Bond Ordering Relation. Incompatibility between Bonds, Essential Single/Double Bonds, and the Nonexistence of Kekulé Structures in Molecular Subgraphs

Tetsuo Morikawa

Chemistry Department, Joetsu University of Education, Yamayashiki, Joetsu, Niigata Prefecture 943, Japan

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An ordering relation between single and/or double bonds, such that one bond gives an order to another, on a set of Kekulé structures (perfect matchings) in hydrogen-suppressed molecular graphs is defined. By use of this binary relation, lemmas relating to both incompatibility between bonds and essential single/double bonds can be described. It is thus possible to estimate the nonexistence of Kekulé structures in a given molecular subgraph.

1. INTRODUCTION

We follow graphic terminology of ref 1. Let v_i and e_i be a vertex and an edge of a hydrogen-suppressed molecular graph G; in a path $v_ie_iv_{i+1}$, e_i joins v_i and v_{i+1} together. When a double bond connects v_i and v_{i+1} in a Kekulé structure (a perfect matching) of G, the bond is denoted by d_i; and when a single bond, by s_i. We use b_i to indicate s_i or d_i; $\bar{b}_i$ represents d_i if $b_i = s_i$; $\bar{b}_i$ represents s_i if $b_i = d_i$; $\bar{\bar{b}}_i = b_i$; also refer to Table 1.

Let $K\{G\}$ be the number of Kekulé structures in G, and let $K\{b_i, r\}$ be the number of Kekulé structures containing b_i in G. Here $\{r\}$ is an abbreviation for the rest of G. Two identity equations in Kekulé structure counting[1] are thus expressed in the present notation as

$$K\{e_i, r\} = K\{b_i, r\} + K\{\bar{b}_i, r\} \qquad (1)$$

$$K\{e_i, e_j, r\} = K\{b_i, b_j, r\} + K\{b_i, \bar{b}_j, r\} + K\{\bar{b}_i, b_j, r\} + K\{\bar{b}_i, \bar{b}_j, r\}(e_i \neq e_j) \qquad (2)$$

This note is concerned with local properties relating to e_i, b_i, and $\bar{b}_i$ in Kekulé structures.

It is a well-known fact in Kekulé structure counting that the selection of a bond b_i in paths and cycles uniquely determines the local conjugated structures containing this b_i. In a hexagon (benzene), for example, a bond b_i fixes all the other bonds in a Kekulé structure. This propagation of bonds can be interpreted as an ordering relation in mathematics. An edge e_i between v_i and v_{i+1} in polyhexes is called *forcing*[2,3] if it decides Kekulé structures. We first introduce the bond ordering as a mathematical binary relation $\leq$, and secondly define both incompatibility between bonds and essential single/double bonds by using this binary relation. We shall prove lemmas relating these concepts, and, as a result, establish two theorems on the nonexistence of Kekulé structures in hydrogen-suppressed molecular subgraphs.

2. BOND ORDERING RELATION

We begin by defining a binary relation $b_i \leq b_j$, and read it as "b_i precedes or equals b_j". Notice that a Kekulé structure contains only one of b_i and $\bar{b}_i$.

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Table 1. Glossary of Symbols

b_i	s_i or d_i
$\bar{b}_i$	s_i if $b_i = d_i$, or d_i if $b_i = s_i$
d_i	double bond, connecting v_i and v_{i+1} in Kekulé structures
e_i	edge, connecting v_i and v_{i+1} in G
G	hydrogen-suppressed molecular graph
H, H_k	subgraph of G
$K\{b_i, b_j, r\}$	number of Kekulé structures with b_i, b_j in G
$K\{G\}$	number of Kekulé structures in G
q	abbreviation for graphic part such that $K\{H, q\} > 0$
r	abbreviation for the rest of G
s_i	single bond, connecting v_i and v_{i+1} in Kekulé structures
t	abbreviation for the rest of H
v_i	vertex in G
$\rightarrow$	imply (implies)
$\leftarrow$	inverse of $\rightarrow$
$\leftrightarrow$	$\rightarrow$ and $\leftarrow$
$\leq$	precede or equal (precedes or equals)

Definition 1 (Bond Ordering). *A relation $\leq$ between b_i and b_j is written as $b_i \leq b_j$, when* (1), *and when either* (2-1) *or* (2-2). (1) *There is a Kekulé structure with a bond b_i.* (2-1) *($e_i = e_j$) Every Kekulé structure containing b_i becomes a Kekulé structure containing $\bar{b}_i$ by the replacement of b_i with $\bar{b}_i$.* (2-2) *($e_i \neq e_j$) Every Kekulé structure containing b_i has a bond b_j.*

The restriction $K\{G\} > 0$ is an implicit assumption in Definition 1. It is easy to extend this assumption to $K\{G\} \geq 0$. Let $H = \{e_i, e_j, t\}$ be a subgraph of $G = \{H, r\}$. In a manner similar to Definition 1, it is possible to define $b_i \leq b_j$ in H if there is graphic part $\{q\}$ such that $K\{H, q\} > 0$, because $\{H, q\}$ can be chosen as a hydrogen-suppressed molecular graph. This extension makes it possible for us to estimate whether or not a given G is non-Kekuléan by means of $\leq$. A bond ordering relation $\leq$ hereafter means the one for such H.

Clearly the relation $\leq$ satisfies $b_i \leq b_i$ (reflexivity). If $b_i \leq b_j$, and if $b_j \leq b_k$, then $b_i \leq b_k$ (transitivity). In the chemical meaning, the ordering relation $b_i \leq b_j$ is not antisymmetric; i.e., b_i is not equivalent to b_j, even if $b_i \leq b_j$ and $b_j \leq b_i$.

Let us define a binary relation $\equiv$ by $b_i \equiv b_j$ if and only if $b_i \leq b_j$ and $b_j \leq b_i$. This relation $\equiv$ has, needless to say, no valid meaning of chemistry but is a proper definition from the point of view of Kekulé structure counting. We then have $b_i \leq b_i \rightarrow b_i \equiv b_i$ (reflexivity); $b_i \equiv b_j$ and $b_j \equiv b_k \rightarrow b_i \leq b_j$, $b_j \leq b_i$, $b_j \leq b_k$ and $b_k \leq b_j \rightarrow b_i \leq b_k$ and $b_k \leq b_i \rightarrow b_i \equiv b_k$ (transitivity); $b_i \equiv b_j \rightarrow b_i \leq b_j$ and $b_j \leq b_i \rightarrow b_j$

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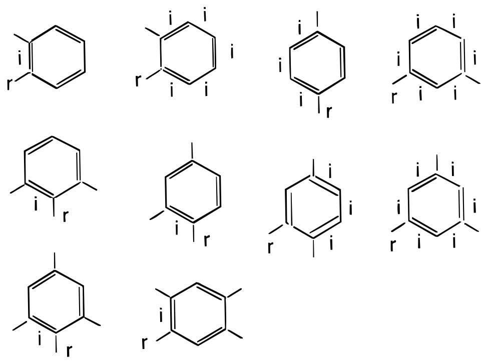

Figure 1. All 10 hexagonal subgraphs of G, each of which has at least one b_i that precedes or equals all the bonds in the hexagon. r indicates the rest of G. Mirror images of the subgraph about the vertical line and/or the horizontal line are all omitted.

$\leq b_i$ and $b_i \leq b_j \rightarrow b_j \equiv b_i$ (symmetry); namely, $\equiv$ is an equivalence relation. On a set of $\{b_i\}$ divided by $\equiv$, i.e., on the quotient set $\{b_i\}/\equiv$, a binary relation $\leq^*$ is defined by $C(b_i) \leq^* C(b_j) \leftrightarrow b_i \leq b_j$, where $C(b_i)$ is a class containing b_i in the quotient set. Clearly $\leq^*$ satisfies reflexivity and transitivity, because $\leq$ satisfies reflexivity and transitivity. Suppose that $C(b_i) \leq^* C(b_j)$ and $C(b_j) \leq^* C(b_i)$, then, $b_i \leq b_j$ and $b_j \leq b_i \rightarrow b_i \equiv b_j$; therefore, $C(b_i) = C(b_j)$; namely, the antisymmetry for $\leq^*$ holds; i.e., $\leq^*$ is a partial ordering relation.[5] The failure of antisymmetry is illustrated by two subpolyhexes (called *alternate cycles* below) in the last column of Figure 1. We use only $\leq$ hereafter.

Definition 1 leads to Lemmas 1 and 2.

Lemma 1. *$(e_i = e_j)$ $b_i \leq b_j \leftrightarrow K\{b_i, r\} \leq K\{b_j, r\}$.*

Lemma 2. *$(e_i \neq e_j)$ $b_i \leq b_j \rightarrow K\{b_i, e_j, r\} = K\{b_i, b_j, r\} \leq K\{e_i, b_j, r\} \leftrightarrow K\{e_i, \bar{b}_j, r\} = K\{\bar{b}_i, \bar{b}_j, r\} \leq K\{\bar{b}_i, e_j, r\}$.*

Note the direction of arrows in Lemmas 1 and 2,[4] and $e_i \neq e_j$ means $b_j \neq b_i, \bar{b}_i$. It is plain that $b_j \leq \bar{b}_k$ implies $K\{e_j, b_k, r\} \leq K\{\bar{b}_j, e_k, r\}$. Hence we get Lemma 3.

Lemma 3. *$b_i \leq b_k$ and $b_j \leq \bar{b}_k$ $(e_i \neq e_j) \rightarrow K\{b_i, e_j, r\} \leq K\{e_i, \bar{b}_j, r\}$.*

The application of Lemma 2 to a set of bond ordering relations, $b_i \leq b_j$, $b_i \leq b_k$, ..., and $b_i \leq b_m$, gives

$$K\{b_i, e_j, e_k, ..., e_m, r\} = K\{b_i, b_j, b_k, ..., b_m, r\}$$

and

$$K\{\bar{b}_i, \bar{b}_j, \bar{b}_k, ..., \bar{b}_m, r\} \leq K\{\bar{b}_i, e_j, e_k, ..., e_m, r\}$$

Using Lemma 1, we thus have Lemma 4.

Lemma 4. *A set of bond ordering relations, $b_i \leq b_j$, $b_i \leq b_k$, ..., and $b_i \leq b_m$ $(e_i \neq e_j, e_k, ..., e_m)$, such that*

$$K\{b_i, b_j, b_k, ..., b_m, r\} = K\{\bar{b}_i, \bar{b}_j, \bar{b}_k, ..., \bar{b}_m, r\}$$

is given. Then $b_i \leq \bar{b}_i$.

Figure 1 shows all 10 hexagonal subgraphs, each of which fulfills all the sufficient conditions of Lemma 4; i.e., $b_i \leq \bar{b}_i$ for each hexagonal subgraph.

Lemma 1 and eq 1 yield the upper and lower bonds for $K\{e_i, r\}$.

Lemma 5. *If $b_i \leq \bar{b}_i$, then $2K\{b_i, r\} \leq K\{e_i, r\} \leq 2K\{\bar{b}_i, r\}$.* Repeating three times the combination of Lemmas 4 and 5 and the elimination of single bonds, we can derive the subgraph (right) from the polyhex subgraph (left) in Figure 2, where

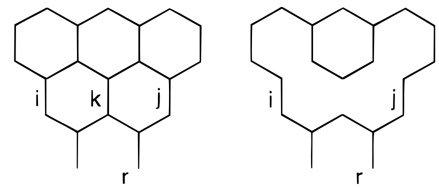

Figure 2. A subgraph (polyhex, left) is reducible to another subgraph (right) by means of Lemmas 4 and 5. Three edges, indicated by i, j, and k, of the subgraphs (left and right) are all essential single bonds for any $\{r\}$.

$$K\{\text{given subgraph(left)}, r\} \leq 2^3 K\{\text{reduced subgraph(right)}, r\} \quad (3)$$

The right-hand side of this inequality will be estimated in the last section.

3. INCOMPATIBILITY BETWEEN BONDS

Let us consider, as an example, a path $v_1e_1v_2e_2v_3e_3 ... v_{2k}e_{2k}v_{2k+1}$ $(k \geq 1)$ in G such that

$$s_1 \leq d_2 \leq s_3 \leq ... \leq s_{2k-1} \leq d_{2k}$$

Such a path may be called *alternate*,[6] because single and double bonds appear one after the other. A path beginning and ending at vertices with degree 3 in the subgraph (right) of Figure 2 is an example of alternate paths. For an alternate path, we get $s_1 \leq d_{2k}$ and $d_1 \geq s_{2k}$, then Lemma 2 gives

$$K\{s_1, v_2e_2v_3e_3 ... v_{2k}, s_{2k}, r\} = 0$$

In other words, we can say that s_1 is incompatible with s_{2k}. A pair of bonds, d_k and d_{k+1}, where the bonds are both incident with a common vertex, is another example; clearly $K\{d_k, d_{k+1}, r\} = 0$. In general, we define the incompatibility between bonds by the following.

Definition 2 (Incompatibility). *Two distinct bonds are said to be incompatible (with each other) when they both are in no Kekulé structure.*

A mathematical expression of incompatibility for G such that $K\{G\} \geq 0$ is given by the following lemma.

Lemma 6. *A subgraph $H = \{e_i, e_j, t\}$ $(e_i \neq e_j)$ of $G = \{H, r\}$, such that $K\{H, q\} > 0$ is given. If $K\{\{b_i, b_j, t\}, q\} = 0$, then b_i and b_j are incompatible in G; if b_i and b_j are incompatible in G, then $K\{\{b_i, b_j, t\}, q\} = 0$.*

Since a Kekulé structure contains only one of b_i and $\bar{b}_i$, we may say as a special case $(e_i = e_j)$ that b_i and $\bar{b}_i$ are incompatible. Lemma 2 suggests $K\{b_i, \bar{b}_j, r\} = 0$ for $e_i \neq e_j$. Hence using Lemma 6, we have the following.

Lemma 7. *If $b_i \leq b_j$, then b_i is incompatible with $\bar{b}_j$.*

Lemma 7 and eqs 1 and 2 suggest the following.

Lemma 8. *If $b_i \leq b_j$ and $\bar{b}_i \leq b_j$ $(e_i \neq e_j)$, then $K\{e_i, e_j, r\} = K\{e_i, b_j, r\}$.*

Two conditions, $b_i \leq b_k$ and $b_j \leq b_l$ $(e_i \neq e_j)$, for Lemmas 1 and 2, give

$$K\{b_i, b_j, r\} \leq K\{b_k, b_j, r\} \leq K\{b_k, b_l, r\}$$

Hence we obtain the following.

Lemma 9. *If $b_i \leq b_k$ and $b_j \leq b_l$ $(e_i \neq e_j)$, and if b_k is incompatible with b_l, then b_i is incompatible with b_j.* This lemma is useful for determining whether b_i and b_j are incompatible in a subgraph H of G. It is clear that if the K

value in the right-hand side of $\leq$ is equal to zero, then that in the left-hand side also equals zero. We can thus state the following.

Lemma 10. *A subgraph H of G is given: H is decomposed into n subgraphs, H_1, H_2, ..., and H_n, such that*

$$0 < K\{H, r\} \leq cK\{H_1, r\}K\{H_2, r\} \ldots K\{H_n, r\}$$

H and one H_k of the subgraphs both have two bonds b_i and b_j (c being a positive number). Then, if b_i and b_j are incompatible in a subgraph H_k, then they are also incompatible in H.

Lemma 11. *A subgraph H of G is given: H is decomposed into n subgraphs, H_1, H_2, ..., and H_n, such that*

$$0 < K\{H, r\} \leq c_1K\{H_1, r\} + c_2K\{H_2, r\} + \ldots + c_nK\{H_n, r\}$$

H and all the n subgraphs have two bonds b_i and b_j (c_k with $k = 1, 2, ..., n$, being a positive number). Then, if b_i and b_j are incompatible in H_k for $k = 1, 2, ..., n$, then they are also incompatible in H.

4. ESSENTIAL SINGLE/DOUBLE BONDS

Certain bonds for a given conjugated molecule are single or double in all the possible Kekulé structures that one can write; such a bond is called an essential single or essential double bond.[7] We define an essential bond by the following definition.

Definition 3 (Essential). *A bond is essential when it is in every Kekulé structure*. Definition 3 for G such that $K\{G\} \geq 0$ is rewritten by use of eq 1 as Lemma 12.

Lemma 12. *A subgraph $H = \{e_i, t\}$ of $G = \{H, r\}$, such that $K\{H, q\} > 0$, is given. If $K\{\{b_i, t\}, q\} = 0$, then $\bar{b}_i$ is essential in G; if b_i is essential in G, then $K\{\{\bar{b}_i, t\}, q\} = 0$.*

As an example, let us consider a cycle $[v_1e_1v_2e_2v_3e_3 \ldots v_{2k}e_{2k}]$, in which the last edge e_{2k} connects v_{2k} and v_1, such that

$$d_1 \leq s_2 \leq d_3 \leq s_4 \leq \ldots \leq d_{2k-1} \leq s_{2k} \leq d_1$$

Such a cycle may be called *alternate*,[6] because alternating single and double bonds occurs. We can observe three alternate cycles in the subgraph (right) of Figure 2. For an alternate cycle, we have

$$K\{[d_1, v_2e_2v_3e_3 \ldots v_{2k}e_{2k}], r\}$$
$$= K\{[d_1, s_2, d_3, s_4, \ldots, d_{2k-1}, s_{2k}], r\}$$
$$= K\{[s_1, d_2, s_3, d_4, \ldots, s_{2k-1}, d_{2k}], r\}$$
$$= K[\{s_1, v_2e_2v_3e_3 \ldots v_{2k}e_{2k}], r\}$$

This equality suggests that the K value of an alternate cycle vanishes if an external edge attached to the cycle is double; i.e., every external edge of alternate cycles is single; hence, such a single bond becomes essential if the K value is positive.

If b_i is essential, then $K\{\bar{b}_i, r\} = 0 \leq K\{b_i, r\}$; therefore, Lemma 1 suggests the following.

Lemma 13. *If b_i is essential, then $\bar{b}_i \leq b_i$.*

Remembering that $b_i \leq b_j$ implies $K\{e_i, \bar{b}_j, r\} \leq K\{\bar{b}_i, e_j, r\}$, and using Lemmas 1, 2, and 12, we get the following two lemmas.

Lemma 14. *If b_i, such that $b_i \leq b_j$, is essential, then b_j is also essential.*

Lemma 15. *If $\bar{b}_j$, such that $b_i \leq b_j$, is essential, then $\bar{b}_i$ is also essential.*

Easily Lemma 12 and eq 2 give Lemma 16.

Lemma 16. *If both of b_i and b_j ($e_i \neq e_j$) are essential, then*

$$K\{e_i, e_j, r\} = K\{b_i, b_j, r\}$$

Two ordering relations, $b_i \leq b_k$ and $b_i \leq b_l$, imply

$$k\{b_i, e_k, e_l, r\} = K\{b_i, b_k, e_l, r\} \leq K\{e_i, b_k, b_l, r\}$$

which suggests Lemma 17 below. Lemma 17 is useful when we determine whether b_i is essential in H. This lemma is also applicable to the case when either $b_i \leq b_j$ and $b_i \leq \bar{b}_j$ ($e_i \neq e_j$) or $b_i \leq d_k$ and $b_i \leq d_{k+1}$ ($e_i \neq e_k$, e_{k+1}), where d_k and d_{k+1} are adjacent. Lemma 18 follows at once from repeated use of Lemma 17. A single polygon with an odd number of vertices has the relations $b_i \leq \bar{b}_i$ and $\bar{b}_i \leq b_i$; for such a single polygon, $K = 0$.

Lemma 17. *If $b_i \leq b_k$ and $b_i \leq b_l$ ($e_i \neq e_k$, e_l), and if b_k is incompatible with b_l, then $\bar{b}_i$ is essential.*

Lemma 18. *If $b_i \leq b_j$, $b_i \leq \bar{b}_j$, $\bar{b}_i \leq b_j$ and $\bar{b}_i \leq \bar{b}_j$ ($e_i \neq e_j$), then $K\{b_i, r\} = K\{\bar{b}_i, r\} = K\{b_j, r\} = K\{\bar{b}_j, r\} = 0$.*

It is similar to the derivation of Lemmas 10 and 11 to get the following two lemmas.

Lemma 19. *A subgraph H of G is given: H is decomposed into n subgraphs, H_1, H_2, ..., and H_n, such that*

$$0 < K\{H, r\} \leq cK\{H_1, r\}K\{H_2, r\} \ldots K\{H_n, r\}$$

both of H and one H_k of the subgraphs have b_i (c being a positive number). Then, if b_i is essential in a subgraph H_k, then b_i is also essential in H.

Lemma 20. *A subgraph H of G is given: H is decomposed into n subgraphs, H_1, H_2, ..., and H_n, such that*

$$0 < K\{H, r\} \leq c_1K\{H_1, r\} + c_2K\{H_2, r\} + \ldots + c_nK\{H_n, r\}$$

H and the subgraphs all have b_i (c_k with $k = 1, 2, ..., n$, being a positive number). Then, if b_i is essential in H_k for $k = 1, 2, ..., n$, then b_i is also essential in H.

5. ALGORITHMS FOR DETERMINING BOND ORDERING RELATIONS

A vertex v_k of a conjugated path has three different kinds of external bonds that are attached to v_k; namely, double, single, and unfixed; $(=)_k$, $(-)_k$, and $(\ )_k$, respectively, denote such bonds in this section. An algorithm below tries to construct a sequence, composed of b_k and $\bar{b}_k$, from a given path ($v_ie_iv_{i+1} \ldots v_ke_kv_{k+1} \ldots v_je_jv_{j+1}$), and also tries to fix $(\ )_k$ for v_k.

(1) Make b_i (d_i or s_i).
(2) Set $i + 1$ to be k.
(3) Loop:
(a) If $b_{k-1} = d_{k-1}$, and
  i. if $(=)_k$, then Failure,
  ii. if $(-)_k$, then make s_k and set all $(\ )_k$ to be $(-)_k$,

iii. if $(\ )_k$, then make s_k and set all $(\ )_k$ to be $(-)_k$,

(b) If $b_{k-1} = s_{k-1}$, and

i. if $(=)_k$, then make s_k,

ii. if $(-)_k$, then Failure,

iii. if $(\ )_k$, then Failure.

(c) Increase k by 1.

(4) Repeat the loop until either $k = j$ or Failure.

If no sequence beginning at b_i and ending at b_j for a given path is complete, then search for another path. We can conclude that $b_i \leq b_j$ if there is a sequence from b_i to b_j.

When the algorithm above-mentioned is not applicable to a subgraph H of G, we have to reduce H by use of Lemmas 4, 5, 10, 11, 19, and 20. In H, if one cycle shares only s_i with another, then the elimination of s_i from H means the fusion of the two cycles into one cycle; if $\{H, r\}$ is a bipartite graph, then the resultant subgraph by the fusion is also a bipartite graph; see Figure 2.

6. NONEXISTENCE OF KEKULÉ STRUCTURES IN MOLECULAR SUBGRAPHS

The argument of the foregoing sections is summarized as two theorems.

Theorem 1. *A subgraph* $H = \{e_i, t\}$ of $G = \{H, r\}$ is given. *Then* (1) $\leftrightarrow$ (2) $\rightarrow$ (3):

(1) *Both* b_i *and* $\bar{b}_i$ *are essential*.

(2) b_i, *such that* $b_i \leq \bar{b}_i$, *is essential*.

(3) $K\{H, r\} = 0$.

In Theorem 1, Lemma 13 derives item (2) from item (1); inversely, by use of Lemma 14, item (2) gives item (1). Equation (1) and Lemma 12 derives item (3) from (1).

Theorem 2. *A subgraph* $H = \{e_i, e_j, t\}$ *of* $G = \{H, r\}$ *is given* ($e_i \neq e_j$). *Then one of the following statements implies* $K\{H, r\} = 0$.

(1) *Both* b_i *and* $\bar{b}_j$, *such that* $b_i \leq b_j$, *are essential*.

(2) b_i *is essential, and* b_i *and* b_j ($b_i \leq b_j$) *are incompatible*.

(3) b_i, $\bar{b}_i$, b_j and $\bar{b}_j$ *are all essential*.

(4) $b_i \leq b_j$, $b_i \leq \bar{b}_j$, $\bar{b}_i \leq b_j$ *and* $\bar{b}_i \leq \bar{b}_j$.

(5) $\bar{b}_j$, *such that* $\bar{b}_i \leq b_j$ *and* $b_i \leq b_j$, *is essential*.

In Theorem 2, by means of Lemmas 14 and 15, item (1) leads to item (3). Lemma 7 and eq 2 give the sufficiency of item (2). Item (4) implies item (3) (Lemma 18); eq 2 suggests the sufficiency of item (3). The sufficiency of item (5) is proved by Lemma 8. We can observe that item (1) is satisfied in the subgraph (right) of Figure 2; i.e., the subgraph (right) is non-Kekuléan. Equation 3 therefore suggests that the subgraph (left) of Figure 2 is non-Kekuléan for any $\{r\}$.

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