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IRREGULAR NORMAL CORONOID HYDROCARBONS

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Abstract

The definition of 1/2 essentially disconnected single coronoid systems is extended to $1/n$ (n is a positive integer) essentially disconnected multiple coronoid systems. An equivalent definition of 1/2 essentially disconnected single coronoid systems is given. Some properties of $1/n$ essentially disconnected multiple coronoid systems are discussed.

1. Introduction

There has been considerable interest in the enumeration and classification of benzenoid and coronoid systems in the past few years [1-3]. The systems correspond in a natural way to benzenoid hydrocarbons and coronoid hydrocarbons [4]. A benzenoid system [4] is a finite connected subgraph of the infinite hexagonal lattice with no cut vertices or non-hexagonal internal face. A coronoid system [3] is obtained from a benzenoid system by deleting some internal vertices and/or internal edges so that at least one hole with the size of at least two hexagons emerges and is completely surrounded by hexagons. The so-called perfect matching of a benzenoid or coronoid system corresponds to the notion of Kekulé structure from organic and physical chemistry. Thus a Kekulé structure of a benzenoid or coronoid system is a set of disjoint edges covering all the vertices of the system. The significance of Kekulé structures or merely their number is well known in different branches of organic chemistry [5]. According to whether or not benzenoid or coronoid systems have Kekulé structures, the systems are divided into Kekuléan or non-Kekuléan systems. It was realized that Kekulé systems should be divided further to make the classification more appropriate for studies of Kekulé structure counts (i.e. the number of Kekulé structures).

It may happen that an edge of a Kekuléan system in a particular position is or is not selected in all Kekulé structures of that system. The fixed (double or single) bonds are just associated with such edges. The term "essentially disconnected"was used for the first time by Cyvin et al [6] to indicate those Kekuléan systems with fixed bonds. Kekuléan systems without fixed bonds are referred to as "normal". Therefore, the *neo* classification was introduced [7]. This concept stands for normal (n), essentially disconnected (e) and non-Kekuléan (o) benzenoid systems. The same classification can be applied to coronoid systems [8]. Later, extensive studies of Kekulé structures of coronoid systems demonstrated the need for a subdivision of normal coronoid systems. Among the normal single coronoid systems some peculiar systems were identified, which exhibited two schemes of Kekulé structures, each being associated with fixed bonds. The Kekulé structures of the two schemes gave the complete set of Kekulé structures (see Fig.1). These normal single coronoid systems are called 1/2 (half) essentially disconnected systems whose strict definition will be given in the next section. On the other hand, it was found that a subclass of normal single coronoid systems can be generated from a single hexagon by a series of normal additions and a corona-condensation [2]. These normal single coronoid systems are defined as regular single coronoid systems. Then a conjecture about the relation of 1/2 essentially disconnected single coronoid systems and regular single coronoid systems was proposed [2]: A normal single coronoid system which is not 1/2 essentially disconnected is regular. This conjecture was proved to be valid later [3]. As a consequence, the *rheo* classification was introduced: the single coronoid systems are classified into non-Kekuléan (o), essentially disconnected (e), regular (r) and 1/2 (half) essentially disconnected (h).

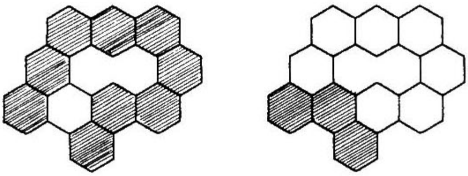

Fig.1 A 1/2 essentially disconnected single coronoid system.The two schemes for Kekulé structures are indicated (the effective units are hatched).

The definition of "regular" can be extended straightforwardly to multiple coronoid systems [9]. Therefore, an extension of the concept "1/2 essentially disconnected" is necessary when multiple coronoid systems are taken into account [10].

In this paper, we give an equivalent definition for 1/2 essentially disconnected single coronoid systems. Then the concept "1/2 essentially disconnected" is extended to "$1/n$ essentailly disconnected" in a natural way. Moreover, some properties concerning $1/n$ essentially disconnected coronoid systems are given.

2. Definitions and known results

It is known that benzenoid and coronoid systems are bipartite. In the following we may assume that the vertices of a coronoid system in question have been colored black and white so that the end vertices of each edge are differently colored. In the following drawings the black vertices are indicated by dots. Let G be a coronoid system, C_o the external boundary of G; C_1,C_2, ..., C_m the boundaries of the holes of G.

Definition 1 A straight line segment P_1P_2 is called an elementary cut segment from C_i to C_j if:

1. P_1 is the centre of an edge e_i on C_i, P_2 is the centre of an edge e_j on C_j;
2. P_1P_2 is orthogonal to both e_i and e_j;
3. every point of P_1P_2 is either an internal or a boundary point of some hexagon of G.

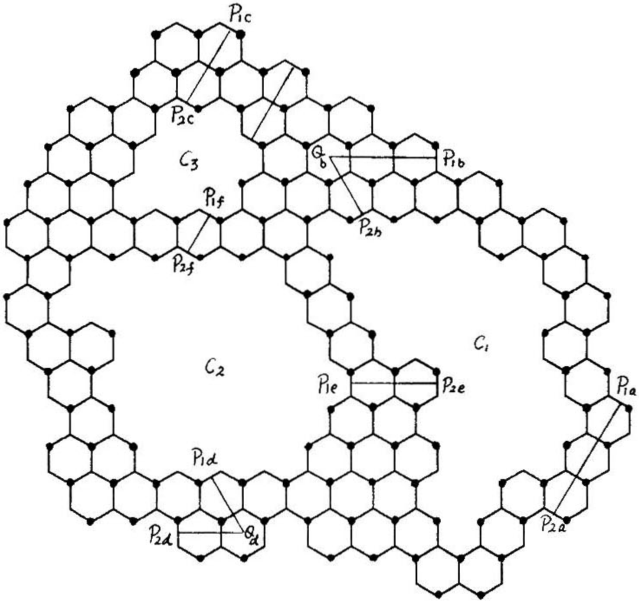

Fig.2 Illustrations of element cuts, generalized cuts and standard combinations.

Definition 2 A broken line segment P_1QP_2 is called a generalized cut segment from C_i to C_j if:

1. P_1 is the centre of an edge e_i on C_i, P_2 is the centre of an edge e_j on C_j, and Q is the centre of a hexagon of G;
2. P_1Q and P_2Q are orthogonal to e_i and e_j, respectively;
3. the angle P_1QP_2 is 60^o or 300^o;
4. every point of P_1QP_2 is either an internal or a boundary point of some hexagon of G.

Definition 3 An elementary cut (generalized cut) E_{ij} is the set of edges intersected by an elementary cut (generalized cut) segment from C_i to C_j. E_{ij} is said to be of type I if $i = j$. Otherwise, E_{ij} is said to be of type II.

Definition 4 Let $E_{i_1i_2}$ $E_{i_2i_3}, \ldots, E_{i_{t-1}i_t}, E_{i_ti_1}$ be pairwise disjoint elementary cuts or generalized cuts of type II, where $E_{i_ji_{j+1}}$ is an elementary cut or generalized cut from C_{i_j} to $C_{i_{j+1}}$, and $i_1 \neq i_2 \neq \ldots \neq i_t$; $E{=}E_{i_1i_2} \bigcup E_{i_2i_3} \bigcup \cdots \bigcup E_{i_{t-1}i_t} \bigcup E_{i_ti_1}$. E is said to be a standard combination if the end vertices of the edges of E have the same color when they lie in the same component of $G - E$, where $G - E$ is the subgraph of G obtained from G by deleting all the edges of E.

In Fig.2 let E_{01} be the generalized cut corresponding to the generalized cut segment $P_{1b}Q_bP_{2b}$, E_{12} the elementary cut corresponding to the elementary cut segment $P_{1e}P_{2e}$, E_{20} the generalized cut corresponding to the generalized cut segment $P_{1d}Q_dP_{2d}$.Then $E = E_{01} \bigcup E_{12} \bigcup E_{20}$ is a standard combination. While the two elementary cuts corresponding to elementary cut segments $P_{1c}P_{2c}$ and $P_{1f}P_{2f}$, respectively; and the generalized cut corresponding to the generalized cut segment $P_{1d}Q_dP_{2d}$ do not constitute a standard combination.

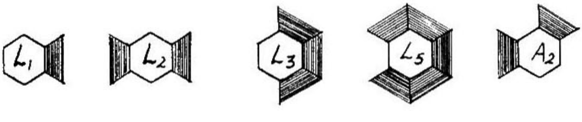

Fig.3 Five modes of hexagons in a coronoid system

Definition 5 A normal addition [2] is adding one hexagon to a benzenoid or coronoid system such that the added hexagon acquires the mode L_1, L_3 or L_5. A corona condensation [3] is adding one hexagon to a coronoid system such that the added hexagon acquires the mode L_2 or A_2 (see Fig.3). A normal tearing down is the opposite process of a normal addition. Similarly, a corona tearing down is the opposite process of a corona condensation.

Definition 6 A normal coronoid system with m holes [2,9] is said to be regular if it can be subjected to a series of normal tearings down plus m corona tearings down, each time only one hexagon being removed, right down to a single hexagon.

Definition 7 A normal single coronoid system G is said to be 1/2 essentially disconnected if and only if:

1. the set of Kekulé structures of G can be divided into two disjoint subsets K_1 and K_2;
2. $K_i(i = 1, 2)$ contains some fixed single bonds which form an elementary cut or generalized cut E_i of type II;
3. $E_1 \bigcup E_2$ is a standard combination.

Recall that for a Kekulé structure M of a coronoid system G, a cycle P is said to be an M−alternating cycle if the edges of P are alternately in M and $E(G) - M$, where $E(G)$ is the edge set of G.The following results are known:

Theorem 1 [3,9] A normal coronoid system G with m holes is regular if and only if there is a Kekulé structure M of G such that the external perimeter and all the perimeters of the holes are simultaneously M−alternating cycles.

Theorem 2 [3] A normal single coronoid system is 1/2 essentially disconnected if and only if it is not regular.

The above theorem guarantees that regular and 1/2 essentially disconnected single coronoid systems constitute a division of normal single coronoid systems.

3. An equivalent definition for "1/2 essentially disconncted"

Lemma 1 [11] Assume that G is a benzenoid or coronoid system.Let e', e and e'' be three consecutive edges of a hexagon s of G. Edges $e_1, e_2, ..., e_n$ are geometrically parallel to e, where e_n is on the external perimeter or the perimeter of some hole of G, while e_i is not on the external perimeter or the perimeter of any hole of G for $i = 1, 2, ..., n-1$. If e is a fixed single bond of G, and there is a Kekulé structure containing e' and e'', then all the edges $e_1, e_2, ..., e_n$ are fixed single bonds of G (see Fig.4)

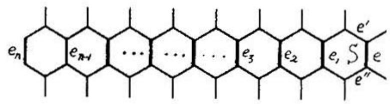

Fig.4 An illustration of Lemma 1.

Lemma 2 Let G be a coronoid system with a fixed single bond e on the external perimeter or the perimeter of some hole of G. Then e determines an elementary cut or generalized cut consisting of fixed single bonds of G.

Proof We distinguish two cases:

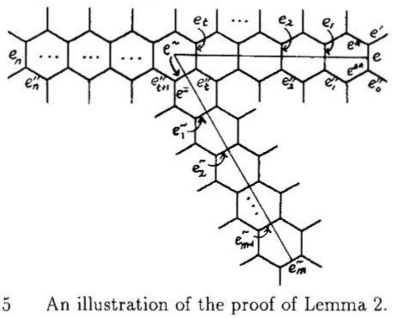

Fig.5 An illustration of the proof of Lemma 2.

Case 1 Edge e' is not a fixed double bond or e' does not belong to G (see Fig.5). Then there is a Kekulé structure M of G such that e^* is an M−double bond. If e^{**} is an M−double bond too, then by Lemma 1 all the edges $e_1, e_2, ..., e_n$ are fixed single bonds, where e_n is on some perimeter of G. Thus $\{e, e_1, ..., e_n\}$ is an elementary cut (if e and e_n are on the same perimeter of G) or a generalized cut (if e and e_n are on different perimeters of G) consisting of fixed single bonds of G. If e^{**} is an M−single bond, then e''_0 is an M−double bond. We consider the following two subcases.

Subcase 1.1 Edge e''_0 is a fixed doule bond of G. If all the edges $e''_1, ..., e''_n$ are fixed double bonds of G, then $\{e, e_1, ..., e_n\}$ is an elementary cut consisting of fixed single bonds of G. Now suppose that $e''_1, e''_2, ..., e''_t (t < n)$ are fixed double bonds, but e''_{t+1} is not a fixed double bond. Then there is a Kekulé structure M' of G such that $e^{=}$ is an M'−double bond. Edge e''_t is certainly an M'−double bond since it is a fixed double bond of G. Note that $e^{\sim}$ is a fixed single bond of G. By Lemma 1 all the edges $e^{\sim}, e^{\sim}_1, ..., e^{\sim}_m$ are fixed single bonds. Hence $\{e, e_1, ..., e_n, e^{\sim}, e^{\sim}_1, ..., e^{\sim}_m\}$ is a generalized cut consisting of fixed single bonds of G.

Subcase 1.2 Edge e''_0 is not a fixed double bond of G. Then there is a Kekulé structure $M^* \neq M$ such that e^{**} is an M^*−double bond. It is not difficult to see that the edges of $(M^* \bigcup M) - (M^* \bigcap M)$ constitute several M−alternating cycles, these cycles are also M^*− alternating cycles. Edges e''_0 and e^{**} belong to one of them, say C^*. We claim that e^* cannot be on C^*. Otherwise, an odd length cycle C^{**} consisting of a segment of C^* and the edge e is found, contradicting that G is bipartite. Now let $M^{\sim} = (E(C^*) \bigcup M) - (E(C^*) \bigcap M)$. Evidently, $M^{\sim}$ is a Kekulé structure of G. Both e^* and e^{**} are $M^{\sim}$−double bonds. $\{e, e_1, ..., e_n\}$ is a required elementary cut as mentioned at the beginning of Case 1.

Case 2 Edge e' is a fixed double bond. By the symmetry between e' and e''_0, it can be dealt with as in Subcase 1.2.

Lemma 3 [11] A coronoid system G is normal if and only if for each perimeter C of G , there is a Kekulé structure M of G such that C is an M−alternating cycle.

Lemma 4 [12] Let G be a Kekuléan coronoid system. Then G is essentially disconnected if and only if G possesses an elementary cut or generalized cut E of type I or a standard combination E of type II such that $|B(G_1)| - |W(G_1)| = |W(G_2)| - |B(G_2)| = 0$, where $G_i, i = 1, 2$ is the component of $G - E$ (the subgraph of G obtained from G by deleting all the edges of E), $|B(G_i)|$ and $|W(G_i)|$ are the numbers of black and white vertices of G_i, respectively.

Theorem 3 A normal single coronoid system G is 1/2 essentially disconnected if and only if there is a standard combination E of type II such that $|B(G_1)| - |W(G_1)| = |W(G_2)| - |B(G_2)| = 1$ or $|B(G_1)| - |W(G_1)| = |W(G_2)| - |B(G_2)| = -1$.

Proof **Necessity.** Let C_0 denote the external perimeter of G, C_1 the perimeter of the hole. $G' = G - C_0$ is the subgraph obtained from G by deleting all the vertices of C_0 together with their incident edges. If G' has some pendent edges, then these pendent edges are fixed double bonds of G', while those edges incident with the pendent edges are fixed single bonds. If G' has no pendent edges, then G' is a coronoid system. We infer that $G' - C_1$ has no Kekulé structures. Otherwise, $G - C_0 - C_1 = G' - C_1$ has Kekulé structures, and G is regular (Theorem 1), contradicting that G is 1/2 essentially disconnected and is not regular (Theorem 2). Hence G' is essentially disconnected (Lemma 3), and has fixed single bonds. We have proved that no matter G' has pendent edges or not, G' has fixed single bonds. Now delete from G' all the fixed single bonds , and all the fixed double bonds together with their end vertices. Denote the remaining subgraph by G''. Then each component of G'' is normal. We claim that in the process of deleting fixed bonds of G', the perimeter C_1 of the hole must be broken. If not, $G'' - C_1$ has Kekulé structures. Bear in mind that G'' is obtained from G by deleting the external perimeter C_0 and all the fixed bonds of $G' = G - C_0$. Hence, the fact $G'' - C_1$ has Kekulé structures implies that $G - C_0 - C_1$ has Kekulé structures, contradicting that G is not regular. There are two possibilities for C_1 to be broken. There may be a standard combination E of G' such that $|B(G_i)| = |W(G_i)|, i = 1, 2$, where G_1 and G_2 are the two components of $G' - E$; or there may be a fixed double bond which does not lie on C_1 but is incident with a vertex of C_1, say v. Assume that e_1 and e_2 are the two edges on C_1 whose common end vertex is v. Then e_1 and e_2 are two fixed single bonds of G'. By Lemma 2, e_i determines an elementary cut or generalized cut E_i consisting of fixed single bonds of G'. Note that E_i must be of type II. Otherwise, E_i is also an elementary cut or generalized cut of type I of G, and the edges of E_i are also fixed single bonds of G, contradicting that G is normal. It is not difficult to see that $E = E_1 \bigcup E_2$ is a standard combination. Now let $E_1 = \{e_1, e_{11}, ..., e_{1p}\}$, $E_2 = \{e_2, e_{21}, ... e_{2q}\}$, where e_1 and e_2 are on C_1, e_{1p} and e_{2q} are on the external perimeter of G'. Let e'_p (resp. e'_q) be the edges on C_0 which is parallel to e_{1p} (resp. e_{2q}) and is in the same hexagon with e_{1p} (resp. e_{2q}). Let $E'_1 = E_1 \bigcup \{e'_p\}$, $E'_2 = E_2 \bigcup \{e'_q\}$. It is evident that $E' = E'_1 \bigcup E'_2$ is a standard combination of G. Delete from C_0 the two edges e'_p and e'_q, C_0 is broken into two paths such that the end vertices of each path have the same color, namely, the difference between the numbers of white vertices and black vertices is 1 or

-1 for each path. Therefore, $|B(G_1)| - |W(G_1)| = |W(G_2)| - |B(G_2)| = 1$ or $|B(G_1)| - |W(G_1)| = |W(G_2)| - |B(G_2)| = -1$. The necessity is thus proved.
Sufficiency. Assume that G has a standard combination $E = E_1 \bigcup E_2$ such that for the two components $G_i, i = 1, 2$, $|B(G_1)| - |W(G_1)| = |W(G_2)| - |B(G_2)| = 1$ or $|B(G_1)| - |W(G_1)| = |W(G_2)| - |B(G_2)| = -1$. This means that for any Kekulé structure M of G, one and only one vertex of G_1 is matched by an edge of E_1 or E_2 to a vertex of G_2. Namely, one and only one edge of $E_1 \bigcup E_2$ is an $M-$double bond. Now denote by K the set of all Kekulé structures of G, K_i the set of Kekulé structures of G with an double bond in $E_i, i = 1, 2$. Then the edges of E_1 are fixed single bonds of K_2, and the edges of E_2 are fixed single bonds of K_1. By definition 7 G is $1/2$ essentially disconnected.

With the above theorem, we are now in the position to give an equivalent definition for $1/2$ essentially disconnected single normal coronoid systems.
Definition 7′ A normal single coronoid system G is said to be $1/2$ essentially disconnected if and only if there is a standard combination $E = E_1 \bigcup E_2$ such that $|B(G_1)| - |W(G_1)| = |W(G_2)| - |B(G_2)| = 1$ or $|B(G_1)| - |W(G_1)| = |W(G_2)| - |B(G_2)| = -1$

4. $1/n$ essentially disconnected coronoid systems

With the equivalent definition for $1/2$ essentially disconnected single coronoid systems, the definition of "$1/2$ essentially disconnected" can be extended in a natural way to irregular normal multiple coronoid systems.

Let G be a coronoid system, E an elementary cut or a generalized cut of G. Delete from G all the edges of E, and the pendent edges (if any) together with their end-vertices one by one until no pendent edge is found. Then each component of the remaining subgraph is said to be an effective unit of $G - E$. For example, in Fig.6 each of $G - E_{11}$ (above) and $G - E_{12}$ (below) has only one effective unit.

Definition 8 Two standard combinations $E_1 = E_{11} \bigcup ... \bigcup E_{1n_1}$ and $E_2 = E_{21} \bigcup ... \bigcup E_{2n_2}$ are said to be independent if E_1 is contained in the same effective unit of $G - E_{2i}$ for all $i = 1, ..., n_2$, or E_2 is contained in the same effective unit of $G - E_{1j}$ for all $j = 1, ..., n_1$(see Fig.6).

Definition 9 An irregular normal multiple coronoid system is said to be $1/n(n > 1)$ essentially disconnected if and only if there are $t(\geq 1)$ mutually independent standard combinations $E_i = E_{i1} \bigcup ... \bigcup E_{in_i} (i = 1, ..., t)$ such that for the two components $G_{ij}, j = 1, 2$ of $G - E_i$, $|B(G_{i1})| - |W(G_{i1})| = |W(G_{i2})| - B(G_{i2})| = 1$ or $|B(G_{i1})| - |W(G_{i1})| = |W(G_{i2})| - B(G_{i2})| = -1$, where $n = \prod_{i=1}^{t} n_i$.

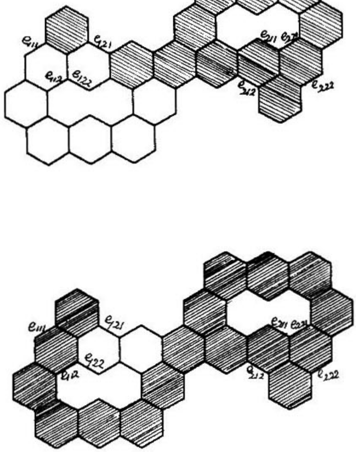

Fig.6 An illustration of Definition 8, where $E_1 = E_{11} \bigcup E_{12}, E_2 = E_{21} \bigcup E_{22}, E_{ij} = \{e_{ij1}, e_{ij2}\}$, for i,j=1,2.

In section 2 we already knew that for a normal single coronoid system, if it is not regular, then it must be 1/2 essentially disconnected. For irregular normal multiple coronoid systems, however, the situation is much more complicated. We have the following properties.

Property 1 An irregular normal multiple coronoid system needs not be $1/n$ essentially disconnected for $n > 1$. One can check that the multiple coronoid G_1 depicted in Fig.7 is normal since each of $G_1 - C_1$, $G_1 - C_2$ and $G_1 - C_3$ has Kekulé structures. G_1 is not regular since $G_1 - C_1 - C_2 - C_3$ has no Kekulé structure. But G_1 is not $1/n$ essentially disconnected (later we will know why this is so).

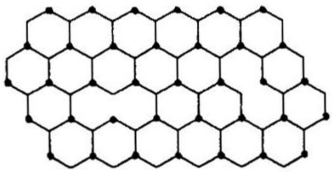

Fig.7 An irregular normal multiple coronoid system G_1 which is not $1/n$ essentially disconnected

Property 2 An irregular normal multiple coronoid system with m holes may be $1/n$ essentially disconnected for $2 \leq n \leq 2^m$. The irregular normal

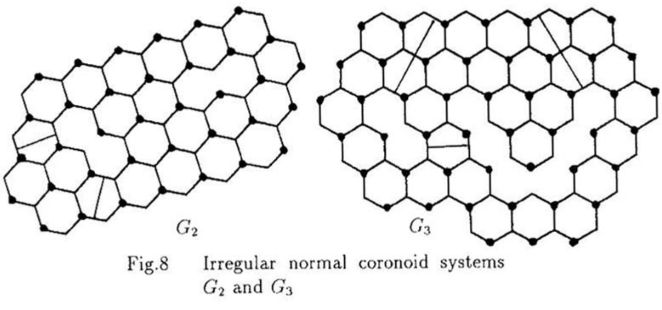

Fig.8 Irregular normal coronoid systems G_2 and G_3

coronoid systems G_2, G_3 (see Fig.8) and the coronoid system depicted in Fig.6 each with 2 holes are 1/2 essentially disconnected, 1/3 essentially disconnected and 1/4 essentially disconnected, respectively.

In the following we give a criterion for an irregular normal multiple coronoid system to be $1/n$ essentially disconnected.

Theorem 4 Let G be an irregular normal multiple coronoid system, C_0 the boundary of the external perimeter, $C_1, C_2, ..., C_m$ the boundaries of the holes. If there is a $C_i, (0 \le i \le m)$ such that $G - C_i$ is essentially disconnected and for $G - C_i$ there is a standard combination $E = E_{i_1 i_2} \bigcup E_{i_2 i_3} \bigcup ... \bigcup E_{i_{h-1} i_h} \bigcup E_{i_h i_1}$, where $E_{i_j i_{j+1}}$ is an elementary cut or generalized cut from C_{i_j} to $C_{i_{j+1}}$, satisfying $|B(G'_1)| - |W(G'_1)| = |W(G'_2)| - |B(G'_2)| = 0$, where $G'_i, i = 1,2$ is the component of $G - C_i - E$, then G is $1/h$ essentially disconnected.

Proof. One can check that if E is a standard combination of $G - C_i$ such that $|B(G'_1)| - |W(G'_1)| = |W(G'_2)| - |B(G'_2)| = 0$, where $G'_i, i = 1,2$ is the component of $G - C_i - E$, then $E^{*} = E \bigcup \{e_1, e_2\}$ is a standard combination of G such that $|B(G_1)| - |W(G_1)| = |W(G_2)| - |B(G_2)| = 1$ or $|B(G_1)| - |W(G_1)| = |W(G_2)| - |B(G_2)| = -1$, where $G_i, i = 1,2$ is the component of $G - E$, $e_i, i = 1,2$ is the edge on C_i which is parallel to an edge e_i^{*} of E and belongs to the same hexagon as e_i^{*}. By the definition of $1/n$ essentially disconnected, G is $1/h$ essentially disconnected.

It is not difficult to see that the condition in the above theorem is also necessary for an irregular normal multiple coronoid system to be $1/n$ essentially disconnected. Thus we can use the above condition as a criterion to determine whether or not an irregular normal multiple coronoid system is $1/n$ essentially disconnected. Now we can understand why the irregular normal coronoid system G_1 is not $1/n$ essentially disconnected for any integer $n > 1$. One can check that each of $G - C_i, i = 0,1,2$, is not essentially disconnected. Since many techniques and algorithms have been developed to recognize fixed bonds in a coronoid system [9-12], it is easy to know whether or not $G - C_i$ is essentially disconnected.

References

[1] B.N.Cyvin, J.Brunvoll and S.J.Cyvin (1992), in: I.Gutman, S.J.Cyvin (eds), Advances in the Theory of Benzenoid Hydrocarbons, Topics in Current Chemistry 162, Springer, Berlin.

[2] S.J.Cyvin, J.Brunvoll and B.N.Cyvin (1991), Theory of Coronoid Hydrocarbons, Lecture Notes in Chemistry 54, Springer, Berlin.

[3] S.J.Cyvin, J.Brunvoll, R.S.Chen, B.N.Cyvin and F.J.Zhang (1994), Theory of Coronoid Hydrocarbons II,Lecture Notes in Chemistry 62, Springer, Berlin.

[4] I.Gutman and S.J.Cyvin (1989), Introduction to the Theory of Benzenoid Hydrocarbons, Springer-Verlag.

[5] S.J.Cyvin and I.Gutman (1988), Kekulé Structures in Benzenoid Hydrocarbons, Lecture Notes in Chemistry 46, Springer-Verlag.

[6] S.J.Cyvin, B.N.Cyvin and I.Gutman, Z.Naturforsch, 40 a, 1253(1985).

[7] A.T.Balaban,J.Brunvoll,J.Cioslowski,B.N.Cyvin,S.J.Cyvin,I.Gutman, W.J.He,W.C.He,J.V.Knop,M.Kovačević,W.R.Muller,K.Szymanski,R.Tošić, N.Trinajstić,Z.Naturforsch,42a,863(1987).

[8] J.Brunvoll, S.J.Cyvin and B.N.Cyvin , J.Chem.Inf.Comput.Sci. 27(1987)14.

[9] R.S.Chen and F.J.Zhang, Discrete Applied Mathematics 74(1997) 147.

[10] S.J.Cyvin, B.N.Cyvin and J.Brunvoll, Chemical Physics Letters, 140(1987)124.

[11] F.J.Zhang and M.L.Zheng, Discrete Applied Mathematics, 36(1992), 67.

[12] R.S.Chen and F.J.Zhang, J.Molecular Structure 403(1997), 237.