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RESEARCH NOTE:

EXTENDED APPLICATION OF AN ALGORITHM FOR THE NUMBER OF KEKULÉ STRUCTURES

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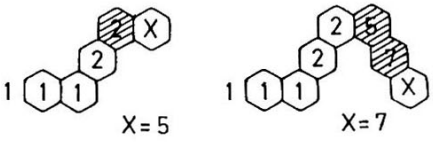
An algorithm has been launched for the number of Kekulé structures (K) of a single (catacondensed) chain by Cyvin and Gutman.[1] It is a modification of a similar well-known algorithm due to Gordon and Davison[2] and has recently been commented on by Živković and Trinajstić.[3] In the present note we give an alternative interpretation of the algorithm and extend it to the case of a single chain annelated to an arbitrary Kekuléan benzenoid, say B.

Single unbranched chain. An algorithm numeral, X, associated with a hexagon X, may be determined by the following rules. (1) Erase X and all hexagons preceding to it until the first kink is encountered. (2) Take the K number of the remaining chain. It may be obtained by adding numerals.

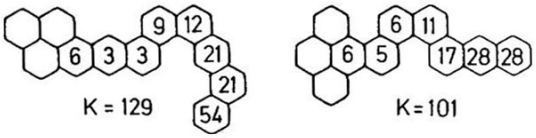
The rules are illustrated below for two numerals of Fig. 1 in Ref. 1.



The remaining chain in the above considerations corresponds to the concept of a "sub-benzenoid" in certain pericondensed systems.[1]

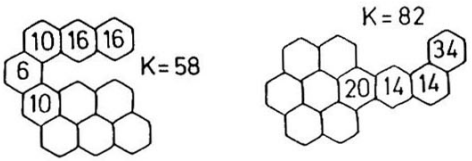
Single unbranched chain annelated to B. Analytical studies have been performed previously for a linear chain annelated to B,[4] and for an annelated zigzag chain.[5] The present algorithm will be adapted to chains with arbitrary kinks. By "annelation" we understand that the chain is added to B so that the two parts have exactly one edge in common.

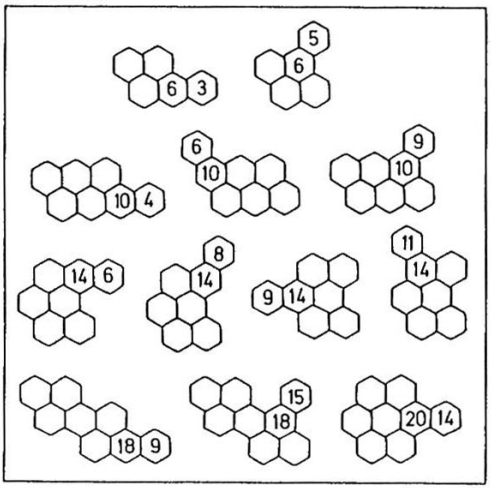
For the number of Kekulé structures set $K\{B\} = B$. Furthermore, let $K\{B'\} = B'$ pertain to a system where a double bond is assigned to the edge of annelation (e), or B' = B - e.[6] For pyrene (B=6) for instance, B' = 3 and B' = 5 for an (a)-type and (e)-type annelation, respectively. We give at once two examples of the algorithm:



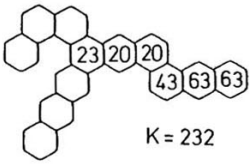
The systems may be treated in the same way as the single chain above. Hence the following rules may be formulated. (1) Start with B and B' on the two sides of the edge of annelation. (2) Continue with B' as long as a linear annelation is experienced. (3) After the first kink use the "sub-benzenoid" method (see above). (3) From now on either the "sub-benzenoid" method or the (simpler) rules for a single chain are applicable.

The chart (next page) shows all the basic (non-annelated) benzenoids with h (number of hexagons) ≤ 7, annelated with one hexagon in all (non-equivalent) positions. The numerals give information about B and B' in all cases. Below is an application of the chart for an annelation to anthanthrene and to coronene.





Single branched chain with one branching hexagon. The title system may be considered as an annelated single chain to B, where B itself is a single chain. Hence the above methods are applicable and may be useful in practice. Example:



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