Efficient Method for Calculating the Resonance Energy Expression of Benzenoid Hydrocarbons Based on the Enumeration of Conjugated Circuits

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To reduce the calculating time for the summations over linearly independent and minimal conjugated circuits of benzenoid hydrocarbons (BHs), an approximate method is proposed that counts only the numbers of the first four classes of conjugated circuits R_1, R_2, R_3, and R_4, respectively. By representation of BHs as custom-made "ring−block chains" and use of the techniques of Database and visual computing, an application software is realized that is much faster and more powerful than the old one based on an enumeration technique.

I. INTRODUCTION

According to the conjugated-circuit model introduced by Randic,[1−4] the resonance energies of conjugated benzenoid hydrocarbons (BHs) can be expressed as the sum of contributions arising from linearly independent and minimal conjugated circuits (LMCCs). By definition,[5] a set **S** of linearly independent and minimal conjugated circuits of a Kekule structure K_i of a benzenoid hydrocarbon **B** consists of a maximum number of linearly independent circuits of **B** in which every circuit is a conjugated circuit of K_i, and has the minimum total length. The manual calculation of LMCCs is very complex, which includes both recognition and counting, and is feasible only for some special types of BH or for very small molecules.

A more precise description is given in Guo and Randic.[5] For any BH **B**, K is a Kekule structure in **B**. We denote $R(K) = \sum_{R_j \in S} R_j = \sum_{n=1,2...} r_n(K) R_n$, where **S** is a set of LMCCs under K, R_j is any K-conjugated circuit (K-CC) in **S**, R_n denotes a circuit of size $4n + 2$ in **S**, and $r_n(K)$ is the number of R_n. It is well-defined that the summation expression of LMCCs of **B** is denoted as

$$R(\mathbf{B}) = \sum_K R(K) = \sum_{n=1,2,...} r_n R_n \qquad (1)$$

where $r_n = \sum_K r_n(K)$, and the sum is over all the Kekule structures in **B**. R(**B**) is also called the LMCC expression of **B**, and it plays a central role in the conjugated-circuit model, because the resonance energy RE(**B**) of BH **B** is simply equal to $R(\mathbf{B})/K(\mathbf{B})$, where K(**B**) is the number of Kekule structures in **B**.

Aimed to realize an automatic calculation for R(**B**) on PC, we have developed some algorithms and a visual solution[6] on the basis of Guo and Randic[5] and the old scheme proposed by Randic:[4] (1) generate all the Kekule structures in a BH; (2) find a set of LMCCs for each Kekule structure; (3) make a summation. With the power of modern PCs, for a reasonable size, the calculation of R(**B**) using this method can be conveniently performed.

This direct method works theoretically for any BH. But it is heavily time-consuming for large BHs, since it depends essentially on the generation and manipulation of all the Kekule structures in the BH considered, while the total number of which grows rapidly as the number of rings increases.

To reduce the calculating time to a reasonable limit, an approximate method is proposed in this paper. By analyzing the problem from a completely different point of view, which is largely rid of enumeration, we calculate only the numbers of the first four classes of conjugated circuits (CCs) R_1, R_2, R_3, and R_4, respectively. For the numerical calculation of molecular resonance energy, Randic and others[4,8] have taken the parametrization as $R_1 = 0.869$ eV, $R_2 = 0.246$ eV, $R_3 = 0.100$ eV, and $R_4 = 0.041$ eV (or 0.140 eV) and have neglected all the other contributions from larger CCs. As a result, our approximate scheme still satisfies well the requirements of numerical calculations for the molecular resonance energy of BHs in the conjugated-circuit model.[4,8−10]

II. APPROXIMATE LMCC EXPRESSION

A BH **B** is said to be normal if **B** contains no fixed bond (i.e. no bond which appears always as a double or always as a single bond of every Kekule structure in **B**). Otherwise **B** is said to be essentially disconnected. A normal component $\mathbf{B}_i$ of **B** is a maximal subgraph of **B** with no fixed bond (possibly, $\mathbf{B}_i = \mathbf{B}$). The total of all the normal components of **B** is denoted by $\mathbf{B}^*$.

A necessary and sufficient condition for a set of K-CCs in a BH **B** to be a set of LMCCs is reported:[5]

Theorem 1. Let K be a Kekule structure in **B**. A set $\mathbf{S} = \{\mathbf{C}_1, \mathbf{C}_2, \mathbf{C}_3, ... \mathbf{C}_t\}$ of K-CCs of **B** is a set of LMCCs of K, if and only if for any ring s_j in all normal components $\mathbf{B}^*$ of **B**, there is exactly one circuit $\mathbf{C}_j$ in **S** such that $\mathbf{C}_j$ is a s_j-MCC (minimally conjugated circuit containing s_j).

On the basis of this theorem, we are sure that if **B** is a normal BH, then there is exactly one s-MCC for any ring s of **B** in each set of LMCCs of K. As a consequence, we

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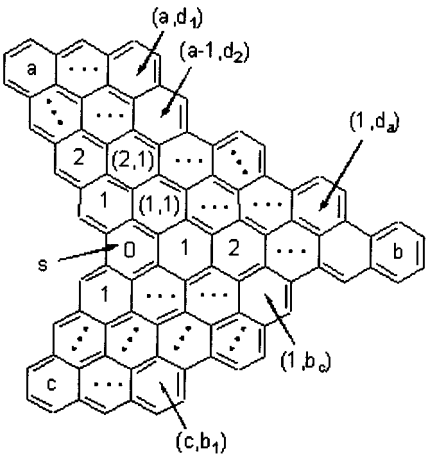

Figure 1. Construction of *s*-MCC.

know that the LMCC expression of **B** can also be represented as

$$R(\mathbf{B}) = \sum_s R_s(\mathbf{B}) = \sum_s \sum_{n=1,2,\ldots} r_n(s) R_n \qquad (2)$$

where *s* is any ring in any normal component of **B**, $R_s(\mathbf{B})$ is the summation of the MCCs of *s*, one for each Kekule structure *K*, and $r_n(s)$ is the total number of the *s*-MCCs of size $4n + 2$, independent of the Kekule structures. In the following, for simplicity, we always suppose that **B** is normal unless special declaration is made.

Form 2 of $R(\mathbf{B})$ has certain advantages from the viewpoint of both computing and approximation, with respect to form 1 of $R(\mathbf{B})$ defined in section I. First, we can restrict the summation of *n* in form 2 to be made only over the first four terms (cf. section IV) and define our approximate LMCC expression of $R(\mathbf{B})$ as

$$R_{\mathrm{ap}}(\mathbf{B}) = \sum_s \sum_{n=1,2,3,4} r_n(s) R_n \qquad (3)$$

in order to match the requirement of chemical application, whereas it is impossible to restrict oneself to a fixed limit in form 1 of $R(\mathbf{B})$. In fact, in the calculation of (1), one should find a *s*-MCC for each *s* under each Kekule structure of **B**, and one could not know the exact size of *s*-MCC for any ring *s* before the search procedure.[6]

Besides, the summation for form 2 of $R(\mathbf{B})$ is only over all the rings *s* in **B**, which can be performed without giving any concrete Kekule structure in **B**, as we shall do in the following, and thus this avoids the generation and manipulation of each Kekule structures in **B**, which is otherwise implicit in using the form of (1) to calculate $R(\mathbf{B})$.

Form 2 is particularly powerful for huge symmetric BHs. In these cases, it is enough to perform the calculation on certain rings, which belong to the asymmetric part of the molecule, and thus we can deal with very large scale problems within reasonable time period.

III. AVAILABLE FORMS OF $R_n(s)$, $n = 1, 2, 3, 4$

In this section, we discuss the available forms of $R_n(s)$, $n = 1, 2, 3, 4$, i.e. the *s*-MCCs of sizes 6, 10, 14, and 18, respectively.

For the general case, the possible forms of a *s*-MCC under a given Kekule structure are given by Guo and Randic.[5] For a circuit **C** in **B**, let $B[\mathbf{C}]$ denote the maximal subgraph of **B** bounded by **C**. Then we have the following:

Theorem 2. Let *K* be a Kekule structure in **B** and **C** a *s*-*K*-MCC of **B**. Then $B[\mathbf{C}]$ is one of the BHs shown in Figure 1, where $a, b, c \geq 0$, $0 \leq d_1 \leq d_2 \leq \ldots \leq d_a \leq b$, $0 \leq b_1 \leq b_2 \leq \ldots \leq b_c \leq b$, and the *K*-double bonds in $B[\mathbf{C}]$ are uniquely determined.

By varying the parameters *a*, *b*, *c*, b_c, and d_a in theorem 2, we obtain seven classes of available forms for a *s*-MCC,[6] which differ from each other by the number of double bond(s) in the ring *s* as well as their distribution. When we focus our attention only on R_1, R_2, R_3, and R_4, all the available asymmetric *s*-MCCs can be well-depicted, as in Figure 2.

IV. CALCULATING THE COEFFICIENTS $r_n(s)$, $n = 1, 2, 3, 4$

Completely different from the enumeration of every *s*-MCC under each Kekule structure, which is used for the general case,[6] here we will follow a simple and valuable scheme which has already been used by Herndon and Klein et al.[11−16] for a long time.

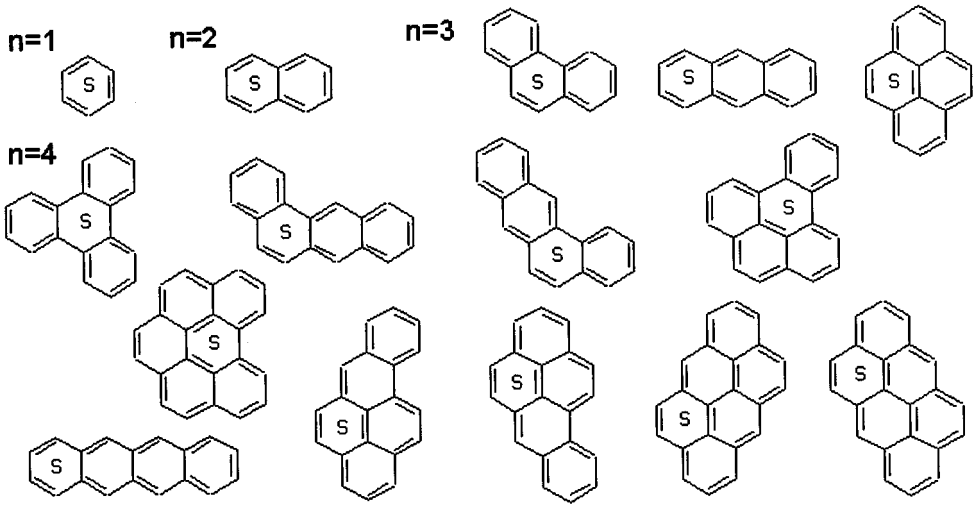

Figure 2. Available asymmetric *s*-MCCs.

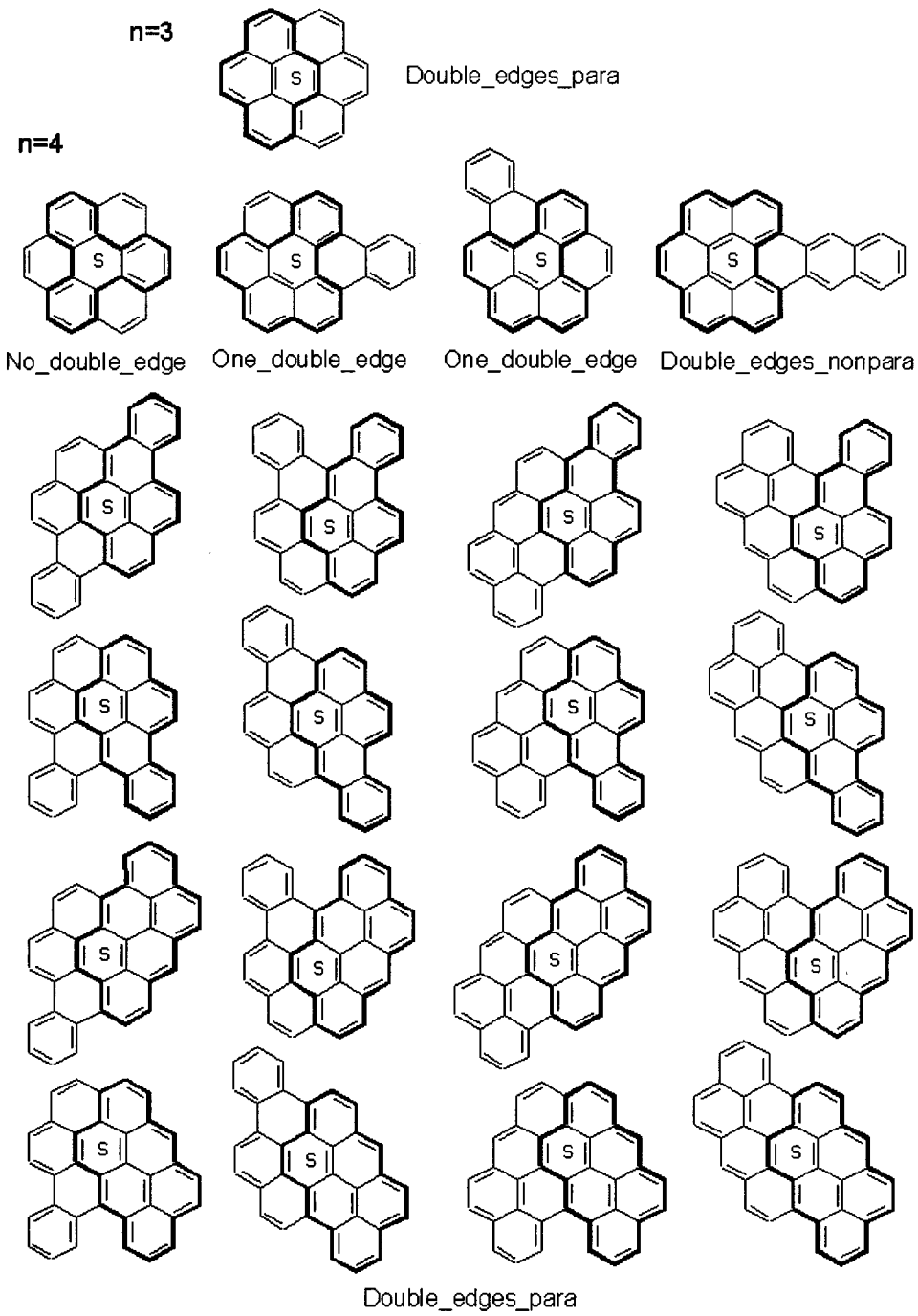

Figure 3. Pairs of *s*-MCCs.

Suppose **C** is a *s*-MCC; then by theorem 2, there exists a unique Kekule structure K' in $B[\mathbf{C}]$. By embedding K' into a larger Kekule structure K (in the case that it exists) in **B**, it becomes obvious that **C** corresponds exactly to $K(\mathbf{B}-B[\mathbf{C}])$ Kekule structures, for each of which **C** is a *s*-MCC in **B**. In this sense, if there is a unique *s*-MCC **C** of size $4n + 2$ for each Kekule structure in **B**, then we have

$$r_n(s) = \sum_c K(\mathbf{B} - B[\mathbf{C}]) \qquad (4)$$

It is proved in Guo et al.[7] that this fact is true for the cases $n = 1$ and 2, but generally false for $n = 3$ and 4. For the latter, there is at most a pair of *s*-MCCs for any ring *s* under any Kekule structure. Thus, for the calculation of the approximate LMCC expression $R_{ap}(\mathbf{B})$ (cf. (3)), we should pay more attention in calculating the coefficients $r_3(s)$ and $r_4(s)$.

Let K be a Kekule structure in **B**. Suppose that for some ring *s* of **B**, there exist two CCs $\mathbf{C}_1$ and $\mathbf{C}_2$, which are both *s*-K-MCCs. We know by the above work[7] that $B[\mathbf{C}_1]$ and $B[\mathbf{C}_2]$ contain a unique ring *s* in common and that each component in $\mathbf{C}_1 \cap \mathbf{C}_2$ is surely a K double bond. We denote by Coexist($\mathbf{C}_1$,$\mathbf{C}_2$) the graph $B[\mathbf{C}_1] \cup B[\mathbf{C}_2]$ together with its Kekule structure, which is exactly the restriction of K. Examples of asymmetric Coexist($\mathbf{C}_1$,$\mathbf{C}_2$) are given in Figure 3.

In the cases of coexistence, the Kekule structure K is counted twice in (4), once by $\mathbf{C}_1$ and the other by $\mathbf{C}_2$. Since $K(\mathbf{B}-B[\mathbf{C}_1] \cup B[\mathbf{C}_2])$ corresponds to the number of Kekule

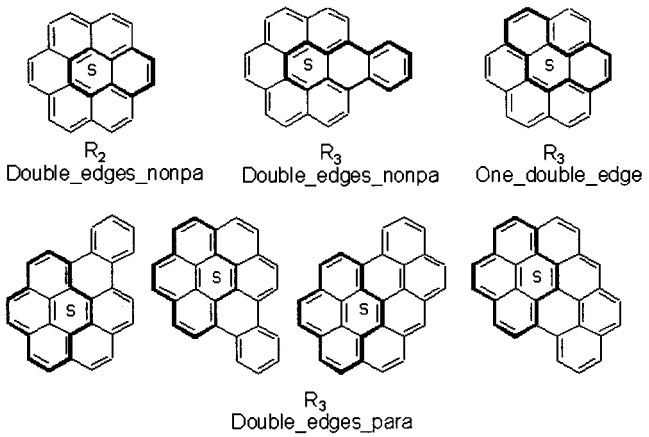

Figure 4. Miscalculated R_4 cases.

structures in **B** under which $\mathbf{C}_1$ and $\mathbf{C}_2$ are both *s*-MCCs, we can write

$$r_3(s) = \sum_c K(\mathbf{B}-B[\mathbf{C}]) - \sum K(\mathbf{B}-B[\mathbf{C}_1] \cup B[\mathbf{C}_2]) \quad (5)$$

where the first sum is over all the possible *s*-MCCs of size 14 and the second sum is over all the possible Coexist($\mathbf{C}_1$,$\mathbf{C}_2$) ($\mathbf{C}_1$, $\mathbf{C}_2$ of size 14).

For $r_4(s)$, we should still exclude some cases of miscalculation. The asymmetric examples are given in Figure 4. In such cases, for each Kekule structure *K* which corresponds to the given *B*[**C**] (or **C**), there is a proper *s*-MCC of size less than 18 (say, exactly, 10 or 14), and thus it should be excluded from $r_4(s)$. At last, we have

$$r_4(s) = \sum_c K(\mathbf{B}-B[\mathbf{C}]) - \sum K(\mathbf{B}-B[\mathbf{C}_1] \cup B[\mathbf{C}_2]) - \sum K(\mathbf{B}-\mathbf{D}) \quad (6)$$

where **C**, $\mathbf{C}_1$, and $\mathbf{C}_2$ in the first and second sums are of size 18, **D** denotes a subgraph of **B** which is corresponding to a miscalculating case, and the third sum is over all the possible **D**s.

V. REPRESENTING HS AS A RING-BLOCK CHAIN

To realize the total procedure on a PC, there are still two problems unsolved: how to produce all the available *s*-MCCs $\mathbf{C}_n$ (n = 2, 3, 4) and the relevant subgraphs of **B** from the asymmetric ones depicted in Figures 2−4; how to generate all the relevant subgraphs automatically and efficiently, such as $\mathbf{B} - B[\mathbf{C}_n]$ and the others involved in the calculations of (4)−(6), for the successive calculation of their numbers of Kekule-structure counts.

To solve such problems, we propose a special representation for every ring *s* in **B**. Here we can consider a hexagonal system as a linear chain of ring-blocks. In each ring-block, we use six edge-pointers in order to reconstruct the whole system. These pointers are numbered from 0 to 5 clockwise, as in Figure 5. Each edge-pointer points to its direct-neighboring ring (i.e. the value of the edge-pointer is equal to the order number of the latter in the linear chain), and it will be null if there is no corresponding neighbor. With this representation, it is not difficult to describe any subgraph,

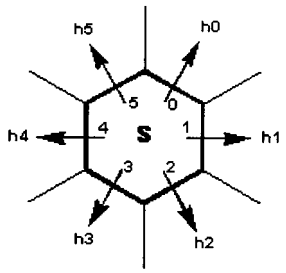

Figure 5. Representation of a hexagon in the chain.

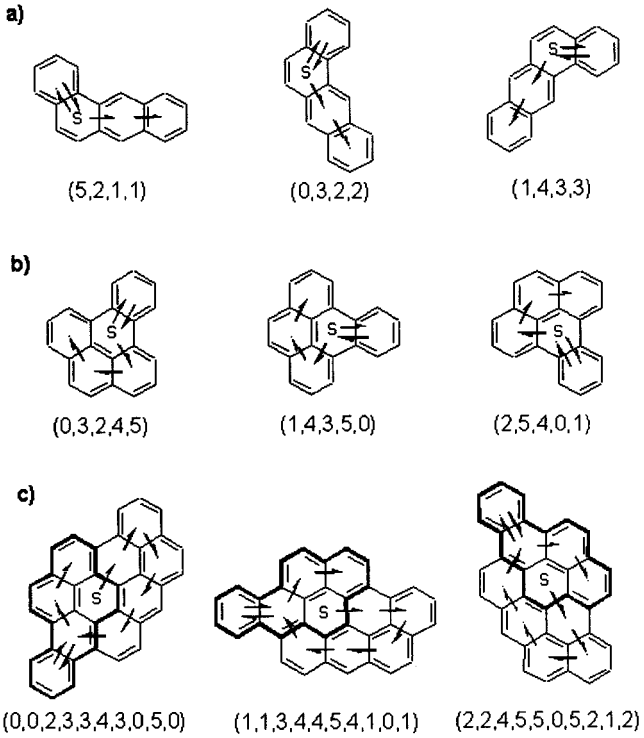

Figure 6. Representation of selected subgraphs.

such as *B*[**C**], $B[\mathbf{C}_1] \cup B[\mathbf{C}_2]$, and **D**, by a pointer-walk from ring-center to ring-center. This walk may then be designated by a sequence of edge-pointer labels. For example, Figure 6a can be denoted as (5,2,1,1), Figure 6b can be denoted as (0,3,2,4,5), and Figure 6c can be denoted as (0,0,2,3,3,4,3,0,5,0), etc.

H denotes a BH, and **G** is generated from **H** by rotating $\pi/3$ clockwise. Suppose that $\boldsymbol{H} = (p_1, p_2, ..., p_n)$ and $\mathbf{G} = (q_1, q_2, ..., q_n)$, then we have simply $q_i = p_i + 1$ (mod 6), $i = 1, ..., n$. By repeating this procedure, it is easy to produce all the available *s*-MCCs and the relevant subgraphs from the asymmetric ones. Some examples are presented in Figure 6.

Furthermore, it becomes only a tracing problem to generate a subgraph of **B**, such as $\mathbf{B} - B[\mathbf{C}]$ or others (cf. Figure 7). Suppose that $B[\mathbf{C}] = (p_1, p_2, ..., p_n)$. We work on the linear chain representation of **B** and start from the ring-block (denoted as $\mathbf{b}_0$) corresponding to *s*. First, we mark $\mathbf{b}_0$ and the ring-block (denoted as $\mathbf{b}_1$) which is pointed by the p_1th edge-pointer of $\mathbf{b}_0$; then mark the ring-block $\mathbf{b}_2$ which is pointed by the p_2th edge-pointer of $\mathbf{b}_1$; and go on until the ring-block $\mathbf{b}_n$ is marked. By neglecting all the ring-blocks marked in the linear chain of **B**, as well as all the relevant edge-pointers in the other ring-blocks, which point to the

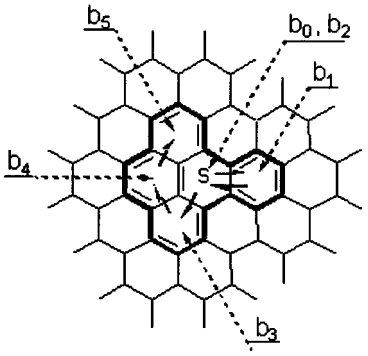

Figure 7. Generation of $\mathbf{B} - B[\mathbf{C}]$.

marked ring-blocks, we can easily construct the subgraph wanted from the ring-blocks remaining.

VI. TOTAL SOLUTION

As preparation, we should first create a Database (DB), which contains all the graphs (or subgraphs as mentioned above) needed for this procedure, such as all the available asymmetric forms of *s*-MCC (cf. Figure 2), all the available asymmetric pairs of *s*-MCCs (cf. Figure 3), and all the available asymmetric miscalculated cases (cf. Figure 4). They are organized with the order determined by the calculating algorithms.

In practice, the ring-blocks in the linear chain, which represents the considered BH, are numbered by their input order using an intelligent graphical user interface. As soon as the user decides to stop his modification on the BH under consideration, the corresponding ring-block chain is determined.

For simplicity of programming, we perform the calculation for the number of Kekule structures in subgraphs of **B**, such as $\mathbf{B} - B[\mathbf{C}]$ (denoted as $K(\mathbf{B}-B[\mathbf{C}])$ above) and others, by using the algorithm reported by us[17] for the moment, which is essentially based on explicitly generating each Kekule structure. A more rapid algorithm, which employs mainly the technique of the matrix of $P - V$ paths instead of the enumeration to calculate the number of Kekule structures concerned, is in development and will be reported in detail in another paper.

B denotes an arbitrary normal BH. Suppose that **B** is composed of *h* hexagons which are denoted respectively with their order numbers as 1, 2, ..., *h*. The main algorithm can be described as the following.

Algorithm:

(1) Take hexagon 1 (all its structural information is recorded in ring-block 1) as *s*; $r_1(\mathbf{B}) = r_2(\mathbf{B}) = r_3(\mathbf{B}) = r_4(\mathbf{B}) = 0$;

(2) Calculate $K(\mathbf{B}-s)$, and then $r_1(s) = 2K(\mathbf{B}-s)$; $r_1(\mathbf{B}) = r_1(\mathbf{B}) + r_1(s)$;

(3) Take the first record (the unique R_2 in Figure 2) in the DB; produce all the symmetric ones and generate the corresponding subgraphs as described in section V; then calculate $r_2(s)$ with formula 4; $r_2(\mathbf{B}) = r_2(\mathbf{B}) + r_2(s)$;

(4) Take the proper *s*-MCCs (all the R_3 in Figure 2) and the relevant pairs of *s*-MCCs (cf. Figure 3) in the DB; produce all the symmetric ones and generate the corresponding subgraphs as described in section V; then calculate $r_3(\mathbf{s})$ with formula 5; $r_3(\mathbf{B}) = r_3(\mathbf{B}) + r_3(s)$;

(5) Take the proper *s*-MCCs (all the R_4 in Figure 2) and the relevant pairs of *s*-MCCs (cf. Figure 3) as well as the miscalculated cases (cf. Figure 4) in the DB; produce all the symmetric ones and generate the corresponding subgraphs as described in section V; then calculate $r_4(s)$ with formula 6; $r_4(\mathbf{B}) = r_4(\mathbf{B}) + r_4(s)$;

(6) If $j < h$, then $j = j + 1$ and take hexagon *j* as *s*; go to 2;

(7) Stop.

When the algorithm ends, we obtain $r_n(\mathbf{B})$, $n = 1, 2, 3, 4$, as the coefficients of R_n, $n = 1, 2, 3, 4$, in the summation expression of $R_{ap}(\mathbf{B})$.

Since all the fixed bonds in any BH can be detected by the algorithm reported by us,[18] we can easily extend this algorithm to a more general case based on the following theorem:[5]

Theorem 3. Let $\mathbf{B}_1$, $\mathbf{B}_2$, ..., $\mathbf{B}_t$ be the normal components of an essentially disconnected BH **B**. Then

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

By replacing all the "$R(...)$" in the above theorem with "$R_{ap}(...)$", we can extend our method to the cases of essentially disconnected BHs.

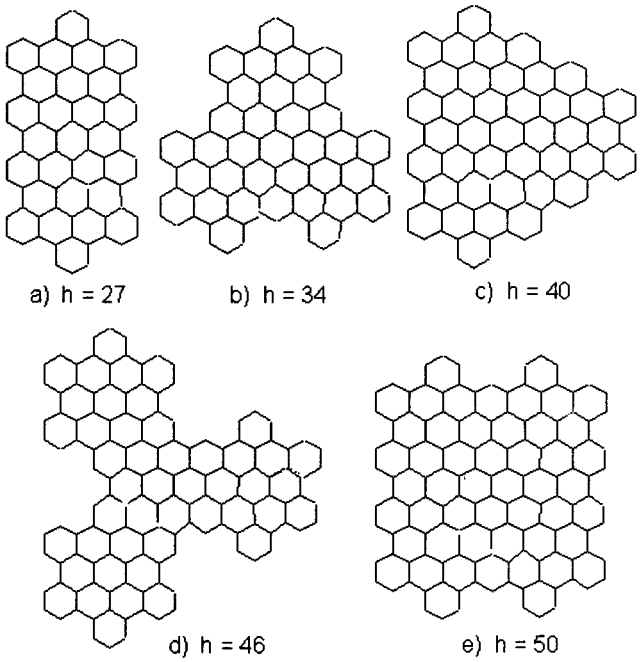

Figure 8. Selected examples of BH.

VII. SELECTED APPLICATIONS

Based on the algorithms reported in this paper and in our early works,[17,18] an application software has been developed. The BHs being considered can be easily input into the system by mouse under an intelligent graphical user interface. All of the calculation is autonomic and visual.

As examples, some large BHs from the works of Mullen and collaborators[19−21] (cf. Figure 8) have been treated, and the results are presented as follows, where *h* is the number

of hexagons in BH considered.

(a) $h = 27$:

$$R_{ap}(\mathbf{B}) = 505200R_1 + 303500R_2 + 204210R_3 + 111300R_4$$

(b) $h = 34$:

$$R_{ap}(\mathbf{B}) = 7897800R_1 + 4772100R_2 + 3294000R_3 + 1853220R_4$$

(c) $h = 40$:

$$R_{ap}(\mathbf{B}) = 61966278R_1 + 41227074R_2 + 29383446R_3 + 15788460R_4$$

(d) $h = 46$:

$$R_{ap}(\mathbf{B}) = 1349940400R_1 + 801906900R_2 + 541051875R_3 + 298602500R_4$$

(e) $h = 50$:

$$R_{ap}(\mathbf{B}) = 2503746592R_1 + 1688655568R_2 + 1228348490R_3 + 679658230R_4$$

(Randic and Guo have already worked on molecules a [10] and b [9] of Figure 8. They have obtained the same results on the counts of R_1 and R_2, as well as that of R_3 for a, but a larger count of R_3 for b, i.e. 3 825 250 instead of 3 294 000.)

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