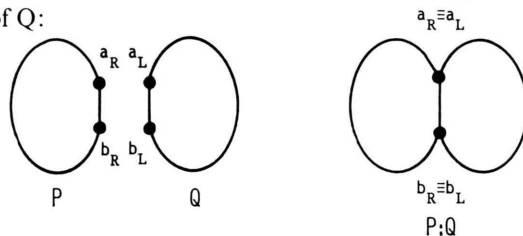
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Then the structure of C_N is expressed by

$$A_0:A_1:A_2:\ldots:A_N:A_\omega.$$

It is consistent to define $C_0 = A_0:A_\omega$.

The system which coincides with C_N except that it does not possess a right terminal fragment will be denoted B_N. Thus, $B_N = A_0:A_1:A_2:\ldots:A_N$, and, in particular, $B_0 = A_0$.

In the following we shall be especially interested in the case when all the units A_i ($i = 1, 2, \ldots, N$) are mutually isomorphic; $A_1 \simeq A_2 \simeq \ldots \simeq A_n$. When we write $A_i \simeq A_j$, we understand not only that A_i and A_j are isomorphic, but also that their vertices are labelled in the same manner.

In order to be able to express our results in a compact form we denote the subgraph obtained from G by deleting the left edge, $G - e_L$ by $'G$. Similarly, the shorthand notation for $G - e_R$ and $G - e_L - e_R$ is G' and $'G'$, respectively.
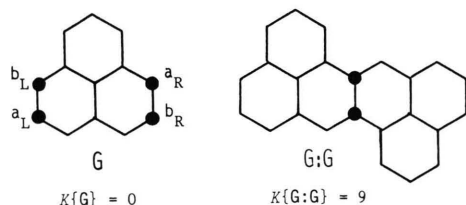
The number of Kekulé structures of the conjugated system whose molecular graph is G will be denoted by $K\{G\}$.

An Auxiliary Result

We demonstrate now that if either P or Q have an even number of vertices, then

$$K\{P:Q\} = K\{P\}\, K\{Q\} - K\{P'\}\, K\{'Q\}. \tag{1}$$

If both P and Q have an odd number of vertices, then (1) needs not to hold, as shown on the following example:

$$K\{G\} = 0 \qquad\qquad K\{G:G\} = 9$$

Of course, if $K\{G\} = 0$, then also $K\{'G\} = K\{G'\} = 0$.

If either P or Q, but not both have an odd number of vertices, then P:Q has an odd number of vertices, $K\{P:Q\} = 0$, and (1) holds in a trivial manner. Hence the only case of interest is when both P and Q have even numbers of vertices.

It has been shown elsewhere [5] that

$$\begin{aligned}
K\{P:Q\} = {}& K\{P\}\, K\{Q - a_L - b_L\} \\
&+ K\{P - a_R - b_R\}\, K\{Q\} \\
&- K\{P - a_R - b_R\}\, K\{Q - a_L - b_L\} \quad (2) \\
&+ K\{P - a_R\}\, K\{Q - b_L\} + K\{P - b_R\}\, K\{Q - a_L\},
\end{aligned}$$

which for P and Q being even systems reduces to

$$\begin{aligned}
K\{P:Q\} = {}& K\{P\}\, K\{Q - a_L - b_L\} \\
&+ K\{P - a_R - b_R\}\, K\{Q\} \\
&- K\{P - a_R - b_R\}\, K\{Q - a_L - b_L\}. \quad (3)
\end{aligned}$$

According to a well-known formula for the number of Kekulé structures [6],

$$K\{P\} = K\{P'\} + K\{P - a_R - b_R\}, \tag{4a}$$

$$K\{Q\} = K\{'Q\} + K\{Q - a_L - b_R\}. \tag{4b}$$

Substituting (4) back into (3) we obtain (1). All results given in the present paper are consequences of (1).

Here we point out an immediate corollary of (1). Let $(P:Q)^*$ be the graph obtained by identifying the vertices a_R and b_R of P, respectively, with the vertices b_L and a_L of Q:
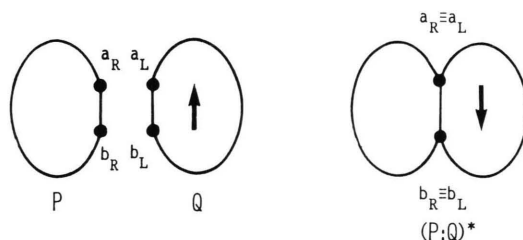
Then

$$K\{(P:Q)^*\} = K\{P:Q\} \tag{5}$$

provided either P or Q or both have an even number of vertices. One should observe that (3) and (4) remain the same if the symbols a_L and b_L exchange places. Therefore

$$K\{(P:Q)^*\} = K\{P\}\, K\{Q\} - K\{P'\}\, K\{'Q\}, \tag{6}$$

which together with (1) implies (5).

Number of Kekulé Structures of B_N

The system B_N has been defined as

$$B_N = A_0:A_1:A_2:\ldots:A_{N-1}:A_N.$$

Let, in addition,

$$B'_N = A_0:A_1:A_2:\ldots:A_{N-1}:A'_N.$$

Applying (1) to B_N and B'_N we immediately get

$$K\{B_N\} = K\{A_N\}\,K\{B_{N-1}\} - K\{'A_N\}\,K\{B'_{N-1}\}, \quad (7a)$$

$$K\{B'_N\} = K\{A'_N\}\,K\{B_{N-1}\} - K\{'A'_N\}\,K\{B'_{N-1}\}, \quad (7b)$$

or in matrix form

$$\begin{bmatrix} K\{B_N\} \\ K\{B'_N\} \end{bmatrix} = \mathbf{M}_N \begin{bmatrix} K\{B_{N-1}\} \\ K\{B'_{N-1}\} \end{bmatrix}, \quad (7c)$$

where the matrices $\mathbf{M}_i;\ i = 1, 2, \ldots, N$ are defined as

$$\mathbf{M}_i = \begin{bmatrix} K\{A_i\} & -K\{'A_i\} \\ K\{A'_i\} & -K\{'A'_i\} \end{bmatrix}. \quad (8)$$

Repeating the same argument additional $N-1$ times, we arrive at

$$\begin{bmatrix} K\{B_N\} \\ K\{B'_N\} \end{bmatrix} = \mathbf{M}_N\,\mathbf{M}_{N-1}\ldots\mathbf{M}_2\,\mathbf{M}_1 \begin{bmatrix} K\{A_0\} \\ K\{A'_0\} \end{bmatrix}. \quad (9)$$

Formula (9) has the following consequences. If at least one of the units from which B_N is composed, say A_j, is non-Kekuléan, then irrespective of the structure of $A_0, A_1, \ldots, A_{j-1}, A_{j+1}, \ldots, A_N$, the entire system B_N is non-Kekuléan. Indeed, if $K\{A_j\} = 0$ then also $K\{'A_j\} = K\{A'_j\} = K\{'A'_j\} = 0$ and thus $\mathbf{M}_j = 0$. Note that B_N is non-Kekuléan also if A_0 is non-Kekuléan.

Equations (7) present a system of coupled recurrence relations. They can be easily decoupled into

$$\alpha_N\,K\{B_N\} + \beta_N\,K\{B_{N-1}\} + \gamma_N\,K\{B_{N-2}\} = 0;\quad N \geq 2, \quad (10a)$$

$$\alpha_N\,K\{B'_N\} + \beta_N\,K\{B'_{N-1}\} + \gamma_N\,K\{B'_{N-2}\} = 0;\quad N \geq 2, \quad (10b)$$

where

$$\alpha_N = K\{'A_{N-1}\}, \quad (11a)$$

$$\beta_N = K\{'A_N\}\,K\{'A'_{N-1}\} - K\{A_N\}\,K\{'A_{N-1}\}, \quad (11b)$$

$$\gamma_N = K\{'A_N\}\,\det \mathbf{M}_{N-1}. \quad (11c)$$

If all the subgraphs A_i, $i = 1, 2, \ldots, N$ are mutually isomorphic, then a significant simplification of the above relations occurs. For $A_i \simeq A$, $i = 1, 2, \ldots, N$, we have

$$\begin{bmatrix} K\{B_N\} \\ K\{B'_N\} \end{bmatrix} = \begin{bmatrix} K\{A\} & -K\{'A\} \\ K\{A'\} & -K\{'A'\} \end{bmatrix}^N \begin{bmatrix} K\{A_0\} \\ K\{A'_0\} \end{bmatrix} \quad (12)$$

and

$$K\{B_N\} = \beta\,K\{B_{N-1}\} + \gamma\,K\{B_{N-2}\};\quad N \geq 2, \quad (13a)$$

$$K\{B'_N\} = \beta\,K\{B'_{N-2}\} + \gamma\,K\{B'_{N-2}\};\quad N \geq 2, \quad (13b)$$

where

$$\beta = K\{A\} - K\{'A'\}, \quad (14a)$$

$$\gamma = K\{A\}\,K\{'A'\} - K\{'A\}\,K\{A'\}. \quad (14b)$$

Using standard techniques of the theory of difference equations [7], the explicit general expressions for $K\{B_N\}$ can be calculated from (13a). We shall not pursue this computation any further because the explicit formula for $K\{B_N\}$ has a very complicated algebraic form; note that $K\{B_N\}$ is a function of N, $K\{A\}$, $K\{'A\}$, $K\{A'\}$, $K\{'A'\}$, $K\{A_0\}$ and $K\{A'_0\}$. It seems quite improbable that such a result ever will be needed in practical applications.

If, however, there is no terminal fragment in B_N, which formally corresponds to the choice $K\{A_0\} = 1$, $K\{A'_0\} = 0$, then we obtain a somewhat simpler expression:

$$K\{B_N\} = (2^{N+1}\,R)^{-1}\,[(K\{A\} + K\{'A'\} + R)$$
$$\cdot (K\{A\} - K\{'A'\} + R)^N - (K\{A\} + K\{'A'\} - R)$$
$$\cdot (K\{A\} - K\{'A'\} - R)^N], \quad (15)$$

where

$$R = [(K\{A\} + K\{'A'\})^2 - 4\,K\{'A\}\,K\{A'\}]^{\frac{1}{2}}. \quad (16)$$

Number of Kekulé Structures of C_N

In the preceding section we pointed out the (not necessarily obvious) fact that both $K\{B_N\}$ and $K\{B'_N\}$ conform to the same recurrence relation (10). This has the immediate consequence that also $K\{C_N\}$ satisfies this relation, viz.

$$\alpha_N\,K\{C_N\} + \beta_N\,K\{C_{N-1}\} + \gamma_N\,K\{C_{N-2}\} = 0;\quad N \geq 2. \quad (10c)$$

In order to see that (10c) holds, observe that $C_N = B_N:A_\omega$ and apply (1). Then

$$K\{C_N\} = K\{A_\omega\}\,K\{B_N\} - K\{'A_\omega\}\,K\{B'_N\}. \quad (17a)$$

Equation (10c) is now obtained by substituting (10a) and (8b) into (17a) and by taking into account that

$$K\{A_\omega\}\,K\{B_{N-1}\} - K\{'A_\omega\}\,K\{B'_{N-1}\} = K\{C_{N-1}\}, \quad (17b)$$

$$K\{A_\omega\}\,K\{B_{N-2}\} - K\{'A_\omega\}\,K\{B'_{N-2}\} = K\{C_{N-2}\}. \quad (17c)$$

If $A_i \simeq A$ for all $i = 1, 2, \ldots, N$, then it immediately follows that the recurrence relation for $K\{C_N\}$ also is of the form (13), namely

$$K\{C_N\} = \beta K\{C_{N-1}\} + \gamma K\{C_{N-2}\}; \quad N \geqq 2. \quad (13c)$$

From (13c) an explicit formula for $K\{C_N\}$ could be obtained, but because of already mentioned reasons we avoid this issue.

We have reached the conclusion that the nature of the terminal fragments A_0 and A_ω does not influence the form of the recurrence relation for $K\{C_N\}$. In particular, (10a) and (10b) are special cases of (10c), as well as (13a) and (13b) are special cases of (13c). The numerical value of $K\{C_N\}$ depends, however, on A_0 and A_ω.

It can be shown that a necessary and sufficient condition for C_N to be Kekuléan (i.e. $K\{C_N\} > 0$) is that all units $A_0, A_1, A_2, \ldots, A_N, A_\omega$ are Kekuléan. As we already have pointed out, this is not true if at least one of the A_i's has odd number of vertices.
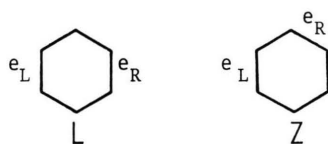
Examples

Two Simple Cases

Consider first the case when C_N contains a linear polyacene fragment [5]. This occurs when $A_i \simeq L$ for all $i = 1, 2, \ldots, N$. Since $K\{L\} = 2$, $K\{'L\} = K\{L'\} = 1$, $K\{'L'\} = 0$ we have $\beta = 2$ and $\gamma = -1$, and (13c) reduces to

$$K\{C_N\} = 2K\{C_{N-1}\} - K\{C_{N-2}\}. \quad (18)$$

It is referred to the below illustration.

The recurrence relation (18) for the number of Kekulé structures of systems containing a linear polyacene fragment has not been observed in [2, 5]. From (18) it immediately follows that $K\{C_N\}$ is a linear function of N, which is a previously known result [5].

The second case is when C_N contains a zigzag polyacene fragment. This means that $A_i \simeq Z$ for all i, and then $K\{Z\} = 2$, $K\{'Z\} = K\{Z'\} = K\{'Z'\} = 1$, $\beta = 1$, $\gamma = 1$, and we reach the previously known [2] Fibonacci-type recurrence formula

$$K\{C_N\} = K\{C_{N-1}\} + K\{C_{N-2}\}. \quad (19)$$

More Advanced Case

As a third, somewhat less elementary example we consider "parallelograms on a string", whose repeated units A_i are all mutually isomorphic and given as
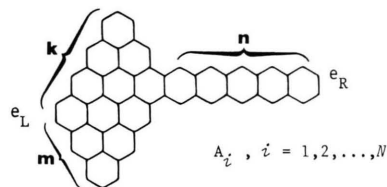

These systems have one terminal fragment A_0, which is the linear polyacene with n hexagons, $L(n)$. The repeated units A_i can be understood as being fused of a parallelogram-shaped benzenoid system $L(m, k)$ and a linear polyacene $L(n)$, i.e. $A_i = L(m, k) : L(n)$:
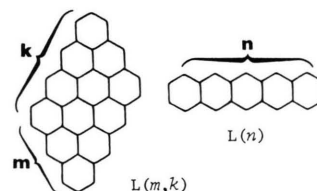
"Parallelograms on a string" containing N repeated units will be denoted by B_N. In addition to N, their structure depends on the parameters n, m and k.

As a special case, the choice $n = 1$, $m = 2$ and $k = 2$ corresponds to the class of "pyrenes on a string". It is a celebrated example of all-benzenoid systems [8, 9]. For $N = 3$ we have the following representative of these benzenoid molecules:
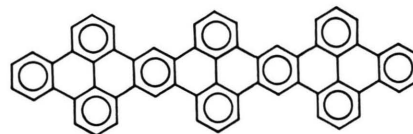
It has been referred specifically to members of this class by several authors [10−13]. One of these papers [10] implies the recurrence relation for the number of Kekulé structures, viz.

$$K\{B_N\} = 10K\{B_{N-1}\} - K\{B_{N-2}\}; \quad N \geqq 2. \quad (20)$$

The explicit combinatorial formula for $K\{B_N\}$ (when $n = 1$, $m = 2$, $k = 2$) has also been reported [14]:

$$K\{B_N\} = \tfrac{1}{2}6^{-\frac{1}{2}}[(5 + 2 \cdot 6^{\frac{1}{2}})^{N+1} - (5 - 2 \cdot 6^{\frac{1}{2}})^{N+1}]. \quad (21)$$

Let us now return to the general case, namely when the parameters n, m and k have arbitrary values. It is well known [15] that

$$K\{L(m, k)\} = \binom{m+k}{k}; \quad K\{L(n)\} = n+1. \quad (22)$$

Knowing that $A_i = L(m, k): L(n)$ and applying (1) we then easily obtain

$$K\{A_i\} = (n+1)\binom{m+k}{k} - n, \quad (23a)$$

$$K\{'A_i\} = n+1, \quad (23b)$$

$$K\{A_i'\} = n\binom{m+k}{k} - (n-1), \quad (23c)$$

$$K\{'A_i'\} = n, \quad (23d)$$

from which $\beta = (n+1)\binom{m+k}{k} - 2n$, $\gamma = -1$, and thus (10a) becomes

$$K\{B_N\} = (r+2) K\{B_{N-1}\} - K\{B_{N-2}\}; \quad N \geq 2, \quad (24)$$

where

$$r = (n+1)\left[\binom{k+m}{k} - 2\right]. \quad (25)$$

Using the initial conditions

$$K\{B_0\} = n+1, \quad K\{B_1\} = (n+1)(r+2) \quad (26)$$

we obtain after a lengthy calculation [7]

$$K\{B_N\} = (n+1) r^{-\frac{1}{2}}(r+4)^{-\frac{1}{2}} \{[\tfrac{1}{2}(r+2+r^{\frac{1}{2}}(r+4)^{\frac{1}{2}})]^{N+1}$$
$$- [\tfrac{1}{2}(r+2-r^{\frac{1}{2}}(r+4)^{\frac{1}{2}})]^{N+1}\}. \quad (27)$$

In particular, for pyrene $L(2, 2)$ one has $r = 4(n+1)$ and consequently

$$K\{B_N\} = 2(2n+3) K\{B_{N-1}\} - K\{B_{N-2}\}; \quad N \geq 2 \quad (28)$$

with

$$K\{B_0\} = n+1, \quad K\{B_1\} = 2(n+1)(2n+3) \quad (29)$$

and

$$K\{B_N\} = \tfrac{1}{4}(n+1)^{\frac{1}{2}}(n+2)^{-\frac{1}{2}}$$
$$\cdot \{[2n+3+2(n+1)^{\frac{1}{2}}(n+2)^{\frac{1}{2}}]^{N+1}$$
$$- [2n+3-2(n+1)^{\frac{1}{2}}(n+2)^{\frac{1}{2}}]^{N+1}\}. \quad (30)$$

Equations (20) and (21) are special cases for $n = 1$ of (28) and (30), respectively.

For anthanthrene $L(2, 3)$ one has $r = 8(n+1)$ and

$$K\{B_N\} = 2(4n+5) K\{B_{N-1}\} - K\{B_{N-2}\}; \quad N \geq 2 \quad (31)$$

with

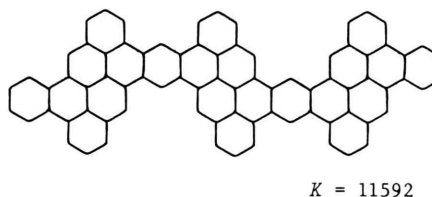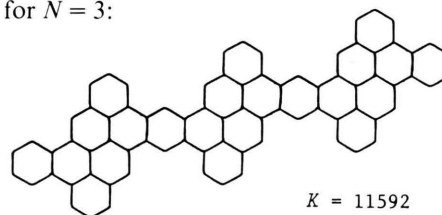$$K\{B_0\} = n+1, \quad K\{B_1\} = 2(n+1)(4n+5) \quad (32)$$

and

$$K\{B_N\} = \tfrac{1}{4}(n+1)^{\frac{1}{2}}(4n+6)^{-\frac{1}{2}}$$
$$\cdot \{[4n+5+8^{\frac{1}{2}}(n+1)^{\frac{1}{2}}(2n+3)^{\frac{1}{2}}]^{N+1}$$
$$- [4n+5-8^{\frac{1}{2}}(n+1)^{\frac{1}{2}}(2n+3)^{\frac{1}{2}}]^{N+1}\}, \quad (33)$$

Especially, for $n = 1$:

$$K\{[L(1): L(2, 3)]^N: L(1)\}$$
$$= \tfrac{1}{4} 5^{-\frac{1}{2}}[(9+4\cdot 5^{\frac{1}{2}})^{N+1} - (9-4\cdot 5^{\frac{1}{2}})^{N+1}]. \quad (34)$$

This case of anthanthrene with $n = 1$ is illustrated below for $N = 3$:

$$K = 11592$$

$$K = 11592$$

The fact that the above two isomers have equal number of Kekulé structures is a consequence of (5). This feature is well known in connection with the kinks (angular annelation) in single-chain benzenoids [15−18]. Such two variants of a benzenoid chain have been referred to as isoarithmic [16]. The above example shows that isoarithmicity is just a particular manifestation of a more general topological phenomenon. In the above examined case, namely of the parallelograms on a (linear) string, isoarithmic structures occur whenever $k \neq m$.

Conclusion

The present paper gives a contribution to the enumeration of Kekulé structures, which has

attained a considerable interest during the last years. It is sufficient to document this fact by the numerous relevant papers which have appeared only in 1986 [3, 19–33]. The chemical importance of benzenoids with repeated units among other large or very large benzenoid systems seems not necessary to be documented specifically. The polymers with an infinite number of units come into this category, but we have not attempted to extend our results to $N \to \infty$. The interesting studies of enumeration of Kekulé structures in polymers, which have appeared recently [19, 25], do not interfere with our results.

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