Algorithms for the Count of Linearly Independent and Minimal Conjugated Circuits in Benzenoid Hydrocarbons

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Available forms of the minimal conjugated circuits for any ring *s* in a Kekule structure are studied, and appropriate algorithms are found to adapt the different cases. On the basis of these algorithms, a direct method for the calculation of the summation expression of linearly independent and minimal conjugated circuits in benzenoid hydrocarbons is proposed, and it is realized within software on a PC.

1. INTRODUCTION

The concept of conjugated circuit (CC) in polycyclic conjugated systems was first introduced by Randic.[1−3] According to the conjugated-circuit model, the resonance energies of conjugated benzenoid hydrocarbons (BHs) can be expressed as the sum of contributions arising from linearly independent conjugated circuits. [4−7] The sets of linearly independent conjugated circuits of a Kekule structure in a benzenoid hydrocarbon are not necessarily unique; hence, a rigorous definition of linearly independent and minimal (LM) conjugated circuits in benzenoid hydrocarbons is required.[8]

Definition: A set $\boldsymbol{S}$ of linearly independent and minimal conjugated circuits of a Kekule structure K_i of a benzenoid hydrocarbon $\boldsymbol{B}$ consists of a maximum number of linearly independent circuits of $\boldsymbol{B}$ in which every circuit is a conjugated circuit of K_i and has the minimum total length.

It is well-known that the length of any CC in a benzenoid hydrocarbon can be represented as $4n + 2$, where n is a positive integer.[5] We denote a circuit of size $4n + 2$ in $\boldsymbol{S}$ by R_n and the summation expression by $R(K_i) = \sum_{R_j \in S} R_j = \sum_{n=1,2,...} r_n(K_i)R_n$, where $r_n(K_i)$ is the number of the circuits of size $4n + 2$ in S. The summation expression $R(K_i)$ is uniquely determined; hence, the summation expression of all sets of LM-conjugated circuits of all Kekule structures in $\boldsymbol{B}$ is also unique and can be denoted by $R(\boldsymbol{B}) = R = \sum_{K_i} R(K_i) = \sum_{n=1,2...} r_n R_n$, where $r_n = \sum_{K_i} r_n(K_i)$. We say that $R(\boldsymbol{B})$ is the summation expression of LM-conjugated circuits of $\boldsymbol{B}$, or simply the LMCC expression of $\boldsymbol{B}$. $R(\boldsymbol{B})$ may also be represented by a sequence of numbers (r_1, r_2, ..., r_n, ...), called the LMC code of B.

The LM-conjugated circuits of benzenoid hydrocarbons plays a central role in the conjugated-circuit model, as the resonance energy RE($\boldsymbol{B}$) of benzenoid hydrocarbon $\boldsymbol{B}$ is simply equal to RE($\boldsymbol{B}$) = $R(\boldsymbol{B})$/K($\boldsymbol{B}$), where K(**B**) is the number of Kekule structures of **B** and has been resolved by various methods for a long time. In recent years, Guo and Randic have gotten some important results in identifying LMCC and calculating $R(\boldsymbol{B})$.[8,9] For certain classes of BHs, the recursive relations in their calculations have been pointed out,[8] and an analytical expression for the count of LMCC of any BH have also been reported.[9]

With the aim of realizing an automatic calculation for $R(\boldsymbol{B})$ on PC, we will use the basis of the above works[8] and the old scheme proposed by Randic:[4] (1) generate all the Kekule structures of a benzenoid hydrocarbon; (2) find out a set of LMCCs for every Kekule structure (or calculate its LMC code); (3) make summation. Although the performance of calculating by hands for steps 1 and 2 will become tedious when the sizes of molecules increase, the enumeration method is still suitable to the machines. Some convenient methods for enumerating the Kekule structures on a PC have been reported by us.[10] In this paper, we will make further analysis based on the results revealed by Guo and Randic,[8] and propose the algorithms to perform step 2 more efficiently. With the power of a modern PC and for a reasonable size, the calculating time using this method is acceptable in practice.

On the basis of the algorithms reported in this paper and in our early works,[10,11] an application software has been developed with VISUAL BASIC. The benzenoid hydrocarbons under consideration can be input directly to the system by the mouse under a graphic interface. Several calculations, such as those for the enumeration of Kekule structures, the spectrums, the Clar covering polynomials, and the summation expressions, etc., can be performed efficiently. As a practice, we have used it to calculate the molecular resonance energy for the families I−X of benzenoid hydrocarbons mentioned by Randic.[4] The number of rings concerned in each family is augmented to 30−40, and the computing times on a 586-PC are still acceptable. (In fact, the computing time depends largely on the number of Kekule structures of the BH concerned. For the BHs having small numbers of Kekule strucures, such as 40 rings of families I−VI, the calculations finish in a few minutes. But for the BHs with huge numbers of Kekule structures, such as 30 rings of the triphenylene−dibenzpyrene family (IX), 30 rings of the pyrene−benzoperylene family (X), and 31 rings of the pyrene−peropyrene family (VIII), it takes more or less than 20 h each on a PC-AMD/PR-133.)

2. PROPERTIES AND FORMS OF MINIMAL CONJUGATED CIRCUITS

2.1. Concepts and Basic Theorems. A benzenoid hydrocarbon is a two-connected-plane graph with each of its

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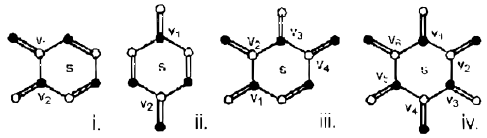


Figure 1. Distribution of double bonds incident with the vertexes of the ring ***s***.

interior faces bounded by a regular hexagon. A connected subgraph of a BH is said to be a BH fragment (BHF). A two-connected BHF is said to be a generalized BH (GBH). ***B*** denotes a BH or GBH. ***B*** is said to be normal if ***B*** contains no fixed bond (i.e. bond appearing as a double or a single bond in every Kekule structure of ***B***); otherwise ***B*** is said to be essentially disconnected. A normal component $\boldsymbol{B}_i$ of ***B*** is a maximal subgraph of ***B*** with no fixed bond (possibly, $\boldsymbol{B}_i = \boldsymbol{B}$). The total of all the normal components of ***B*** is denoted by $\boldsymbol{B}^*$. The boundary of an interior face of a BH or BHF ***B*** is called a ring of ***B***.

s denotes a ring of a BH ***B***, and K_i, a Kekule structure of ***B***. A conjugated circuit ***C*** of K_i (simply, a K_i-conjugated circuit or K_i-CC) is said to be a minimal conjugated circuit of the ring ***s*** (a ***s***-K_i-MCC, or simply a ***s***-MCC when there's no confusion) if the interior of ***C*** contains the interior of ***s*** and ***C*** has the minimum length. Apparently, for a Kekule structure K_i, the minimal conjugated circuit of ring ***s*** may be not unique, but they have all the same length.

Since ***B*** is bipartite, we can color the vertexes of ***B*** black and white so that any two adjacent vertexes have different colors. For a circuit ***C*** in ***B***, B[***C***] denotes the maximal subgraph of ***B*** bounded by ***C***. A K_i-alternating path in ***B*** is a path which is compounded alternatively with double and single bonds of K_i, and it will be denoted as AP-D if it starts and ends both on double bonds.

A necessary and sufficient condition for a set of K_i-conjugated circuits of a benzenoid hydrocarbon ***B*** to be a set of LM-conjugated circuits is reported in Theorem 1:[8]

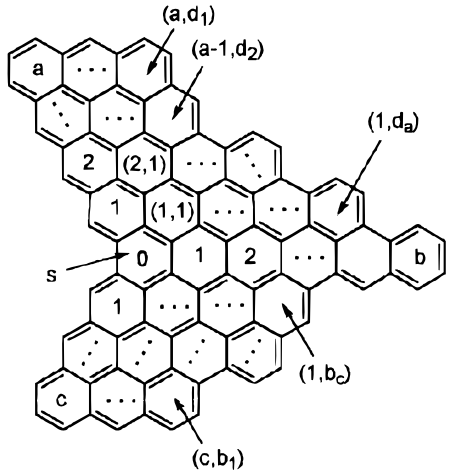
Theorem 1. Let K_i be a Kekule structure of a BH ***B***. A set $\boldsymbol{S} = \{\boldsymbol{C}_1, \boldsymbol{C}_2, \boldsymbol{C}_3, ..., \boldsymbol{C}_t\}$ of K_i-conjugated circuits of ***B*** is a set of LM-conjugated circuits of K_i if and only if for any ring $\boldsymbol{s}_j$ in all normal components $\boldsymbol{B}^*$ of ***B***, there is exactly one circuit $\boldsymbol{C}_j$ in ***S*** such that $\boldsymbol{C}_j$ is a minimal conjugated circuits of $\boldsymbol{s}_j$.

On the basis of this theorem, we are sure that if ***B*** is a normal BH; then there is at least one ***s***-MCC for any ring ***s*** of ***B***. Furthermore, there is another theorem (below) which describes the available forms of a ***s***-MCC.

For any ring (hexagon) ***s*** of ***B***, let K_i be a Kekule structure of ***B*** and ***C*** a ***s***-K_i-MCC; we have $\boldsymbol{C} \cap \boldsymbol{s} \neq \varnothing$. In fact, if ***s*** is not its own K_i-MCC, then there are four cases for the distribution of double bonds incident with the vertexes of the ring ***s*** (cf. Figure 1). On the basis of this result, the form of the ***s***-MCC is well-defined by the following basic theorem:[8]

Theorem 2. Let K_i be a Kekule structure of a benzenoid hydrocarbon ***B*** and ***C*** a minimal K_i-conjugated circuit of a ring ***s*** of ***B***. Then B[***C***] is one of the BHs shown in Figure 2, and the K_i-double bonds in B[***C***] are uniquely determined.

2.2. Available Forms for *s*-MCC. On the basis of the basic theorem above, we can discuss all the possible forms of ***s***-MCC of any fixed Kekule structure K_i (cf. Figure 3).We perform this analysis by varying the parameters a, b, c, b_c, and d_a:



$$a, b, c \geq 0$$
$$0 \leq b_1 \leq b_2 \leq \ldots \leq b_c \leq b$$
$$0 \leq d_1 \leq d_2 \leq \ldots \leq d_a \leq b$$

Figure 2. Construction of a ***s***-MCC.

$$a = b = c = 0 \quad \text{(trivial, and } \boldsymbol{s} \text{ is its own MCC)} \quad \text{(i)}$$

$$a = b = 0, \quad c > 0; \quad \text{or} \quad a = c = 0, \quad b > 0 \quad \text{or} \quad b = c = 0, \quad a > 0 \quad \text{(ii)}$$

$$a = 0, \quad b, c > 0, \quad b_c > 0 \quad \text{or} \quad c = 0, \quad a, b > 0, \quad d_a > 0 \quad \text{(iii)}$$

$$b = 0, \quad a, c > 0 \quad \text{or} \quad a = 0, \quad b, c > 0, \quad b_c = 0 \quad \text{or} \quad c = 0, \quad a, b > 0, \quad d_a = 0 \quad \text{(iv)}$$

$$a, b, c, b_c, d_a > 0 \quad \text{(v)}$$

$$a, b, c > 0, \quad b_c = 0, \quad d_a > 0 \quad \text{or} \quad a, b, c > 0, \quad b_c > 0, \quad d_a = 0 \quad \text{(vi)}$$

$$a, b, c > 0, \quad b_c = d_a = 0 \quad \text{(vii)}$$

Figure 4 shows all the symmetry nonequivalent Kekule structures of coronene, in which the number marked in each ring represents its corresponding case in Figure 3. We denote the Kekule structures in Figure 4 by K_1, K_2, ..., K_6, respectively. By observation, $R(K_1) = R_1 + 3R_2 + 3R_3$, $R(K_2) = 4R_1 + 3R_3$, $R(K_3) = 3R_1 + 3R_2 + R_3$, $R(K_4) = 2R_1 + 4R_2 + R_3$, $R(K_5) = 4R_1 + 2R_2 + R_3$, and $R(K_6) = 6R_1 + R_4$. Then, on considering the symmetry, we have $R(\boldsymbol{B}) = 64R_1 + 48R_2 + 27R_3 + R_4$.

The discussion above gives us an idea on constructing the ***s***-MCC. In fact, the ***s***-MCC is composed of some edge(s) of ***s*** and some minimal K_i-alternating path(s) between two vertexes of ***s***. In the following scheme, we will first find the relevant alternating paths by the method "labeling forward" and "tracing backward". Then, with the suitable choice of the edge(s) of ***s***, we can construct a ***s***-MCC needed.

3. FINDING ITS MCC FOR ANY GIVEN RING *S* UNDER A K_i

3.1. Finding the minimal K_i-alternating paths between two vertexes of *B*. ***B*** denotes a normal component of a BH,

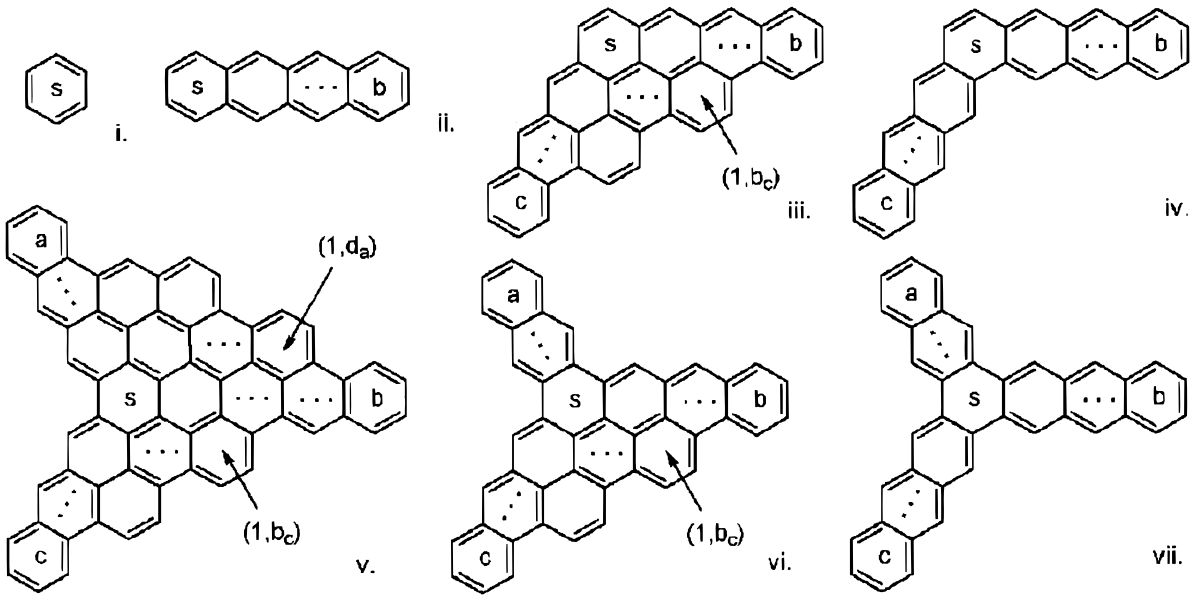


Figure 3. Available forms of **s**-MCC.

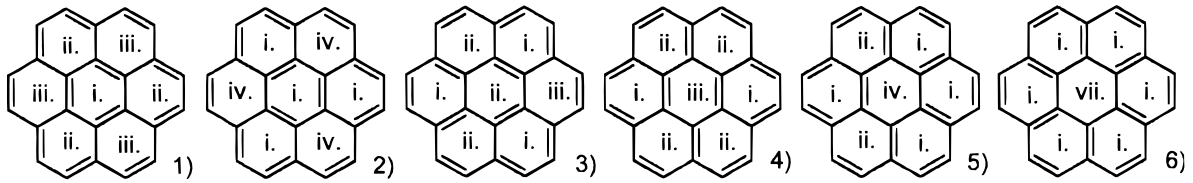


Figure 4. Symmetry nonequivalent Kekule structures of coronene.

and *A*, *B* are two arbitrary vertexes of ***B***; the following algorithm will find out the minimal alternated path *P*(*AB*)s which start from *A* with a double bond and also end by a double bond to *B*. In the following, L denotes the length of *P*(*AB*) and *F* is an indicator of the existence of *P*(*AB*).

Algorithm 1. Part 1: "Labeling forward".

(1) Mark the vertex *A* as 0 and all the other vertexes of ***B*** as -1; $i := 0$, $L := 0$, $F := 0$.

(2) Find out all the vertexes, which are marked as -1 and incident by a double bond with the vertexes labeled *i*, and then remark these vertexes as $i + 1$; if there is no such vertex, then goto 7.

(3) If the label of vertex *B* is not -1, then $F := 1$, $L := i + 1$, goto 7.

(4) $i := i + 1$.

(5) Find out all the vertexes, which are marked as -1 and incident by a single bond with the vertexes labeled *i*, and then remark these vertexes as $i + 1$; if there is no such vertex, then goto 7.

(6) $i := i + 1$; goto 2.

(7) Stop.

At the end of this procedure, *F* takes a value of either 0 or 1. If $F = 1$, then there is at least one *P*(*AB*) (obviously, all the *P*(*AB*)s have the same length); otherwise, such *P*(*AB*) does not exist, and then algorithm 1 terminates at this step. Furthermore, in the case $F = 1$, we should use the following procedure to get explicitly one or all of the *P*(*AB*)s according to the vertexes labeled and the maximal value of the label (i.e. *L*, which must be odd).

Part 2: "Tracing Backward". This stage can be distinguished into two cases: (a) finding out one *P*(*AB*) and (b) finding out all the *P*(*AB*)s. Case a is much simpler than case b. For the algorithms which will be proposed in the following section, we will use one of these two cases.

Case a: Let *V*(*j*) denote the currently tracing vertex (the vertexes of *P*(*AB*) will be {*V*(*j*), $j = L, L$-1, ..., 1}), and ***M*** denotes the set of edges which constitute *P*(*AB*).

(1) $j := 1$, $V(0) := B$ (i.e. *V*(0) takes the order number of vertex *B*).

(2) Find out an edge *e* which links vertex $V(j-1)$ and a vertex labeled $L - j$; take the later vertex as *V*(*j*); $\boldsymbol{M} := \boldsymbol{M} \cup e$:

(3) If $j < L$, then $j := j + 1$; goto 2.

(4) Stop.

Case b: Let n_path denote the number of *P*(*AB*)s found, ***M***(*i*) be the set of the edges which constitute the *i*th *P*(*AB*), and *V*(*j*,*n*) denote the order number of the *n*th currently tracing vertex with label $L - j$.

(1) $j := 1$, n_path: $= 1$, $\boldsymbol{M}(1) := \varnothing$, $V(1,1) := B$.

(2) $k := 1$.

(3) Find out an edge *e* which links vertex $V(j-1,k)$ and a vertex labeled as $L - j$; take the later vertex as *V*(*j*,*k*); $\boldsymbol{M}(k) := \boldsymbol{M}(k) \cup e$.

(4) If *j* is odd, then goto 6.

(5) If there is an edge *f* which links vertex $V(j-1,k)$ and another vertex also labeled as $L - j$, then n_path: $=$ n_path $+ 1$, ***M***(n_path): $= (\boldsymbol{M}(k) \backslash e) \cup f$ and denote the later vertex as *V*(*j*,n_path).

(6) If $k <$ n_path, then $k := k + 1$; goto 3.

(7) If $j < L$, then $j := j + 1$, goto 2.

(8) Stop.

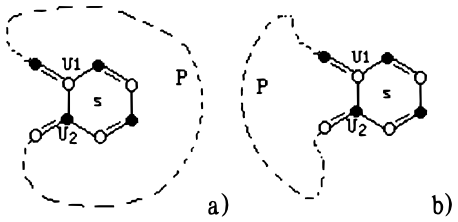


Figure 5. Case 1.

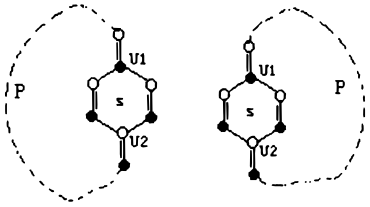
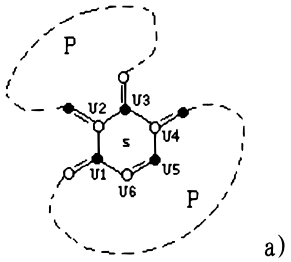


Figure 6. Case 2.



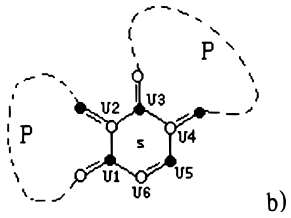
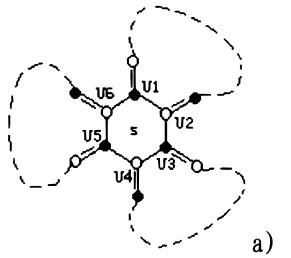


Figure 7. Case 3.



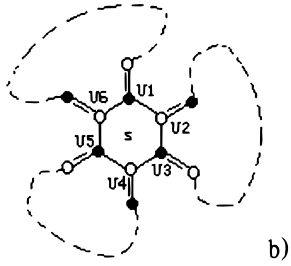


Figure 8. Case 4.

3.2. Construction of the *s*-MCC. On the basis of the analysis of section 2.2, the ***s***-MCC is composed of some edge(s) of ***s*** and some minimal K_i-alternated path(s) between two vertexes of ***s***, each of which starts and ends with double bonds (in Figure 5−8, *P* represents such alternating path-(s)). Effectively, beside the case in which ***s*** has three double bonds, we can characterize them by the following four cases depending on the position of the double bond(s) of ***s***.

Case 1: Ring ***s*** has two double bonds which are not parallel, corresponding to (ii) and (v) of section 2.2 (cf. Figure 3). They can also be simplified as Figure 5, in which the difference between a and b is whether ***s*** is within the interior of the circuit $P \cup v_1v_2$.

In this case, we first find some minimal AP−D *P* between v_1 and v_2 and denote its length by *L*. If the conjugated circuit compounded of *P* and v_1v_2 (denoted as $\boldsymbol{C}_1$) has ***s*** in its interior, then this CC is obviously a ***s***-MCC (with length $L + 1$); otherwise, if there is no such *P*, then the CC compounded of *P* (any minimal AP−D between v_1 and v_2 without being arbitrary) and the rest remaining five edges of ***s*** (denoted as $\boldsymbol{C}_2$) is surely a ***s***-MCC.

In fact, if ***s*** is not in the interior of $\boldsymbol{C}_1$, then ***s*** must be in the interior of $\boldsymbol{C}_2$. Suppose that $\boldsymbol{C}_3$ is a ***s***-MCC which has shorter length than $\boldsymbol{C}_2$. From Figure 5, $\boldsymbol{C}_3$ must be compounded of v_1v_2 and an another AP−D between v_1 and v_2. Since the length of $\boldsymbol{C}_2$ is $L + 5$ and $\boldsymbol{C}_3$ has a length greater than $L + 1$, the length of $\boldsymbol{C}_3$ must be $L + 3$. On the other hand, the length of all the CCs in any BH can be represented as $4n + 2$, where *n* is a positive integer. Thus, we have $L + 5 \equiv L + 3 \pmod 4$, which is impossible.

Furthermore, by observation, ring ***s*** being in the interior of $\boldsymbol{C}_1$ is corresponding to case v of Figure 3, and ***s*** being outside of $\boldsymbol{C}_1$ is corresponding to case (ii) of Figure 3. They may be well distinguished by the fact that the vertexes of *P* are positioned to both sides or all in one side of the straight line v_1v_2. For this case, we use the following.

Algorithm 2:

(1) Find out all the minimal AP−Ds $\{P(i), i = 1, 2, ...\}$ between v_1 and v_2 by using algorithm 1; denote its length as *L*.

(2) If $\exists\, i$ such that the vertexes of $P(i)$ are at both sides of the straight line v_1v_2, then $\boldsymbol{C}: = P(i) \cup v_1v_2$ is a ***s***-MCC with its length equal to $L + 1$; goto 4.

(3) Take the CC compounded of $P(i)$ (the last minimal AP−D between v_1 and v_2 tested in step 2) and the remaining five edges of ***s*** as $\boldsymbol{C}$; $\boldsymbol{C}$ is a ***s***-MCC with length $L + 5$.

(4) Stop.

Case 2: Ring ***s*** has two double bonds which are parallel, corresponding to (iii) of section 2.2 (cf. Figure 3).

For this case, it is rather easy to get the length of a ***s***-MCC. And for the application below, it's not necessary to find out the right form of the ***s***-MCC, but for completeness we will still make it clear (cf. Figure 6).

Algorithm 3:

(1) Find out a minimal AP−D *P* between v_1 and v_2 by using algorithm 1; denote its length as L.

(2) Take as $\boldsymbol{C}$ the CC compounded of *P* and the three edges of ***s*** which are all on the other side of the straight line v_1v_2 with respect to the position of *P*; $\boldsymbol{C}$ is a ***s***-MCC with length $L + 3$.

(3) Stop.

Case 3: Ring ***s*** has only one double bond, corresponding to (iv) and (vi) of section 2.2 (cf. Figure 3). They can also be simplified as Figure 7. The difference between a and b is similar to those in case 1.

By observation, if there is a AP−D $P(v_1v_2)$ which is minimal between v_1 and v_2, and which passes by vertexes v_3 and v_4, then $\boldsymbol{C}_1 = P(v_1v_2) \cup v_1v_2$ will be a CC with $\boldsymbol{s}$ in its interior. Similarly, if there is a AP−D $P(v_3v_4)$ which is minimal between v_3 and v_4, and which passes by vertexes v_1 and v_2, then $\boldsymbol{C}_2 = P(v_3v_4) \cup v_3v_4$ will also be a CC with $\boldsymbol{s}$ in its interior. Let the lengths of $\boldsymbol{C}_1$ and $\boldsymbol{C}_2$ be respectively L_1 and L_2; then $L_1 = L_2$. In fact, without loss of generality, we can suppose that $L_1 > L_2$, then $\boldsymbol{C}_2 \backslash v_1v_2$ is obviously a AP−D between v_1 and v_2, and with its length $L_2 - 1$. This is contradictory with the fact that $P(v_1v_2)$, with its length $L_1 - 1$, is a minimal AP−D between v_1 and v_2. Thus, we know that both $\boldsymbol{C}_1$ and $\boldsymbol{C}_2$ are $\boldsymbol{s}$-MCCs, and we can take any one of them as we like.

If all of the minimal AP−Ds between v_1 and v_2 do not pass by vertexes v_3 and v_4, and all of the minimal AP−Ds between v_3 and v_4 do not pass by vertexes v_1 and v_2, then for any pair of $P(v_1v_2)$ and $P(v_3v_4)$, $\boldsymbol{C}_3 = P(v_1v_2) \cup v_2v_3 \cup P(v_3v_4) \cup v_4v_5 \cup v_5v_6 \cup v_6v_1$ is a CC with $\boldsymbol{s}$ in its interior, and the length of $\boldsymbol{C}_3$ is not greater than that of any CC which has a form as the kind (iv) of Figure 3.

Suppose $\boldsymbol{C}_4 = v_1v_2 \cup P(v_2v_3) \cup v_3v_4 \cup P(v_4v_1)$, where $P(v_2v_3)$ is a minimal AP−D between v_2 and v_3 and $P(v_4v_1)$ between v_4 and v_1, respectively. $\boldsymbol{C}_4$ is a CC with $\boldsymbol{s}$ in its interior, and the length of $\boldsymbol{C}_4$ is not greater than that of any CC which has a form as the kind (vi) of Figure 3. Compare the lengths of $\boldsymbol{C}_3$ and $\boldsymbol{C}_4$; the shorter one (includes not being longer than the other) is obviously a $\boldsymbol{s}$-MCC wanted.

Algorithm 4:

(1) Find out all the minimal AP−Ds $\{P_1(i), i = 1, 2, ...\}$ between v_1 and v_2 by using algorithm 1; denote its length as L_1.

(2) If $\exists$ i such that $P_1(i)$ passes by v_3 and v_4, then $\boldsymbol{C}_1 := P_1(i) \cup v_1v_2$ is a $\boldsymbol{s}$-MCC with its length equal to $L_1 + 1$; goto 8.

(3) Find out all the minimal AP−Ds $\{P_2(i), i = 1, 2, ...\}$ between v_3 and v_4 by using algorithm 1; denote its length as L_2.

(4) If $\exists$ i such that $P_2(i)$ passes by v_1 and v_2, then $\boldsymbol{C}_2 := P_2(i) \cup v_3v_4$ is a $\boldsymbol{s}$-MCC with its length equal to $L_2 + 1$, goto 8.

(5) Find out a minimal AP−D $P(v_2v_3)$ between v_2 and v_3 by using algorithm 1; denote its length as L_3.

(6) Find out a minimal AP−D $P(v_4v_1)$ between v_4 and v_1 by using algorithm 1; denote its length as L_4.

(7) If $L_1 + L_2 \leq L_3 + L_4 - 2$, then $\boldsymbol{C}_3 := P(v_1v_2) \cup v_2v_3 \cup P(v_3v_4) \cup v_4v_5 \cup v_5v_6 \cup v_6v_1$ is a $\boldsymbol{s}$-MCC with its length equal to $L_1 + L_2 + 4$, where $P(v_1v_2)$ and $P(v_3v_4)$ are any representatives of $\{P_1(i), i = 1, 2, ...\}$ and $\{P_2(i), i = 1, 2, ...\}$ respectively; otherwise, $\boldsymbol{C}_4 := v_1v_2 \cup P(v_2v_3) \cup v_3v_4 \cup P(v_4v_1)$ is a $\boldsymbol{s}$-MCC with its length equal to $L_3 + L_4 + 2$.

(8) Stop.

Case 4: Ring $\boldsymbol{s}$ has no double bond, corresponding to (vii) of section 2.2 (cf. Figure 3). For this case, by observation (cf. Figure 8) the analysis is rather direct and will thus be omitted.

Algorithm 5:

(1) Find a minimal AP−D between v_1 and v_2 by using algorithm 1, which will be denoted as $P(v_1v_2)$ and with its length equal to L_1; if there is no such AP−D, then $L_1 := \infty$; goto 5.

(2) Find a minimal AP−D between v_3 and v_4 by using algorithm 1, which will be denoted as $P(v_3v_4)$ and with its length equal to L_2; if there is no such AP−D, then $L_2 := \infty$; goto 5.

(3) Find a minimal AP−D between v_5 and v_6 by using algorithm 1, which will be denoted as $P(v_5v_6)$ and with its length equal to L_3; if there is no such AP−D, then $L_3 := \infty$; goto 5.

(4) $\boldsymbol{C}_1 := P(v_1v_2) \cup v_2v_3 \cup P(v_3v_4) \cup v_4v_5 \cup P(v_5v_6) \cup v_6v_1$.

(5) Find a minimal AP−D between v_2 and v_3 by using algorithm 1, which will be denoted as $P(v_2v_3)$ and with its length equal to L_4; if there is no such AP−D, then $L_4 := \infty$; goto 9.

(6) Find a minimal AP−D between v_4 and v_5 by using algorithm 1, which will be denoted as $P(v_4v_5)$ and with its length equal to L_5; if there is no such AP−D, then $L_5 := \infty$; goto 9.

(7) Find a minimal AP−D between v_6 and v_1 by using algorithm 1, which will be denoted as $P(v_6v_1)$ and with its length equal to L_6; if there is no such AP−D, then $L_6 := \infty$; goto 9.

(8) $\boldsymbol{C}_2 := P(v_2v_3) \cup v_3v_4 \cup P(v_4v_5) \cup v_5v_6 \cup P(v_6v_1) \cup v_1v_2$.

(9) If $L_1 + L_2 + L_3 > L_4 + L_5 + L_6$, then $\boldsymbol{C}_2$ is a $\boldsymbol{s}$-MCC with its length equal to $L_4 + L_5 + L_6 + 3$; otherwise, $\boldsymbol{C}_1$ is a $\boldsymbol{s}$-MCC with its length equal to $L_1 + L_2 + L_3 + 3$.

(10) Stop.

4. CALCULATING THE SUMMATION EXPRESSIONS OF LM-CONJUGATED CIRCUITS IN BENZENOID HYDROCARBONS

The following algorithm can be used to get the summation expression of any normal benzenoid hydrocarbon $\boldsymbol{B}$. Suppose that $\boldsymbol{B}$ is composed of h hexagons which are denoted respectively with their order numbers as 1, 2, ..., h. We can input its graph directly on the screen of PC with the mouse by using the method proposed in ref 10. Denote the LMC code of $\boldsymbol{B}$ under a Kekule structure K_i as $(r_1, r_2, ..., r_n, ...)$.

Algorithm 6:

(1) Enumerate a new Kekule structure K_i for $\boldsymbol{B}$ by using the algorithm proposed in ref 10; If there is no new one, then goto 7.

(2) $j := 1$.

(3) If the hexagon j has 3 double bonds, then $r_1 := r_1 + 1$; goto 5.

(4) For the hexagon j, find one of its K_i-MCC and its length L by using one of the above algorithms 2, 3, 4, and 5 with respect to the distribution of K_i-double bond(s) in it; $n := (L - 2)/4$, $r_n := r_n + 1$.

(5) If $j < h$, then $j := j + 1$; goto 3.

(6) $R(K_i) := \sum_n r_n R_n$; goto 1.

(7) $R(\boldsymbol{B}) := \sum_i R(K_i)$.

(8) Stop.

As all the fixed bonds within any BH can be detected by the algorithms reported in refs 11 and 12, we can easily extend this algorithm to a more general case based on the following theorem:[8]

Theorem 3. Let $\boldsymbol{B}_1$, $\boldsymbol{B}_2$, ..., $\boldsymbol{B}_t$ be the normal components of an essentially disconnected BH or a BH-fragment $\boldsymbol{B}$. Then

$$R(\boldsymbol{B}) = R(\boldsymbol{B}^*) = \sum_i (K(\boldsymbol{B})/K(\boldsymbol{B}_i))R(\boldsymbol{B}_i) \qquad i = 1, ..., t$$

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