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A NOTE ON PROPERTIES OF NORMAL BENZENOIDS AND CORONOIDS*

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ABSTRACT

A serious error of Theorem 7 in [1] is pointed out and the emergence of falsehood is analysed. An error on the total energies of essentially disconnected benzenoids is also pointed out.

The terms "benzenoid" and "coronoid" are defined in the usual way [2,3]. Thus a coronoid can be obtained from a benzenoid by deleting at least one internal vertex together with its incident edges, or one internal edge from a benzenoid such that each edge belongs to at least a hexagon (see Fig.1).

A benzenoid (coronoid) is said to be Kekuléan if it possesses Kekulé structures. In a given Kekulé structure of a benzenoid or a coronoid, if a circuit with h edges has h/2 conjugated

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double bonds, then it is called a conjugated circuit. Kekuléan benzenoid and coronoids are divided into two classes: the normal and the essentially disconnected according to whether or not they possess fixed bonds. It is known that the normal and the essentially disconnected behave quite differently [4]. The study of distinguishing the normal from the essentially disconnected is of importance in classification and enumeration of Kekuléan benzenoids and coronoids [5], and in certain enumeration techniques for Kekulé structures [6]. It also constitutes an interesting mathematical problem. Many attempts have been made to find criterions of normal benzenoids and coronoids [1,4,5,7-10]. The authors of [1] gave the following result after making convention that "whenever a Kekuléan system is mentioned, it involves a Kekuléan benzenoid or a Kekuléan coronoid, and the following theorems hold not only for benzenoids but also for coronoids" ([1], pp. 226-7): A Kekuléan system G is normal if and only is there exists a Kekulé structure K_e where the external perimeter C_e of G is a conjugated circuit (Theorem 7 in [1]).

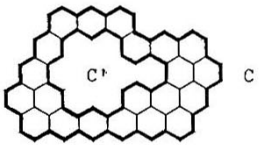


Fig.1 A coronoid with external perimeter C and internal perimeter C'.

Fig.2 A Kekuléan coronoid with a Kekulé structure where the external perimeter is a conjugated cycle, but not being normal.

Unfortunately, the above theorem is actually not valid for Kekuléan coronoids. A glance at the coronoid depicted in Fig.2 will indicate why this is so.

The error emerges from the proof of sufficiency. The authors of [1] first suppose that the external perimeter C_e is conjugated and in the interior of C_e an edge ab is fixed, and then claim " in the interior of C_e an alternating path passing through the edge ab can extend to and terminate on C_e ". But this assertion is not true. One can check that for the coronoid shown in Fig.2 the fixed single bond ab can never be on an alternating path with both ends on the external perimeter C_e.

In consequence of the falsehood of Theorem 7 in [1], the related results, i.e. Corollary, Theorem 8 and the proof of Theorem 9 are also false. Note that Theorem 9 itself is correct [5].

The necessary and sufficient conditions in the following theorems are the simplest ones which is known up to now.

<u>Theorem 1 [10].</u> A benzenoid is normal if and only if its perimeter is a conjugated circuit for some Kekulé structure.

<u>Theorem 2 [11].</u> A coronoid is normal if and only if each of the external and internal perimeters is a conjugated circuit for some Kekulé structure.

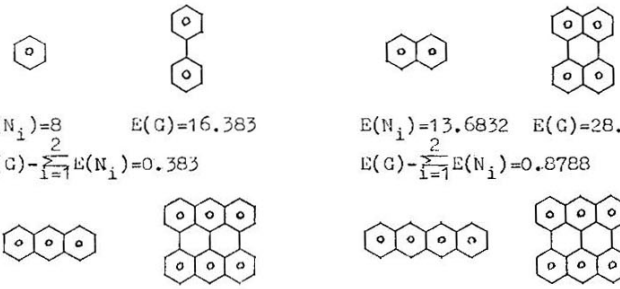
Now we point out another error in [1].

The total energies of essentially disconnected Kekuléan benzenoids were also considered in [1]. Let G be a Kekuléan benzenoid which contains two or more normal components $N_1, N_2, \ldots, N_s$ connected by fixed bonds. The authors of [1] claim that

$$E(G) = \sum_{i=1}^{s} E(N_i) \qquad \ldots\ldots \quad (1)$$

In fact this equation is not true. A glance at the examples shown in Fig.3 will indicate that the difference between two sides of equation (1) increases when the number of hexagons

increases.



$E(N_i)=8$ $E(G)=16.383$ $E(N_i)=13.6832$ $E(G)=28.2453$

$E(G)-\sum_{i=1}^{2}E(N_i)=0.383$ $E(G)-\sum_{i=1}^{2}E(N_i)=0.8788$

$E(N_i)=19.3137$ $E(G)=40.0778$ $E(N_i)=24.93$ $E(G)=51.9261$

$E(G)-\sum_{i=1}^{2}E(N_i)=1.4504$ $E(G)-\sum_{i=1}^{2}E(N_i)=2.0661$

Fig. 3

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