match no. 22 pp. 105-109 1987

THERE ARE EXACTLY EIGHT CONCEALED NON-KEKULÉAN BENZENOIDS WITH ELEVEN HEXAGONS

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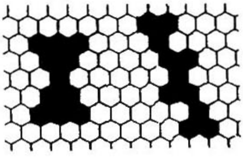
(Received: March 1987)

The eight smallest concealed non-Kekuléan benzenoids (K=0, Δ=0), which have been detected during the years 1974-1986, are proved to be the only existing systems of this kind (for h=11). They can all be built up from phenalene and triangulene units. The same feature is conjectures to be present in (obvious non-Kekuléan) benzenoid systems with $h = 3\Delta$.

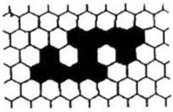
The existence of concealed non-Kekuléan benzenoids was pointed out by one of the present authors in 1974 [1]. These systems are non-Kekuléan (K=0) while Δ=0, i.e. they have the same number of black and white vertices (or peaks and valleys, or upright and upset triangles in the dualist graph). Those with Δ>0 are referred to as obvious non-Kekuléans.

In the mentioned work [1] two of the smallest concealed non-Kekuléans were discovered by trial and error. It was also stated that no such systems exist for h<11, where h is the number of hexagons. The two examples are:



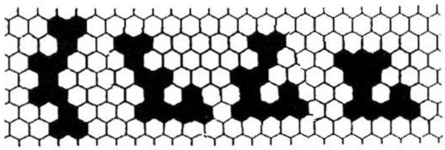
(1974) (1974)

Balaban [2] shares the credit for the first one of these systems between Gutman and Mallion (according to a personal communication). Balaban [3] also pointed out the existence of another concealed non-Kekuléan with h=11 in 1981:



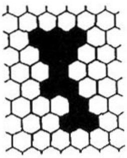
(1981)

One year later the same author [2] depicted four additional examples:



(1982) (1982) (1982) (1982)

Finally one more member was added to the list by Hosoya [4] in 1986:



(1986)

Independently of this work two of the present authors also detected the last concealed non-Kekuléan system in question [5]. In this paper we questioned whether the collection of eight smallest (h=11) concealed non-Kekuléans is complete.

Hosoya [4] devised the concept of inactive V-regions for obvious non-Kekuléans and used these systems as building stones for concealed non-Kekuléans. In this way he constructed the eight systems with h=11, K=0 and Δ=0. But he did not claim to have proved that these are the only concealed non-Kekuléans of that size. Especially the sign of interrogation in the title of Hosoya's paper indicates his uncertainty on this point. To-day we can answer that this is in fact the case: there are exactly eight smallest (h=11) concealed non-Kekuléans. Any further search for concealed non-Kekuléan benzenoids with eleven hexagons is futile.

In the meantime a successful search for concealed non-Kekuléans among the regular hexagonal (D_{6h} and C_{6h}) benzenoids was accomplished. It started with a work of Hosoya [6], who depicted a concealed non-Kekuléan D_{6h} benzenoid with h=43 and conjectured that this is the smallest system of that kind. Some of us [7] found three more examples of the same size and collected the four systems, one D_{6h} and three C_{6h}. Recently the regular hexagonal benzenoids were enumerated and classified by computer aid [8]. During this work it was definitely proved that no smaller system of this kind exists, and that there are five (not four) regular hexagonal non-Kekuléan benzenoids, one D_{6h} and four C_{6h}, among the total of 540 for h=43.

Turning back to the problem of concealed non-Kekuléans for h=11 we are faced with a quantitatively more complex task. Since the general problem of enumeration for h=11 was solved by Stojmenović et al. [9] we know that the question is whether the eight systems, which have been found, are the only concealed non-Kekuléans among the total of 120114 pericondensed benzenoids for h=11 (not counting the 21115 catacondensed systems, which are known to be Kekuléan).

As a matter of fact the Δ value can only change ± 1 or remain unchanged when one hexagon is added to a benzenoid. Therefore all benzenoids of h=11 and Δ=0 can be generated from the h=10 benzenoids with Δ=0 or Δ=1; their number was found to be 28131 together.

During the computer-generation [10] of h=11 benzenoids for every generated benzenoid it was tested whether Δ=0 and K=0 is fulfilled. The computation of Δ was performed by the program described elsewhere [10]. The K numbers were obtained by incorporating a procedure into the program, which basically follows the principles of Brown [11]. The benzenoids where Δ=K=0 was not fulfilled, were removed.

The computation resulted in a generation of exactly eight benzenoids, identical with the concealed non-Kekuléans reported above.

We observe that the eight concealed non-Kekuléans with h=11 can be described in the following way. They consist of two types of triangular conformations or triangles, viz. the smallest (phenalene) and the next-smallest (triangulene). Each member has either (a) two triangulenes, (b) one triangulene and two phenalenes or (c) four phenalenes. In each case one hexagon is shared by two triangles, whereby a perylene sub-unit emerges.

This pattern with the two smallest triangles resembles some forms encountered during a problem in which we have been engaged for a while, concerning the (obvious non-Kekuléan) benzenoid systems with maximum Δ values. We have demonstrated (by a reasoning invoking an inductive procedure) that

$$\Delta_{max} = \left[\frac{h}{3} \right]$$

In consequence, the smallest h value (h_{min}) for which a given Δ is realized, is

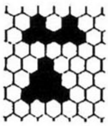
$$h_{min} = 3\Delta$$

Special attention was given to the benzenoids with h = 3, 6, 9, ... and Δ = 1, 2, 3, ..., respectively.

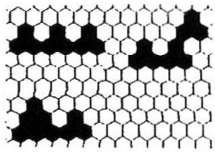
Conjecture: Benzenoids with $h = 3\Delta$ consist exclusively of fused phenalenes and triangulenes.

In this case there are no overlapping hexagons, and one apex from each triangle points the same way, conventionally upwards. The conjecture was verified by computer generation of the benzenoids for h = 3, 6, 9 and 12. The derived forms are shown below.

h=3

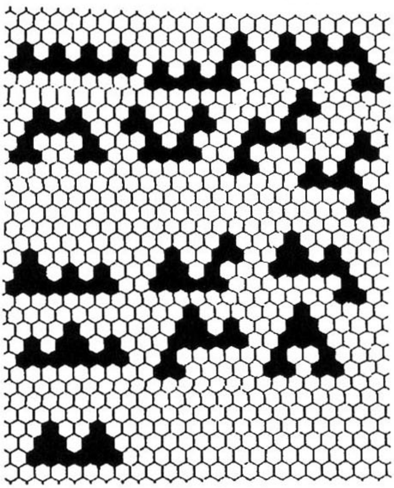


h=6



h=9

h=12



Acknowledgement: Financial support to BNC from the Norwegian Research Council for Science and the Humanities is gratefully acknowledged.

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