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A NOTE ON THE NUMBER OF CIRCULENES

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"When things are going well,
something will go wrong."

Chisholm's Second Law[2]

Abstract

The numbers of the lowest isomeric (h)circulenes are as follows: (8)circulene - 1, (9)circulene - 5, and (10)circulene - 43. In our previous works (Refs. 3 and 4) there was an incorrect number (48) given for the isomeric (10)circulenes.

In his recent letter[5] Professor Cyvin[6] pointed out that there is a discrepancy concerning the count of circulenes with 10 hexagons in our publications.[3,4] He detected exactly 43 circulenes (or corona-condensed polyhexes)[7] with h=10, where h is the number of hexagons making up the polyhex.[8] Our published value was 48 circulenes with 10 hexagons.[3,4]

Even before the letter of Professor Cyvin, Professor Gimarc[13] remarked during our discussions on the computer enumeration and generation of chemical structures this spring in Athens, Georgia[14] that he was also involved in the enumeration of circulenes and has found only 43 (10)-circulenes.

The above prompted us to look through our records on the enumeration and generation of polyhexes, and to repeat the computations for the lowest isomeric (h)circulenes. The records show that the value obtained for the isomeric (10)circulenes was 43 and that the value of 48 which appeared in the paper published here[3] was a result of typing error which remained unfortunately undetected. Later the same value (48) was used without checking in our book on computer generation of certain classes of molecules.[4] Therefore, the correct values for the lowest isomeric (h)-circulenes are as follows:

(h)circulene	the number of isomeric forms
(8)	1
(9)	5

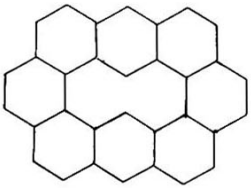
(10) 43

Graphs corresponding to the lowest isomeric circulenes are given in the Figure.

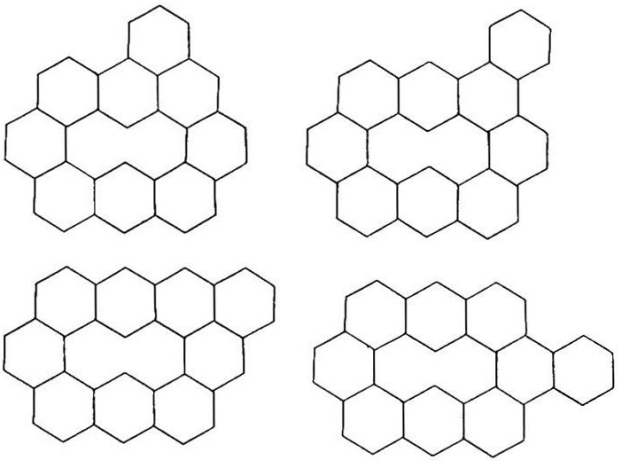
Figure

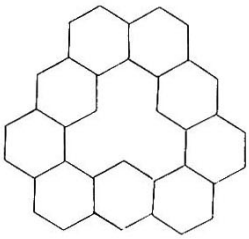
Diagrams of the lowest isomeric (h)circulenes

(i) (8)circulenes

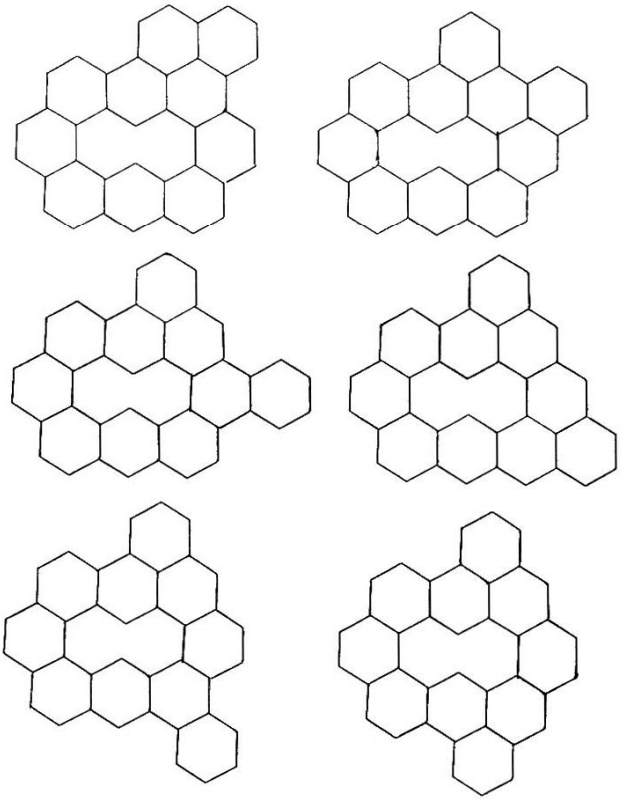


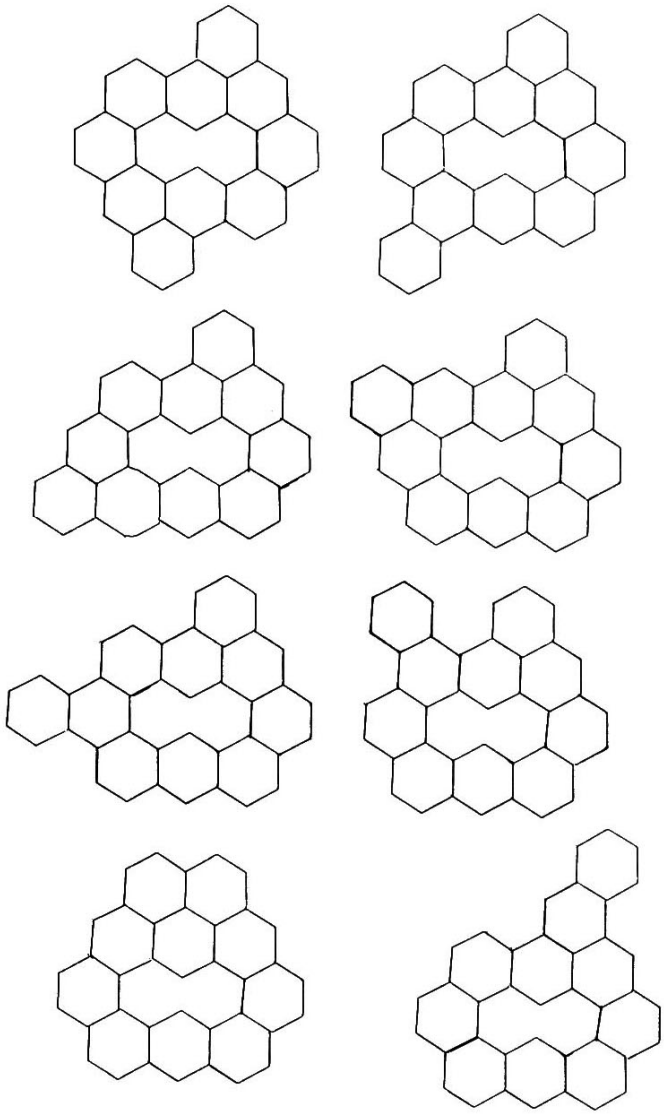
(ii) (9)circulenes

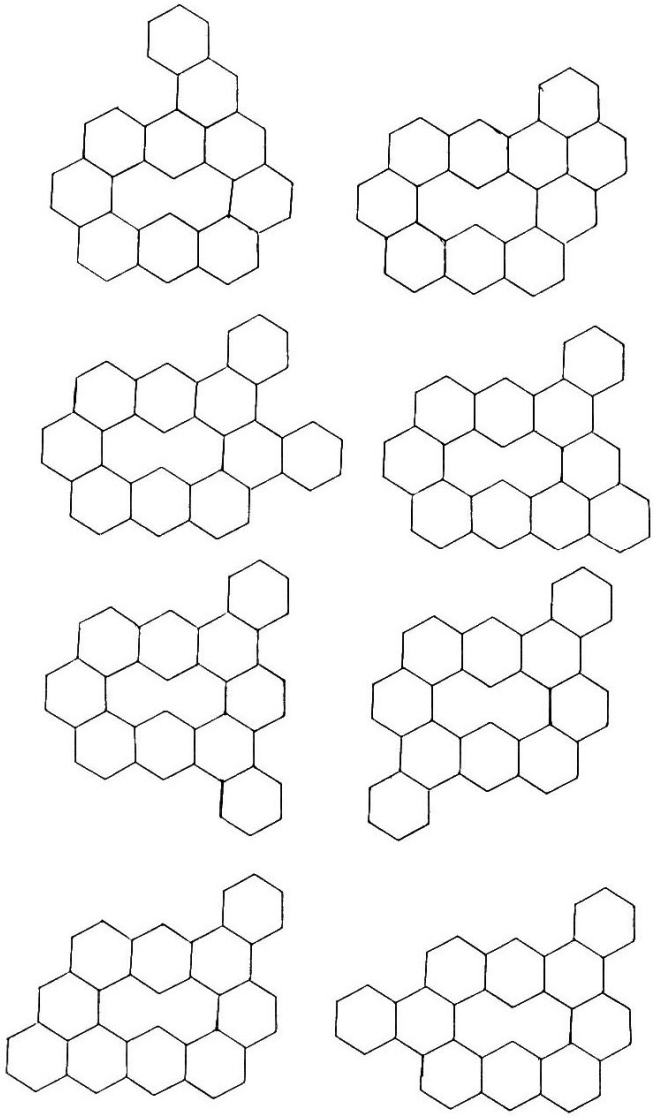


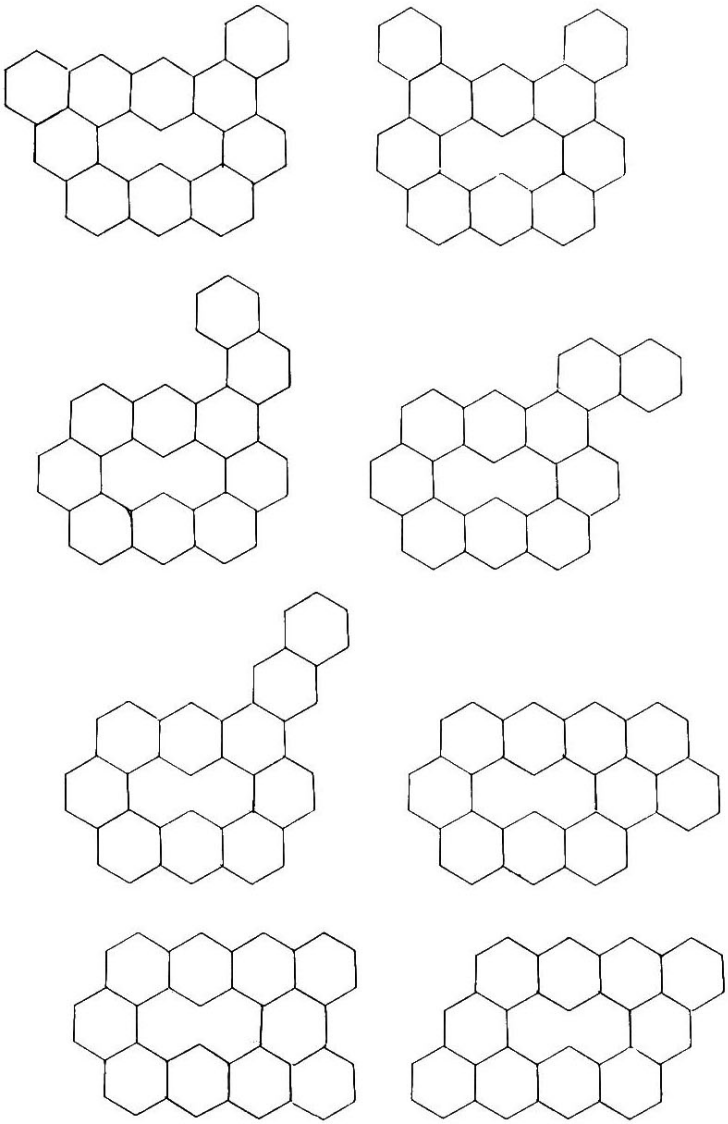


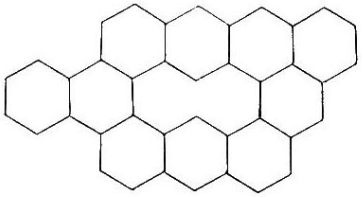
(iii) (10)circulenes

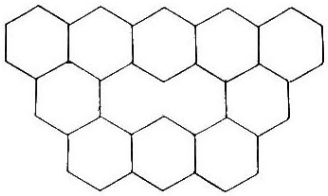


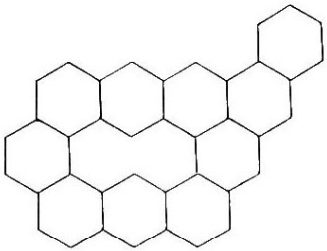


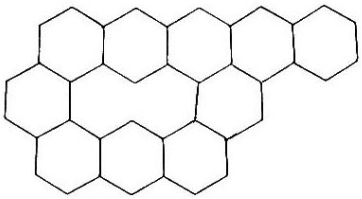


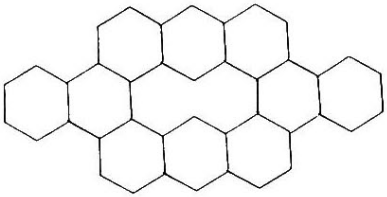


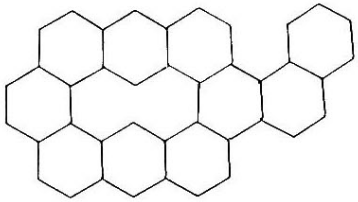


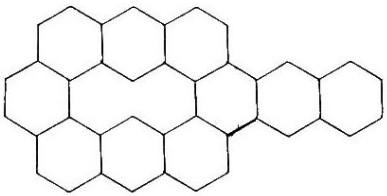


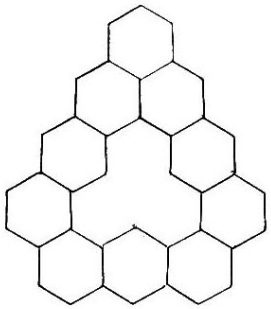


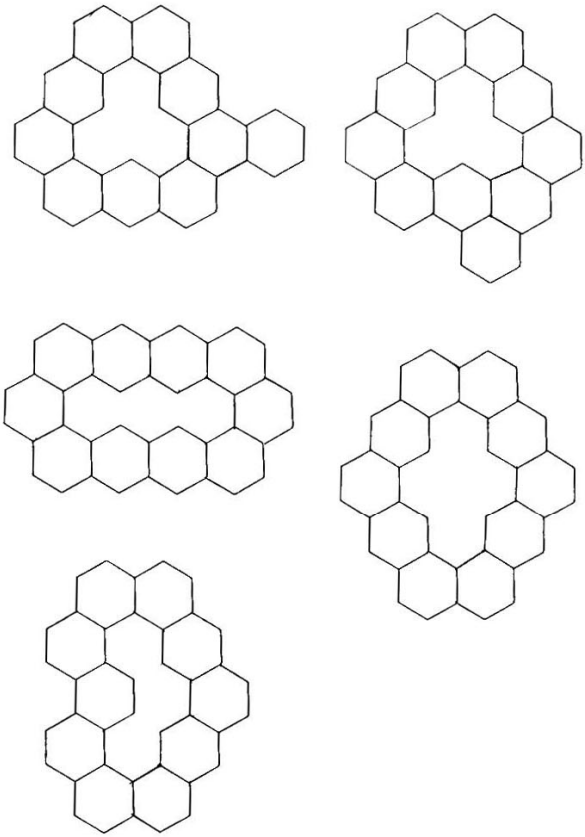












We also detected an error in the grand total number of polyhexes with h=10. This number (34350) should be corrected to 34347 (total number of geometrically planar simply connected 10-polyhexes: 30086 + total number of planar mono-10-circulenes: 404 + total number of 10-helicenes wi-

thout holes: 3857). This error was due to incorrect summation of three sets of numbers above stated. The total numbers of polyhexes (with the contributing terms) with up to 10 six-membered rings are given in the Table.

Table

The total number of polyhexes

Number of hexagons	Number of geometrically planar simply connected polyhexes	Number of planar mono-circulenes	Number of helicenes without holes	Grand total number of polyhexes
1	1			1
2	1			1
3	3			3
4	7			7
5	22			22
6	81	1	1	83
7	331	2	8	341
8	1435	13	71	1519
9	6505	67	542	7114
10	30086	404	3857	34347

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8. Circulenes are polyhexes with holes.[9] A hole is a (N)-annulene-like internal cycle, where N is the size of a cycle. The size of the inner cycle must be $N \geqslant 10$ in order that the polyhex is a "true" circulene. Thus, the smallest "true" circulene, (8) circulene, contains eight hexagons. Note, that circulenes are also referred to as corrannulenes.[10-12]

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