

## CHEMICAL GRAPHS—XII<sup>1</sup> CONFIGURATIONS OF ANNULENES

A. T. BALABAN

Institute of Atomic Physics, P.O.B. 35, Bucharest, Roumania

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**Abstract**—A procedure is developed for finding out all possible configurations of annulenes (both single- and multiple-edge configurations). An exhaustive table for these geometric (*cis-trans*) isomers of all annulenes up to [20]annulene is presented. Every configuration is given a notation by assigning to each edge one of three possible digits indicating its direction.

### INTRODUCTION

IN PREVIOUS papers of this series<sup>2,3</sup> all possible valence-isomers of annulenes were enumerated, disregarding considerations of geometrical isomerism. The purpose of the present paper is to find out a procedure for obtaining all possible *cis-trans* configurations of one valence-isomer, the conjugated cyclopolyenic structure of each annulene  $(\text{CH})_{2n}$ . Other steric factors will be taken into account later; in the beginning, the annulene will be regarded as a closed circuit formed from  $2n$  edges which can only meet at angles of  $120^\circ$ .

The analogous problem for conformations of saturated cycloalkanes was investigated by M. Saunders<sup>4</sup> using a computer programme for finding out medium and large rings superimposable with the diamond lattice; recent investigations<sup>5</sup> show that these are the preferred conformations adopted by cycloalkanes. However, Saunders included other steric factors in the programme discarding from the outset closed circuits with degenerate edges (corresponding to the multiple-edge configurations below).

In a restricted sense, we are interested in finding out all possible closed circuits on a graphite lattice. However, in a more general way, we will also allow multiple-edge circuits in which one or more edges of the graphite lattice can be used more than once ("degenerate or multiple edges"). The example of the helicenes<sup>6</sup> shows that non-planar structures superimposable with the graphite lattice do not introduce insuperable steric strain.

### *Notations, definitions and rules*

To arrive at a numerical notation for any possible configuration, we will use the method first employed by Gordon<sup>7</sup> assigning to the three possible directions of lines in the graphite lattice numbers 1, 2 and 3, as shown in Fig. 1 I (the same method was subsequently followed by Saunders<sup>4</sup> and by us<sup>8</sup>). One could distinguish between the two senses in which these directions are followed, as shown in Fig. 1 II by + and –

signs but this is not necessary because the signs always alternate, e.g. benzene 123123 (Fig. 1 II) will be represented by the simplified notation 123123 (as from Fig. 1 I).

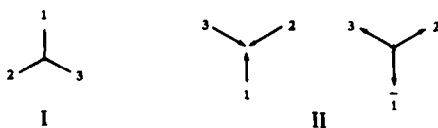


FIG. 1. Conventions of numbering the directions (I) or the directions and senses (II) of edges in the graphite lattice.

The following definitions and rules apply to a circuit :

### Definitions

1. A sequence of three edges is called *cis* whenever it can be noted by 123, or any permutation thereof, otherwise *trans* (e.g. when it can be noted 121).
2. A configuration is called a *single-edge configuration* when no edge is degenerate ; in a *multiple-edge configuration*, one or more edges are degenerate. It must be emphasized that although *single-edge configurations* can be coplanar, this is not a necessary condition (as in the graph theory where a planar graph, e.g. a convex polyhedral graph, is not necessarily embedded in a plane).

### Rules

1. The notation of a circuit consists of a cyclic sequence of  $2n$  digits 1, 2, and 3, so that no two adjacent digits are identical. This represents the fact that edges meet at  $120^\circ$  angles.
2. In the notation of a circuit the number of digits of one kind in even positions equals the number of digits of the same kind in uneven positions (in the notation of Fig. 1 II the sum of digits of the same kind must be zero). One can express this rule differently, by noting that the sequence of digits in even positions is a permutation of the sequence of digits in odd positions. This is the condition for ring closure.<sup>4</sup> All three kinds of digits must be present, otherwise no circuit can result. This rule explains why the number of edges must be even,  $2n$ .
3. By breaking the cyclic sequence in a point, a linear sequence is obtained. From all possible alternative linear sequences (resulting from various points where the numbering can start and from which of the two alternative senses is selected) that one is selected which results in the smallest number. This rule<sup>4,7</sup> assigns an unequivocal notation for each circuit. It results in the fact that the first two digits are always 12, and that the numbering starts at the point which gives the most numerous initial *trans* sequences.
4. The last digit is either 2 or 3. This rule eliminates such structures as 12132121 (III) which do not represent a circuit, and is derived from the fact that the sequence of digits is cyclic (rule 1) so that the first and last digits cannot be identical.



### Enumeration of single-edge configurations

The restricted problem of the single-edge configurations is simpler to solve, taking into account only the outer contours of *cata*-\* or *peri*-condensed benzenoid aromatic hydrocarbons (polyhexes).

The enumeration and nomenclature of *cata*-condensed benzenoid hydrocarbons (catafusenes) was solved by graph-theoretical methods;<sup>8-10</sup> computer programmes for enumerating *peri*-condensed hydrocarbons have also been devised. Such *peri*-condensed systems (perifusenes) have not yet been amenable to mathematical treatment. However, instead of the number of condensed benzenoid rings which was the enumeration parameter for condensed hydrocarbons, for the present problem the number ( $2n$ ) of edges in the circuit is the enumeration parameter.

If the polyhex is represented by its characteristic graph formed from  $h$  vertices† placed in the centers of hexagons, with the adjacency condition that two condensed hexagons lead to adjacent vertices, then catafusenes have characteristic graphs without circuits, whereas characteristic graphs of perifusenes have circuits. With the exception of coronaphenes which will not be considered here, characteristic graphs of perifusenes have circuits of three edges. Let the number of such triangles be represented by  $t$ . For catafusenes,  $t = 0$ , whereas for perifusenes excluding coronaphenes,  $t > 0$ .

The perimeter of such a polyhex (catafusene or perifusene) can be shown to be a single-edge configuration with  $2n = 4h - 2t + 2$  edges. This formula indicates that the perimeters of catafusenes are Hückel-type annulenes, *i.e.* have uneven  $n$  values, whereas those of perifusenes can be either Hückel-type or anti-Hückel-type annulenes.

Based on enumerations of *cata*- and *perifusenes* indicated above,<sup>8-11</sup> the numbers of single-edge configurations of  $[2n]$ annulenes up to and including  $n = 10$  are presented in Table 1. If the computed numbers of perifusenes were listed according to the number of triangles  $t$  of their characteristic graphs in addition to the listing<sup>9, 11</sup> according to the number of hexagons (or vertices of the characteristic graph)  $h$ , it would be easy to extrapolate Table 1 to higher values of  $2n$ .

### Procedures for finding all possible configurations of annulenes

Though a formula allowing the enumeration of configurations has not yet been found, a recurrence procedure is devised in Table 2, in terms of "homologation operations", for increasing the size of the circuit with  $\Delta n$  edges.

By means of this procedure the following configurations for annulenes up to  $[20]$ -annulene were found. Those of  $[6]$ - to  $[16]$ annulenes are listed in Table 3 together with their notations, those of  $[18]$ annulenes are given in Table 4, and those of  $[20]$ -annulenes in Table 5.

In Tables 3-5, characteristic graphs of polyhexes whose perimeters are single-edge configurations are shown within these configurations. Notations of multiple-edge configurations are enclosed in brackets (those of single-edge configurations do not have brackets) in Table 3. In Tables 3-5, single-edge configurations precede multiple-edge ones. The latter are arranged in the order of increasing number of degenerate edges. In addition, as a subordinate criterion, configurations are arranged in the increasing order of the areas they enclose.

\* Some multiple-edge solutions are also hereby obtained, *e.g.* from hexahelicene or higher helicenes.

† The number of hexagons in the polyhex is  $h$ .

TABLE 1. SINGLE-EDGE CONFIGURATIONS OF  $[2n]$ ANNULENES AS PERIMETERS OF CATAFUSENES OR PERIFUSENES






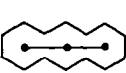
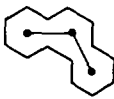

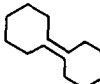
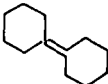


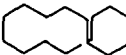
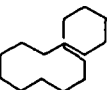
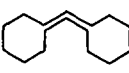
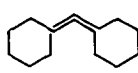
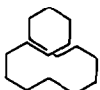

Catafusenes ( $t = 0$ )		Perifusenes ( $t > 0$ )			Total no. of single-edge configurations	Perimeter $2n = 4h - 2t$ $+ 2$
No. of hexagons $h$	No. of catafusenes	No. of hexagons $h$	No. of triangles $t$	No. of perifusenes		
1	1	—	—	—	1	6
—	—	—	—	—	0	8
2	1	—	—	—	1	10
—	—	3	1	1	1	12
3	2	4	2	1	3	14
—	—	4	1	1	2	16
—	—	5	3	1		
—	—	5	2	3	12	18
4	5	6	4	3		
—	—	7	6	1		
—	—	5	1	6	14	20
—	—	6	3	4		
—	—	7	5	3		
—	—	8	7	1		

TABLE 2. HOMOLOGATION OPERATIONS FOR INCREASING THE SIZE OF THE CIRCUIT WITH  $\Delta n$  EDGES

$\Delta n$	Operation	Configuration	
		Initial	Final
0	Rotation of <i>cis</i> -dienic portion		
	By-passing of a vertex		
2	Double bridging		
	Insertion of two vertices		
4	Annelation		
6	Benzologation <sup>a</sup>		
		etc.	etc.
8	Insertion of a loop		

<sup>a</sup> *I.e.* construction of a multiple-edge structure out of the initial configuration and a benzene ring which has 1 to 6 edges overlapping with the initial configuration.

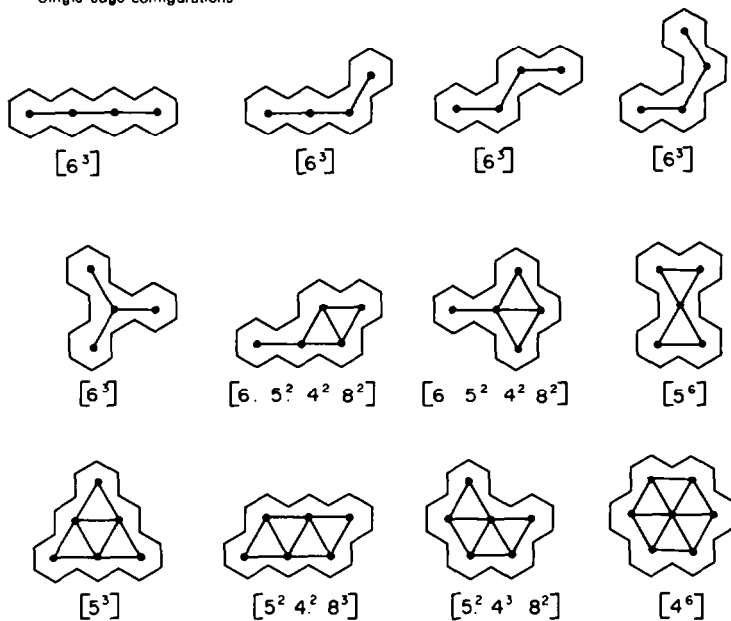
TABLE 3. CONFIGURATIONS AND NOTATIONS OF  $[2n]$ ANNULENES<sup>a</sup>

$2n$	Number of configurations			Configurations
	Total	Single edge	Multiple edge	
6	1	1	0	 123123 [-]
8	0	0	0	—
10	1	1	0	 1212312123 [6]
12	3	1	2	   121231312323      (121321323123)      (123123123123) [5 <sup>3</sup> ]
14	5	3	2	     12121231212123      121231213121313      12123131212313      (121312312131231)      (12121321313123) [6 <sup>2</sup> ]      [6 <sup>2</sup> ]      [5 <sup>2</sup> 4 <sup>2</sup> 8 <sup>2</sup> ]
16	8	2	6	    1212123121312323      1212123131212323      (1212312123213213)      (1212132121323123) [6, 5 <sup>3</sup> ]      [5 <sup>2</sup> 4 <sup>2</sup> 8 <sup>2</sup> ]
				    (1212123123213123)      (1212312321213213)      (1212312132132123)      (1212312123123123)

<sup>a</sup> Symbols in square brackets under formulas in this and subsequent tables are defined by figure 2 below.

TABLE 4. CONFIGURATIONS OF [18]ANNULENES

Single-edge configurations



Multiple-edge configurations

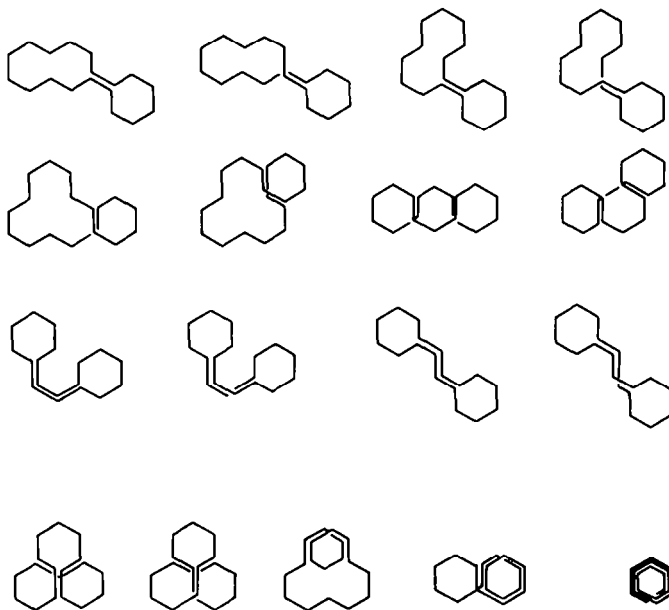
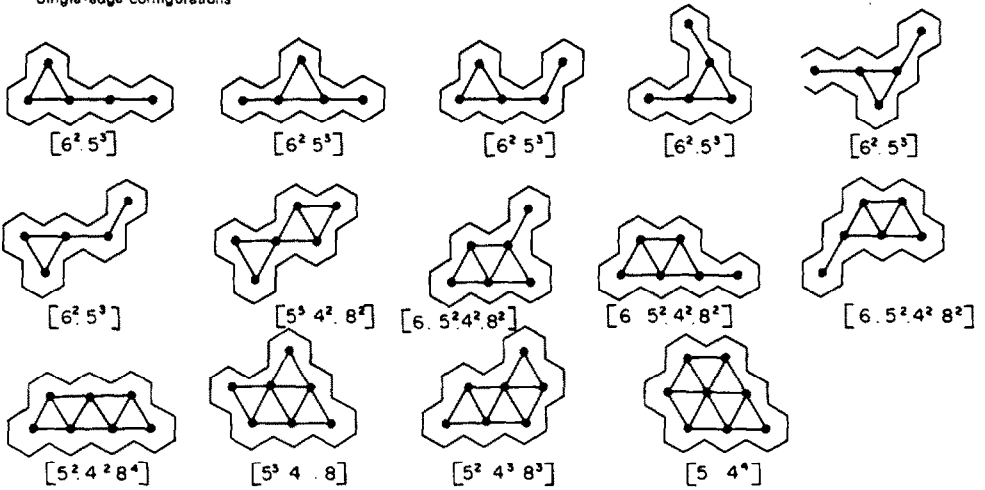


TABLE 5. CONFIGURATIONS OF [20]ANNULENES.

Single-edge configurations



Multiple-edge configurations

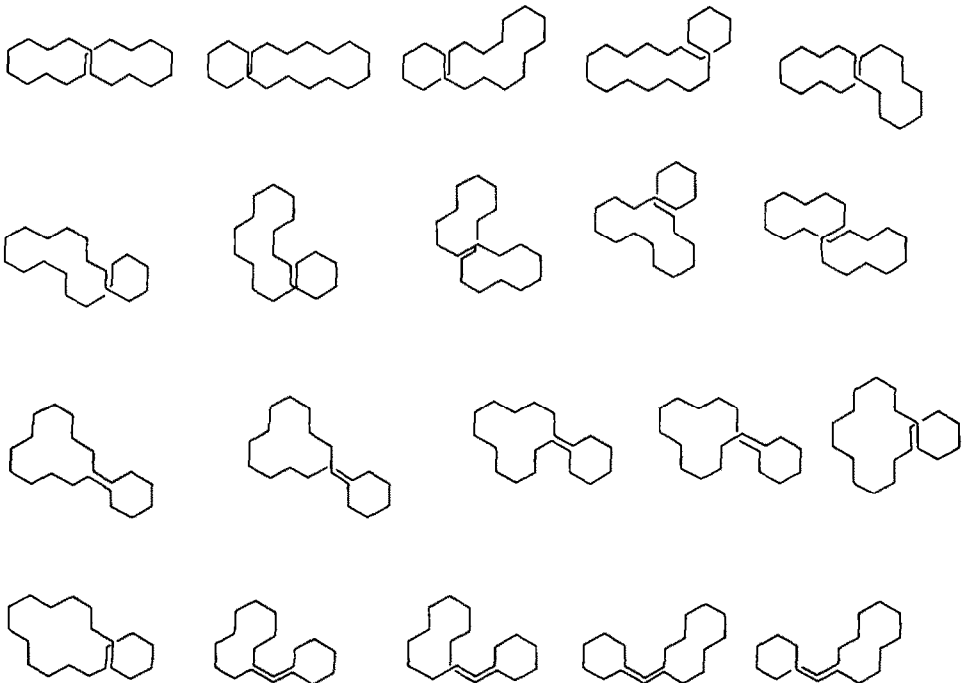
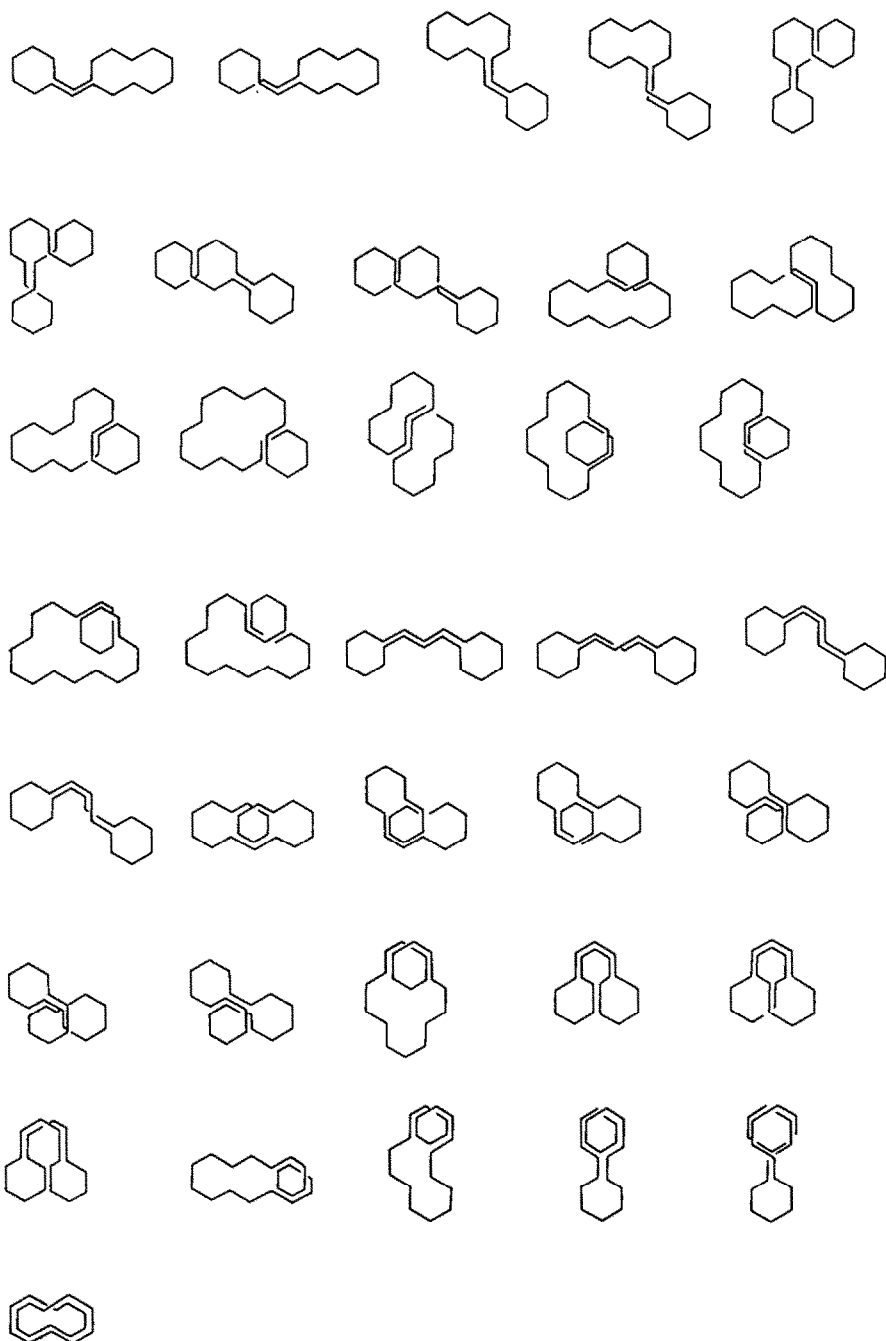




TABLE 5 (Continued)



The numbers of configurations increase steeply with increasing  $n$ , and of multiple-edge configurations more rapidly than of single-edge ones.

Owing to rule 2, the notation of Hückel-type annulenes (with odd  $n$ ) can consist of two identical halves of  $n$  digits, whereas that of anti-Hückel annulenes (with even  $n$ ) cannot, unless all edges are evenly degenerate.

Whenever in a multiple-edge configuration, two vertices are connected only by an evenly ( $2k$ ) degenerate path (not counting paths due to benzologation *cf.* Table 2),  $k + 1$  "cross-isomeric" multiple-edge configurations can result, as illustrated by the first and second multiple-edge configurations for  $2n = 14$  or  $16$  ( $k = 1$ ), or by the two triplets ( $k = 2$ ) for  $2n = 20$ . In turn, the isomers with "crossing bonds" could exist in chiral enantiomers as will be mentioned later.

An alternative procedure for enumerating configurations of annulenes, which could be computerized, is based on the notations introduced above.

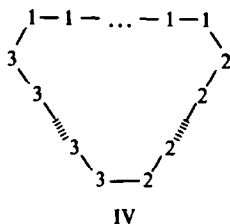
To generate numerically the configurations of a  $[2n]$ annulene, the partitions of  $n$  into three non-zero integers  $n_1$ ,  $n_2$  and  $n_3$  are considered (their number equals the number of the partitions of  $n-3$  into up to three integers)<sup>12</sup>:

$$n = n_1 + n_2 + n_3.$$

Then the cyclic permutations of  $n_1$  symbols 1,  $n_2$  symbols 2, and  $n_3$  symbols 3 are listed (their number can be calculated either by an algebraic procedure,<sup>13</sup> or by applying Pólya's theorem<sup>14</sup>).

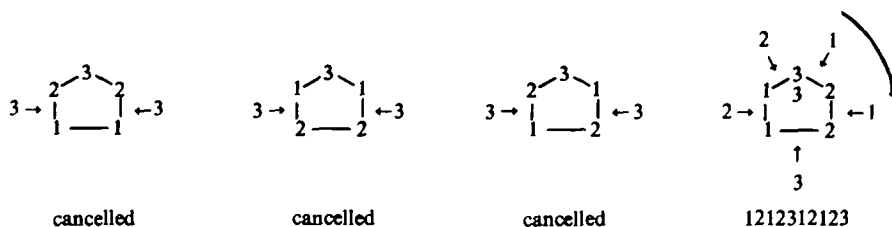
Between the  $n$  symbols of each cyclic permutation derived from a given partition,  $n$  further symbols are inserted by one of the following alternative operations: between two different symbols, the third is inserted; between two identical symbols, one of the other two symbols is inserted so that the totality of inserted symbols adds to the given partition. If  $n_1 \geq n_2 \geq n_3$ , only permutations based on partitions for which  $n_1 \leq n_2 + n_3 - 1$  lead to cyclic sequences of symbols because the highest allowed number of symbols 1 to be inserted is achieved when all symbols 2 and 3 are grouped in one chain (IV); in this case the number of intervals in this chain is  $n_2 + n_3 - 1$ . Some of these permutations can allow several collections of inserted symbols, leading to different cyclic sequences.

The cyclic sequence of symbols is then denoted by the linear sequence which corresponds to the smallest number according to rules 3 and 4 above.



For instance with  $n = 5$  two partitions of 5 into three non-zero integers are possible:  $3 + 1 + 1$  and  $2 + 2 + 1$ ; only the latter partition satisfies the condition  $n_1 \leq n_2 + n_3 - 1$  ( $2 = 2 + 1 - 1$ ) and gives rise to four cyclic permutations. Three of these

cannot lead to  $n$  inserted symbols adding up to the same partition and are therefore cancelled, leaving one cyclic sequence.



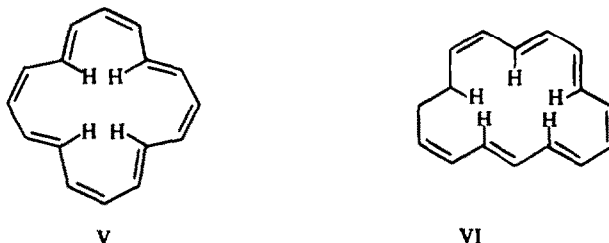
Some permutations afford pairwise the same sequence of symbols (the permutation and the sequence of inserted symbols being complementary); finally, some sequences are equivalent by cyclic permutations of the three symbols. This is illustrated in Table 6 for  $2n \leq 14$ .

TABLE 6. NUMERICAL DERIVATION OF CONFIGURATIONS OF  $[2n]$ ANNULENS

2n	Partition of n			Number of			
	$n_1$	$n_2$	$n_3$	permutations	cyclic sequences	linear sequences	configurations
6	1	1	1	1	1	1	1
8	2	1	1	2	—	—	—
	3	1	1	2	—	—	—
	2	2	1	4	1	1	1
10	4	1	1	3	—	—	—
	3	2	1	6	—	—	—
	2	2	2	11	8	5	3
12	5	1	1	3	—	—	—
	4	2	1	9	—	—	—
	3	3	1	10	1	1	1
	3	2	2	19	6	4	4
14	6	1	1	4	—	—	—
	5	2	1	12	—	—	—
	4	3	1	19	—	—	—
	4	2	2	33	—	—	—
	3	3	2	38	22	10	8

### Other steric factors

The configurations so far presented are not the only ones annulenes may adopt. In a particularly illuminating series of papers this was demonstrated by Oth, Schröder *et al.* for [16]annulene which adopts the interconverting configurations V and VI;<sup>15a</sup> monosubstituted [16]annulenes interconvert more slowly and contain relatively more VI than the unsubstituted [16]annulene.<sup>16</sup> On the contrary, the dianion of [16]annulene which owing to its aromaticity is more planar, adopts configuration V,<sup>15b</sup> which when planar has less overcrowding but possesses angles different from 120°.



There are two further steric factors to be taken into account in such cases.

(1) Steric repulsions between inner hydrogens (more severe in VI than in V), result in distortions of the bond angles, bond lengths and planarity of the molecule to alleviate these steric repulsions.

This increases the energy of the molecule and makes the configuration of comparable energy with configurations such as V which are not superimposable with the graphite lattice.

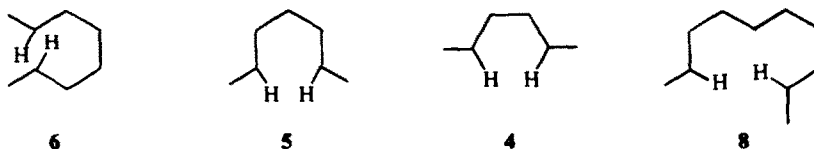


FIG 2. Non-bonding interactions between inner hydrogens: 1,6; 1,5; 1,4; and 1,8

In the order of decreasing steric strain, the repulsions between inner hydrogens can be classified as 1,6-, 1,5-, 1,4- and 1,8-interactions. Scale diagrams for several annulenes are available.<sup>17</sup> As shown in Fig. 2, these 1, *m*-interactions will be noted by the latter digits *m*. In Tables 3–5, under each single-edge configuration, its non-bonded interactions are shown as products of  $m_i^{k_i}$  where each  $k_i$  gives the number of 1, *m*<sub>*i*</sub>-interactions. These products are enclosed in square brackets.

(2) Multiple-edge configurations with crossing bonds can lead to chiral molecules. This is a very attractive field for speculations, but detailed discussions are premature at this stage.

*The least overcrowded single-edge configurations of annulenes superimposable with the graphite lattice*

Consideration of Tables 1 and 3–6 evidences that the least overcrowded configurations of annulenes are single-edge configurations with the largest enclosed areas or,

equivalently, are perimeters of perifusenes whose characteristic graphs have the highest number of triangles.

For a given length  $2n$  of the circuit, equal to the number of carbon or hydrogen atoms of the  $[2n]$ annulene, the maximum numbers of triangles of the characteristic graph ( $t_{\max}$ ) and of hexagons ( $h_{\max}$ ) of the corresponding perifusene are related in one of the following two ways, where  $x$  and  $j$  are integers ( $x \geq 0$ ,  $-2 \leq j \leq 2$ ):

$$\text{For } n = 6x + 3, \quad t_{\max} = \frac{1}{6}(n-3)^2 = 6x^2; \quad h_{\max} = \frac{1}{12}(n^2+3) = 3x^2 + 3x + 1;$$

$$\text{For } n = 6(x+1) + j, \quad t_{\max} = \frac{1}{6}[(n-3)^2 - j^2 - 3] = 6x^2 + 2x(j+3) + j + 1;$$

$$h_{\max} = \frac{1}{12}(n^2 - j^2) = 3x^2 + x(j+6) + j + 3.$$

Table 7 presents the least overcrowded single-edge configurations of  $[2n]$ annulenes up to  $2n = 30$ . An interesting fact is that for any  $2n \geq 22$  the steric repulsion between inner hydrogens remains constant for such configurations.

#### Alternative notations

In addition to the notations system introduced in this paper, which depends on the three external co-ordinates of the graphite lattice, two further notations should be considered, which depend on intrinsic co-ordinates of the carbon chain.\* One of these<sup>15</sup> employs the classical notations of *cis-trans* geometric isomerism (or the newer E, Z notations<sup>18</sup>), which can be converted into digital form by assigning symbol 0 to *cis* and 1 to *trans*, selecting the lowest figure from all possible ones for a given system and converting this figure from the binary into the decimal system. This notation,<sup>15</sup> however, presents ambiguities both for single- and for multiple-edge systems, as shown by VIIB and VIII or by IX B and X.

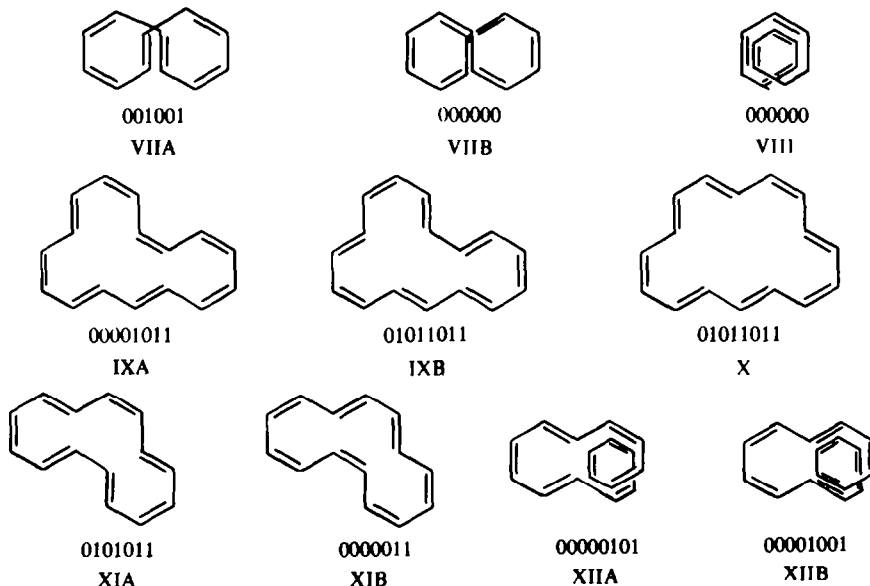











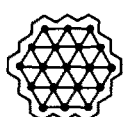


FIG 3. Annulenes with localized double bonds and *cis* (0)-*trans* (1) notation.<sup>15</sup>

\* These two notations can, therefore, be also applied to configurations which are not superimposable with the graphite lattice.

TABLE 7. THE LEAST OVERCROWDED SINGLE-EDGE CONFIGURATIONS OF  $[2n]$ ANNULENES SUPERIMPOSABLE WITH THE GRAPHITE LATTICE

$2n$	$x$	$f$	$f_{\max}$	$h_{\max}$	Configuration	Non-bonding interactions
6	0	-	0	1		$[-]$
8	0	-2	(-1)	-	-	-
10	0	-1	0	2		$[6]$
12	0	0	1	3		$[5^3]$
14	0	1	2	4		$[5^2, 4^2, 8^2]$
16	0	2	3	5		$[5^2, 4^2, 8^2]$
18	1	-	6	7		$[4^6]$
20	1	-2	7	8		$[5, 4^4]$
22	1	-1	10	10		$[4^6]$
24	1	0	13	12		$[4^6]$
26	1	1	16	14		$[4^6]$
28	1	2	19	16		$[4^6]$
30	2	-	24	19		$[4^6]$

Our first notation with three symbols (namely 1, 2, 3) can be converted easily into *cis-trans* notation by definition 1. The reverse is not true, however.

A third notation, similar to that employed for characteristic graphs of polyhexes,<sup>8</sup> would also need two symbols, e.g. *a* and *b*, for right-bend (right-turn) and left-bend, respectively, on passing along the edges of the annulene. Though this notation presents certain attractive features such as a simple expression for the symmetry of the circuit, as shown by XIII–XV, there is no simple condition for ring closure. Therefore these two alternative notations will not be employed.

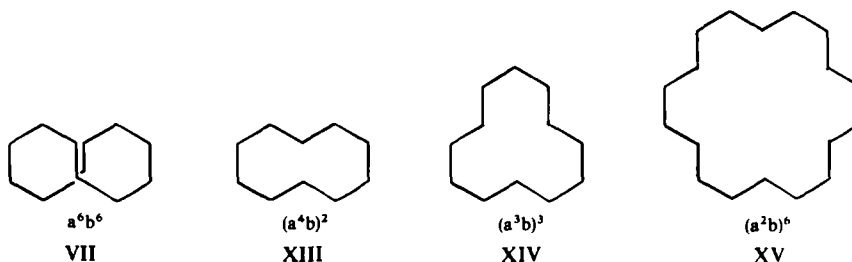


FIG 4. Annulenes with the third notation system

A further problem is presented by alternating bond lengths. Systems devoid of centers of symmetry or symmetry axes passing through vertices (*i.e.* carbon atoms), give rise to two different isomers when localized double bonds are considered. In these cases, the two isomers either have the same number of *trans* double bonds, or one isomer has an even number of *trans* double bonds more than the other (VIIAB, IXAB, XIAB, XIIAB).

All evidence so far available points out that  $[2n]$ annulenes with even  $n$  (anti-Hückel) have indeed localized double bonds, whereas those with odd  $n \leq 11$ , which comply with the Hückel rule, and which can assume a reasonably planar configuration, have averaged bond lengths with electronic delocalization owing to their aromaticity, as shown in the next section.

### Applications

So far, only single-edge configurations are known for those annulenes whose molecular structure was investigated by means of X-ray diffraction analysis (but not all their atoms are necessarily coplanar, *cf.* definition 2).

All  $[2n]$ annulenes from  $[10]$ annulene (cyclodecapentaene)<sup>2, 3, 19, 20</sup> to  $[30]$ -annulene<sup>21</sup> are now known, either as such or as dehydroderivatives (wherein one or more double bonds are replaced by triple bonds, modifying thereby the geometry of the molecule<sup>22, 23</sup>). Other variations include benzoderivatives,<sup>24</sup> or bridged annulenes, where the bridge is formed by O, NR, CH<sub>2</sub> or (CH<sub>2</sub>)<sub>x</sub> groups.<sup>25, 26</sup>

The most striking phenomenon presented by these  $[2n]$ annulenes is the pronounced difference between the two series with odd and even  $n$ . The odd- $n$   $[2n]$ annulenes satisfy the Hückel rule for aromaticity and indeed their NMR spectra indicate the presence of a diamagnetic ring current of  $\pi$ -electrons in an applied magnetic field: protons inside the ring appear at extraordinarily high fields, whereas protons in the plane of, and exterior to, the ring are deshielded more than in benzene itself, because the shielding effect of the ring current is proportional to the area of the ring.<sup>27</sup> This is the case of  $[14]$ - and  $[18]$ annulene,<sup>23, 28</sup> and of  $[22]$ annulene.<sup>29</sup> At the same time the central region above and below the ring is strongly shielded as shown by NMR peaks of the methylene protons of methylene-bridged annulenes.<sup>25</sup> X-ray analysis evidences for  $[14]$ -<sup>30</sup> and  $[18]$ annulene<sup>31</sup> carbon-carbon bond lengths which do not alternate but follow different patterns.

Whereas  $[18]$ annulene is almost planar,  $[14]$ annulene is not, but the distortion is not so important as to make the molecule unable to sustain a diamagnetic ring current

in an external magnetic field; however, two isomers of [14]annulene were isolated which may differ by the reciprocal positions of the four inner crowded hydrogens.<sup>23</sup>

On the other hand, even- $n$  [2 $n$ ]annulenes evidence, in agreement with their antiaromaticity, a paramagnetic ring current in their NMR spectra (e.g. [16]-<sup>15</sup> and [24]-annulene<sup>32</sup>) and bond alternation (for [16]annulene<sup>33</sup>).

In all cases where the structure is known, at least one of the stable configurations of annulenes is the single-edge configuration superimposable with the graphite lattice with the smallest overcrowding (Table 7) namely for [14]-, [16]-, [18]- and [22]-annulene.

Theoretical predictions<sup>34-38</sup> indicate that for  $2n > ca. 22$  the difference between aromatic and antiaromatic systems tends to become negligible so that at higher  $n$  values annulenes will be non-aromatic; one experimental check of this prediction, with tri- and pentahydro [30]annulene<sup>21</sup> seems to confirm it. However, caution must be exercised since only variable-temperature NMR spectra can be relied upon: annulenes undergo easily configurational changes leading to averaged NMR spectra (dehydroannulenes are more stable configurationally), as shown by Sondheimer *et al.*,<sup>23</sup> to whom the major advances in large-ring annulenes are due.

Nuclear magnetic resonance spectra and X-ray structural analysis are the two methods for investigating the geometry (by counting inner and outer protons in the NMR spectra) and the aromaticity of the annulenes (by examining relative bond lengths, or the ring currents). All single-edge configurations superimposable with the graphite lattice of a [2 $n$ ] annulene have  $n-3$  inner hydrogens.

In conclusion, two procedures were presented for the derivation of configuration of annulenes. Single-edge configurations can be classified according to the steric repulsions between inner hydrogens. Multiple-edge configurations have not been discussed in detail, but some of them (e.g. VII) are very interesting and worthy of more detailed theoretical and experimental considerations.

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