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FORMS OF BENZENOID CHEMICAL ISOMERS

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Systematic treatment of the forms of benzenoid chemical isomers (C_nH_s).

INTRODUCTION

The enumeration of the isomers of benzenoid hydrocarbons, say C_nH_s, is mainly due to the pioneering works of Dias: an article series in ten parts [1–10], an early review [11], a monograph [12], and some more recent papers [13,14]. Unfortunately, when the Dias numbers are inspected critically, one finds many errors. The first error was pointed out by Knop et al. [15,16]. In a note to the most recent paper of Dias [14], Cyvin [17] located several errors. Also in the extensive review with supplements Brunvoll and Cyvin [18] had to introduce a number of corrections. That paper [18] tends to list all the

available numbers of benzenoid isomers, if possible divided into Kekuléans (non–radicalic hydrocarbons) and non–Kekuléans (radicals). Specific enumerations of 2–factorable benzenoids (incorporating all–benzenoids) [5–7,11–14,19,20] are not included.

The present work is a continuation of the mentioned review [18]. The forms of benzenoid isomers are surveyed with emphasis on the strictly pericondensed benzenoids. A strictly pericondensed benzenoid [6] has no catacondensed appendage, and its internal vertices are connected. Several sets of the benzenoid isomers are depicted for the first time, and errors in the listings of Dias are corrected.

Here the sets of benzenoid isomers (C_nH_s) are classified according to the "neo" classification [21,22], and more specifically as:

n normal;

e essentially disconnected;

o_i non–Kekuléan with $\Delta = i$.

Here Δ is the color excess [23], viz. the absolute magnitude between the numbers of black and white vertices. The Kekuléan hydrocarbons (n + e) have $\Delta = 0$.

When the chemical formula, C_nH_s, is given, one finds the number of hexagons (h) from

$$h = \frac{1}{2}(n - s) + 1$$

Another important invariant is the number of internal vertices (n_i), given by

$$n_i = n - 2s + 6$$

Finally the Dias parameter (d_s) [1] is obtained from

$$d_s = \frac{1}{2}(3s - n) - 7$$

The excised internal structures [4,6] for strictly pericondensed benzenoids are indicated in the subsequent figures. An excised internal structure is the set of internal vertices with the edges connecting them.

RESULTS AND DISCUSSION

One–isomer series

Already in the early paper Dias [1] pointed out that coronene (see Fig. 1) represents the unique benzenoid isomer of $C_{24}H_{12}$. It is a member of a one–isomer series consisting of the polycircumcoronenes [1], or more generally j–circumbenzenes: $j = 0$ for benzene, $j = 1$ for coronene (circumbenzene), $j = 2$ for circumcoronene (dicircum–benzene), etc. All these benzenoids are normal (n). Other one–isomer series of n benzenoids put forward by Dias [4,6] are the j–circumnaphthalenes and j–circumpyrenes; see Fig. 1 for the ground forms (i. e. those for $j = 0$).

Dias [9] identified also the three one–isomer series for non–Kekuléan (o_1) benzenoids: j–circumphenalenes, j–circumnaphthanthrene and j–circumbenzo[*bc*]–coronene; cf. Fig.1.

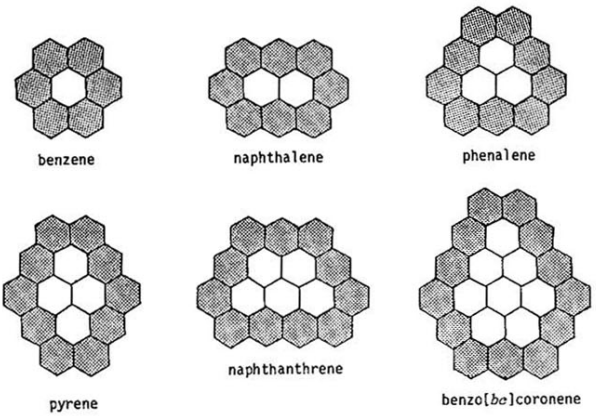


Fig. 1. Ground forms of the one–isomer series of benzenoids (white hexagons). Higher members are obtained by successive circumscribing (indicated by grey hexagons).

Benzenoids with $h \leq 9$

A complete list of the different classes of benzenoid isomers for $h \leq 9$ is given in the following, including the number of isomers according to the above specified classifications. For the individual numbers with references to original sources, here and throughout this work, it is referred to the previous review [18]. Helicenic hydrocarbons are not included.

$h = 1$: C_6H_6 (n);

$h = 2$: $C_{10}H_8$ (n);

$h = 3$: $C_{13}H_9(o_1)$, $C_{14}H_{10}$ (2n);

$h = 4$: $C_{16}H_{10}$(n), $C_{17}H_{11}(o_1)$, $C_{18}H_{12}$(5n);

$h = 5$: $C_{19}H_{11}(o_1)$, $C_{20}H_{12}$(2n+e), $C_{21}H_{13}(6o_1)$, $C_{22}H_{14}$(12n);

$h = 6$: $C_{22}H_{12}(2n+o_2)$, $C_{23}H_{13}(4o_1)$, $C_{24}H_{14}(10n+3e+o_2)$, $C_{25}H_{15}(24o_1)$, $C_{26}H_{16}$(36n);

$h = 7$: $C_{24}H_{12}$(n), $C_{25}H_{13}(3o_1)$, $C_{26}H_{14}(8n+e+o_2)$, $C_{27}H_{15}(25o_1)$, $C_{28}H_{16}(40n+22e+6o_2)$, $C_{29}H_{17}(106o_1)$, $C_{30}H_{18}$(118n);

$h = 8$: $C_{27}H_{13}(o_1)$, $C_{28}H_{14}(7n+e+o_2)$, $C_{29}H_{15}(21o_1)$, $C_{30}H_{16}(45n+13e+9o_2)$, $C_{31}H_{17}(144o_1)$, $C_{32}H_{18}(180n+107e+42o_2)$, $C_{33}H_{19}(453o_1)$, $C_{34}H_{20}$(411n);

$h = 9$: $C_{30}H_{14}(3n+o_2)$, $C_{31}H_{15}(15o_1)$, $C_{32}H_{16}(37n+9e+9o_2)$, $C_{33}H_{17}(153o_1+o_3)$, $C_{34}H_{18}(225n+108e+63o_2)$, $C_{35}H_{19}(823o_1+2o_3)$, $C_{36}H_{20}(777n+575e+249o_2)$, $C_{37}H_{21}(1966o_1)$, $C_{38}H_{22}$(1489n).

In the extensive listings of Knop et al. [16] one finds the forms of all the $h \leq 9$ benzenoids depicted as computer designs. Some of these benzenoids, with special reference to the chemical isomers, are found in the monograph of Dias [12]. This author has also depicted several of the sets together with the corresponding excised internal structures, namely for: $C_{13}H_9(o_1)$, $C_{19}H_{11}(o_1)$, $C_{25}H_{13}(3o_1)$, $C_{27}H_{13}(o_1)$ [9]; $C_{16}H_{10}$(n), $C_{22}H_{12}$(2n), $C_{24}H_{12}$(n) [4,6]; $C_{28}H_{14}(7n+e+o_2)$.

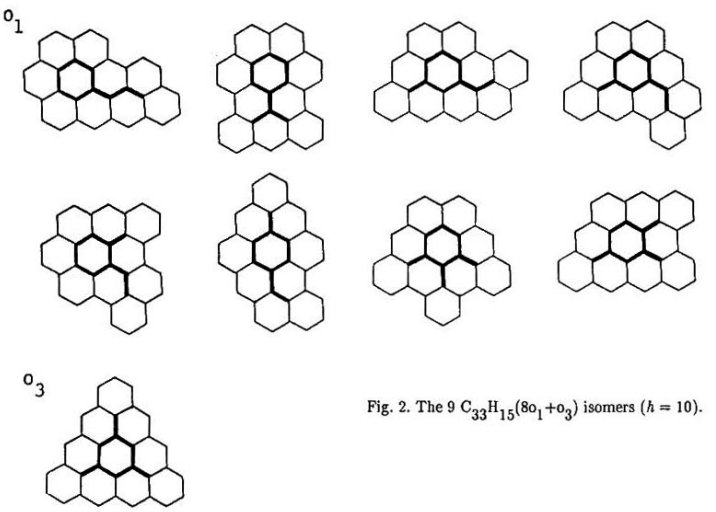


Fig. 2. The 9 $C_{33}H_{15}(8o_1+o_3)$ isomers ($h = 10$).

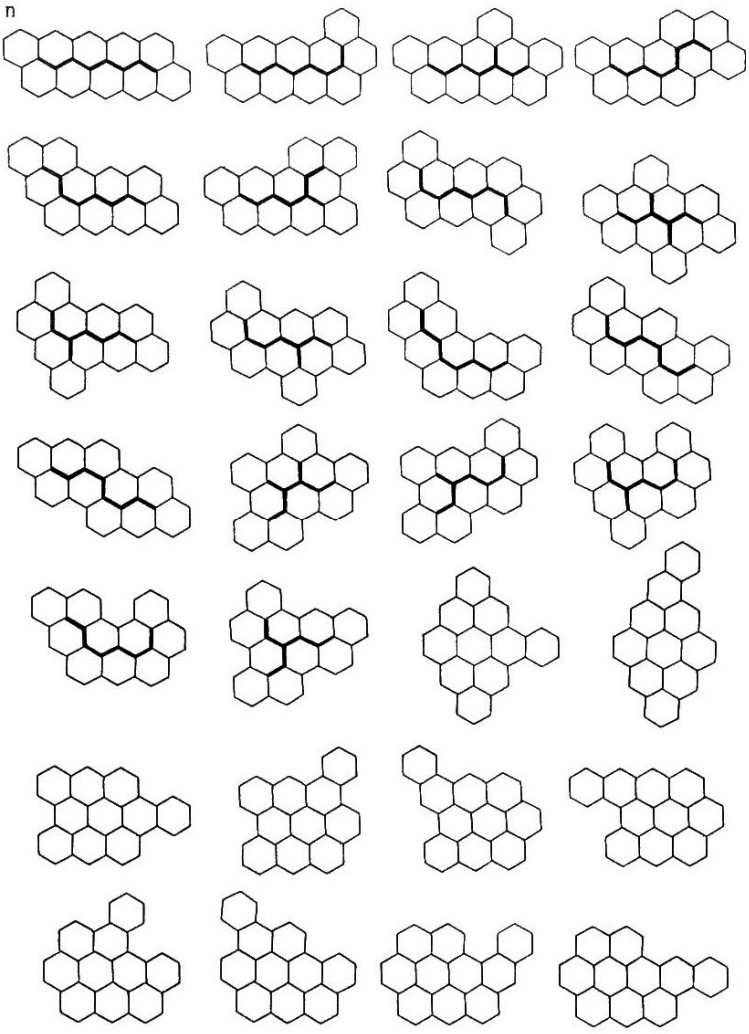
$C_{32}H_{14}$, $C_{33}H_{15}$ and $C_{34}H_{16}$ ($h = 10$)

Among the benzenoids with $h = 10$ we shall consider the title isomers.

$C_{32}H_{14}(n)$ is ovalene or circumnaphthalene, belonging to a one–isomere series [4,6].

For $C_{33}H_{15}(8o_1+o_3)$ Dias [9] has depicted the appropriate forms including their excised internal structures. For the sake of later reference they are reproduced in Fig.2.

Here we wish to clear up the case of $C_{34}H_{16}(31n+3e+8o_2)$. There are 34 Kekuléan benzenoids of these isomers, while Dias [1] gave the number 29, later changed to 37 [6], a number which he repeated several times, also in the monograph [12]. For the non–Kekuléan isomers the number is 8, while Dias [9] reported 5. The appropriate 42 forms are depicted in Fig.3.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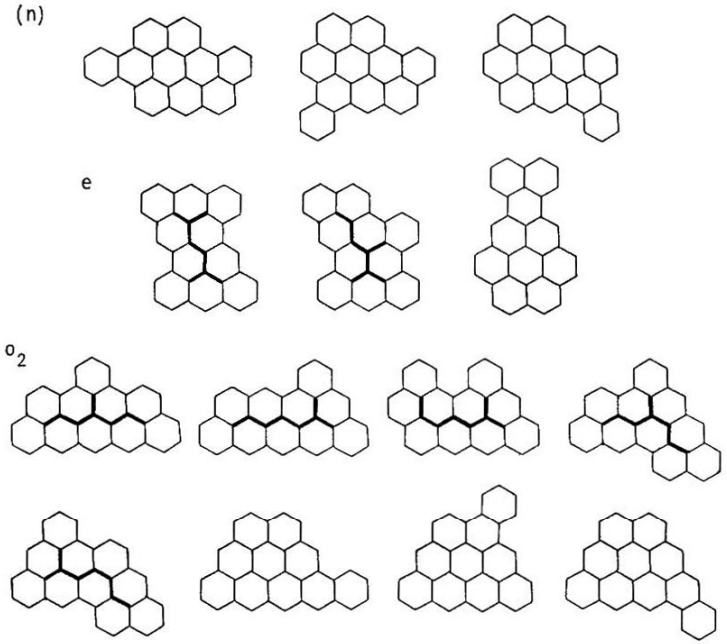


Fig. 3. The 42 $C_{34}H_{16}(31n+3e+8o_2)$ isomers ($h = 10$). Here and throughout the figures, the contours of excised internal structures for the strictly pericondensed benzenoids are drawn in bold. For $C_{34}H_{16}$ there are 17 not strictly pericondensed benzenoids: $13n+e+3o_2$.

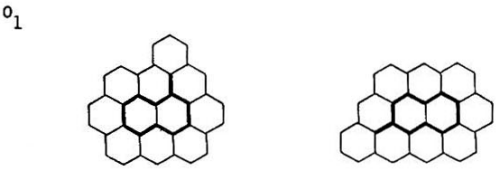
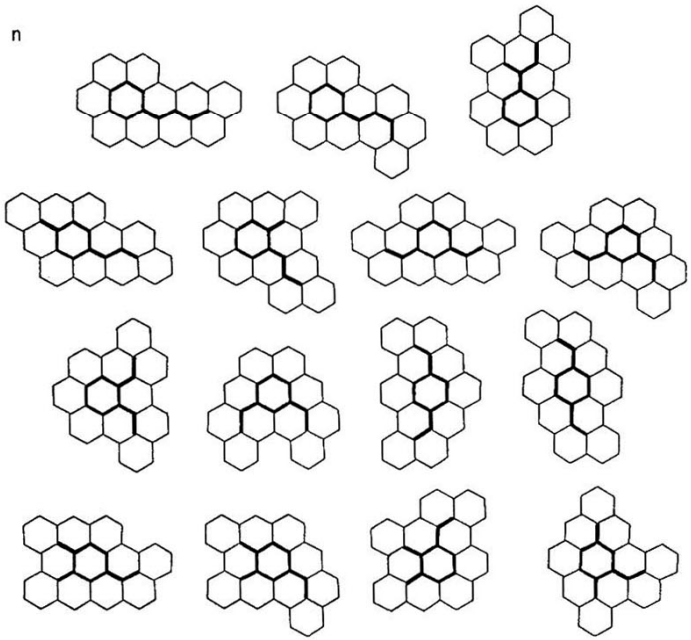


Fig. 4. The 2 $C_{35}H_{15}(2o_1)$ isomers ($h = 11$): ground forms for a two–isomer series.

$C_{35}H_{15}$ and $C_{36}H_{16}$ ($h = 11$)

For $C_{35}H_{15}(2o_1)$ Dias [9] depicted the two forms and their excised internal structures. They are reproduced in Fig. 4 because they are especially important as being the ground forms of a two–isomer series consisting of polycircumbenzo[*bc*]ovalenes and polycircumbenzo[*gh*]ovalenes [18].

The case of $C_{36}H_{16}(18n+2e+6o_2)$ again needs a clarification. Dias [6,9] reported 21 Kekuléan benzenoids of these isomers, but changed the number to 20 in his monograph [12], which also contains the pictures of the pertinent benzenoids. The latter number, viz. 20, is correct. Dias [9] reported also the number 4 for the non–Kekuléan isomers, while it should be 6. For the sake of clarity we show (Fig. 5) all the 26 forms of the $C_{36}H_{16}$ isomers.



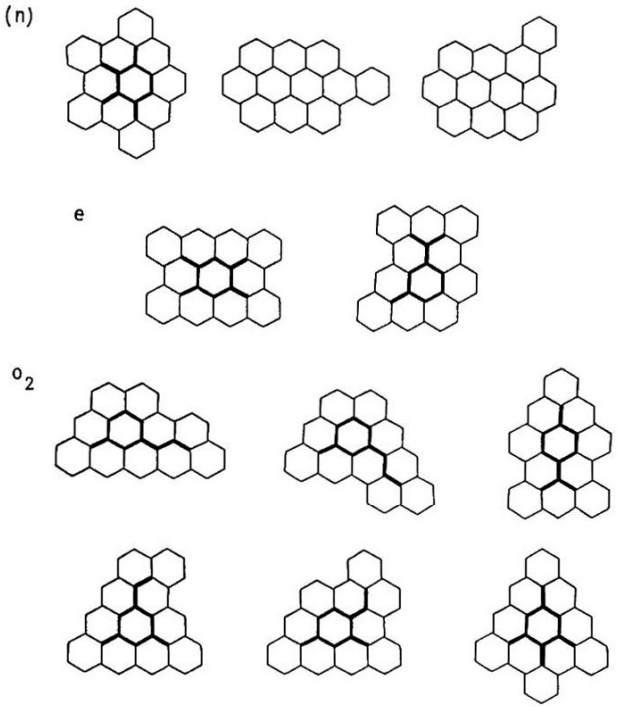


Fig. 5. The 26 $C_{36}H_{16}(18n+2e+6o_2)$ isomers ($h = 11$). The last two of the n benzenoids are not strictly pericondensed.

$C_{37}H_{15}$ and $C_{38}H_{16}$ ($h = 12$)

$C_{37}H_{15}(o_1)$ is circumphenalene, a member of a one–isomer series [9].

For $C_{38}H_{16}(10n+3o_2)$ Dias has correctly indicated the 10 Kekuléan [4,6,12] and 3 non–Kekuléan [9] forms. For the sake of completeness they are reproduced together (in the present style) in Fig. 6.

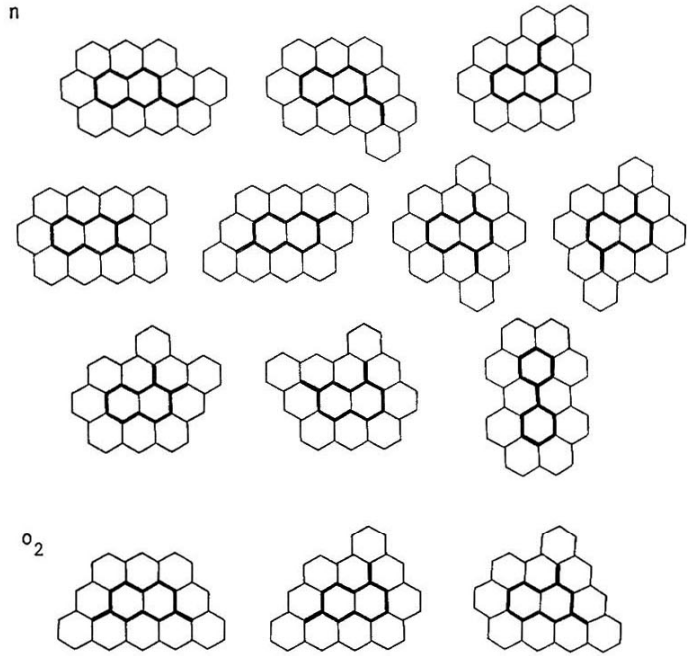


Fig. 6. The 13 $C_{38}H_{16}(10n+3o_2)$ isomers ($h = 12$).

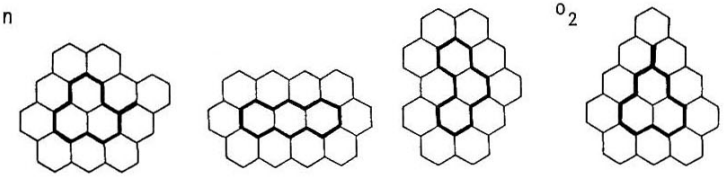


Fig. 7. The 4 $C_{40}H_{16}(3n+o_2)$ isomers ($h = 13$): ground forms for a four–isomer series.

$C_{40}H_{16}$ and $C_{41}H_{17}$ ($h = 13$)

$C_{40}H_{16}(3n+o_2)$ are three normal [4,6,12] and one non–Kekuléan [9] benzenoid (see also Fig. 7). They are the ground forms of a four–isomer series [6].

Figure 8 shows the 35 non–Kekuléan $C_{41}H_{17}(34o_1+o_3)$ isomers, including the one which erroneously was omitted by Dias [9].

$C_{42}H_{16}$ and $C_{43}H_{17}$ ($h = 14$)

$C_{42}H_{16}(n)$ is circumpyrene [4,6,12], a member of a one–isomer series.

For $C_{43}H_{17}(15o_1+o_3)$ Dias [9] depicted two isomorphic forms and missed two others. The 16 non–isomorphic forms are displayed in Fig. 9.

$C_{45}H_{17}$ and $C_{46}H_{18}$ ($h = 15$)

$C_{45}H_{17}(4o_1)$ represents the four non–Kekuléan isomers, of which Dias [9] only identified three forms. They are given in Fig. 10 and are especially important inasmuch as they are the ground forms of a four–isomer series.

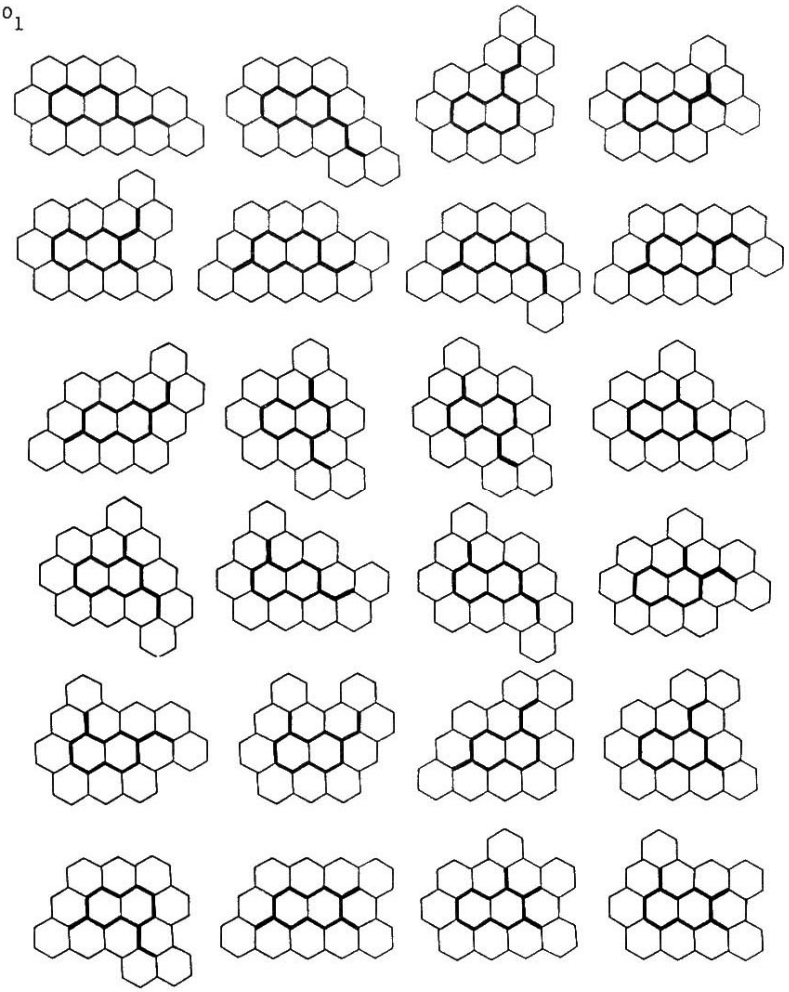
$C_{46}H_{18}(47n+2e+20o_2+o_4)$ is a case which again needs a clarification. Dias [6] reported the number of 56 Kekuléan benzenoids, while we have arrived at 49 [18]. For the non–Kekuléan isomers we derived [18] the number 21 as an original result. The totality of 70 forms are depicted in Fig. 11.

$C_{47}H_{17}$ and $C_{48}H_{18}$ ($h = 16$)

$C_{47}H_{17}(o_1)$ is circumnaphthanthrene, a member of a one–isomer series [9].

$C_{48}H_{18}(22n+8o_2)$ represents the 30 appropriate isomers. With regard to the Kekuléan benzenoids Dias [4] originally depicted 18 forms with their excised internal structures, but corrected the number to 22 shortly thereafter [6,12]. For the non–Kekuléan isomers Dias [9] depicted correctly the 8 excised internal structures. For the sake of completeness we give a reproduction of the forms in Fig. 12.

o_1



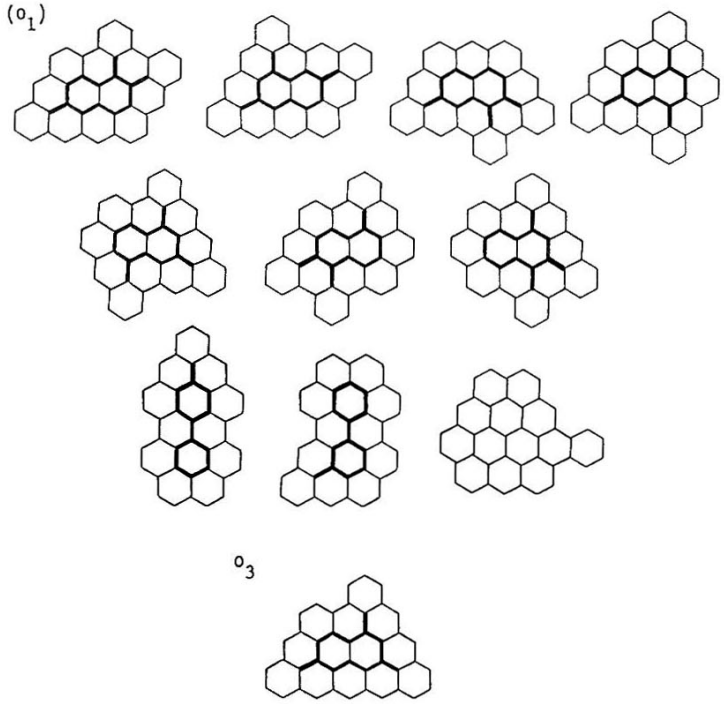


Fig. 8. The 35 $C_{41}H_{17}(34o_1+o_3)$ isomers (h =13). The last one of the o_1 benzenoids is not strictly pericondensed,

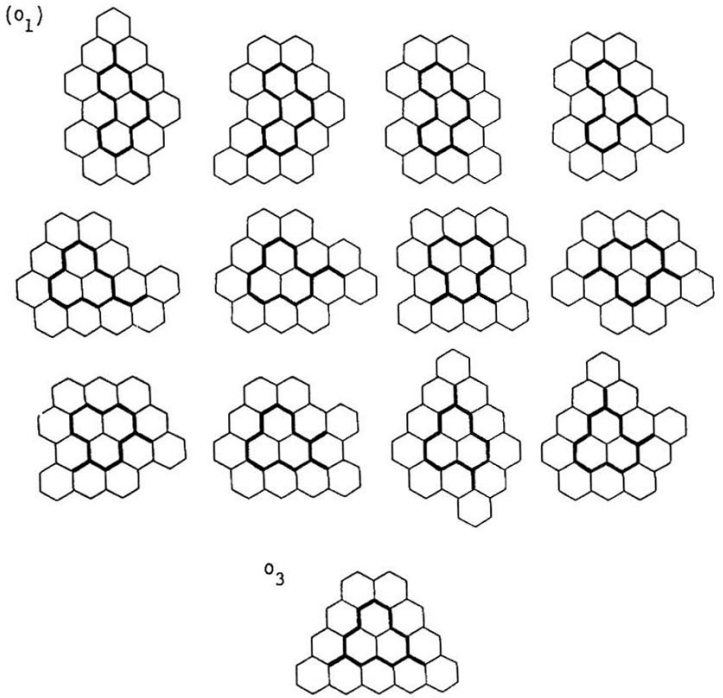


Fig. 9. The 16 $C_{43}H_{17}(15o_1+o_3)$ isomers ($h = 14$).

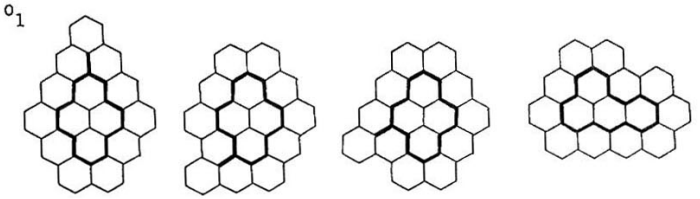
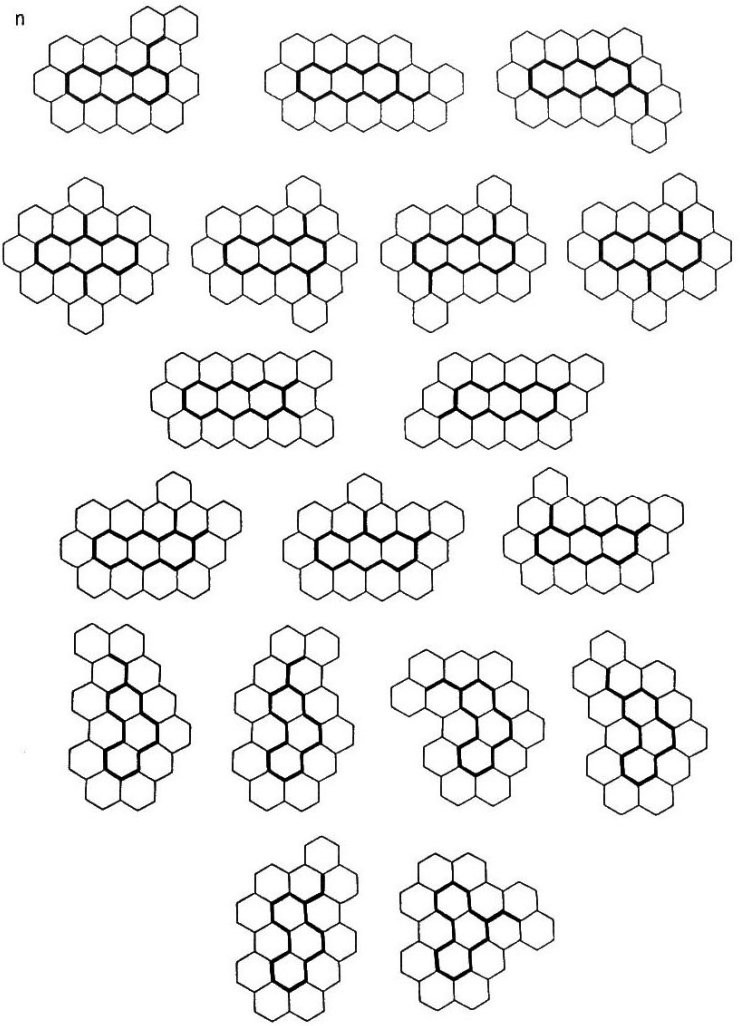


Fig. 10. The 4 $C_{45}H_{17}(4o_1)$ isomers ($h = 15$): ground forms for a four–isomer series.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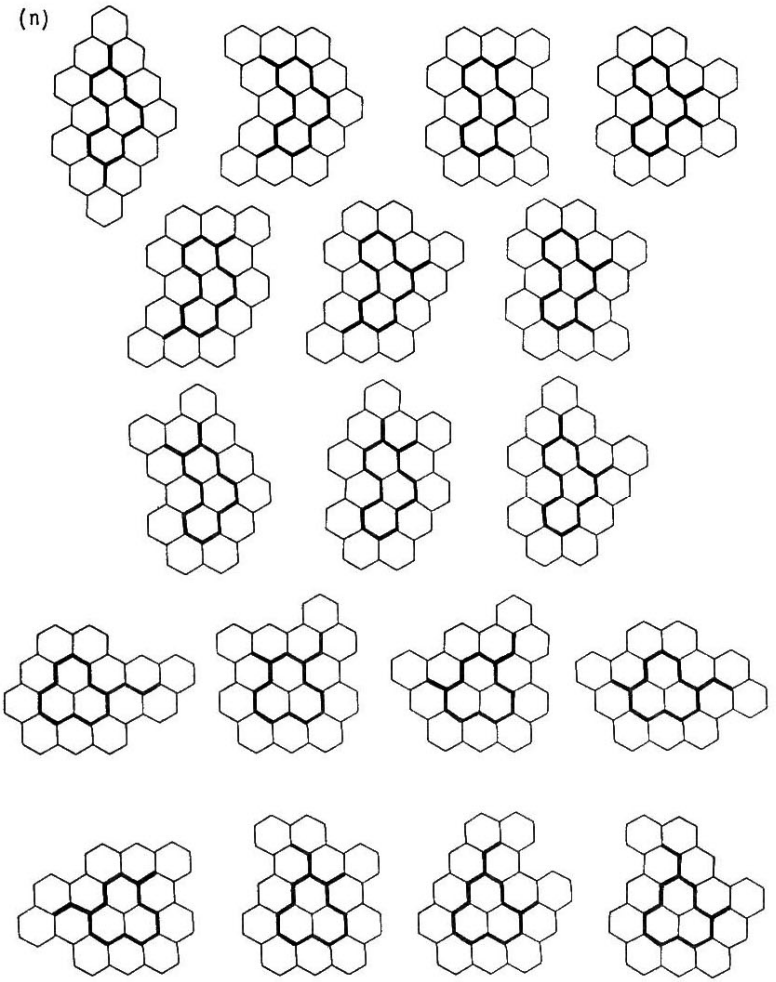
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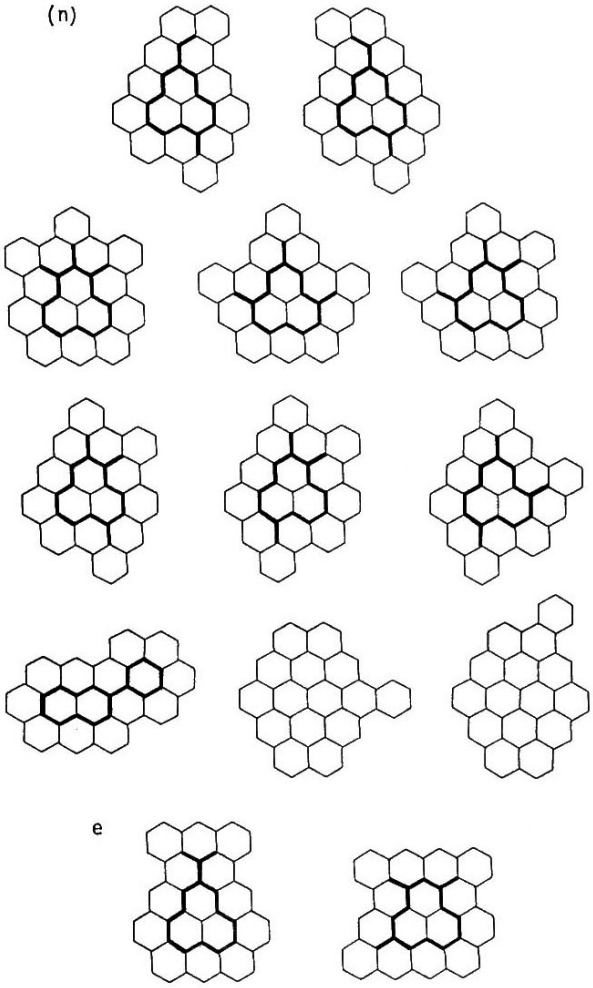
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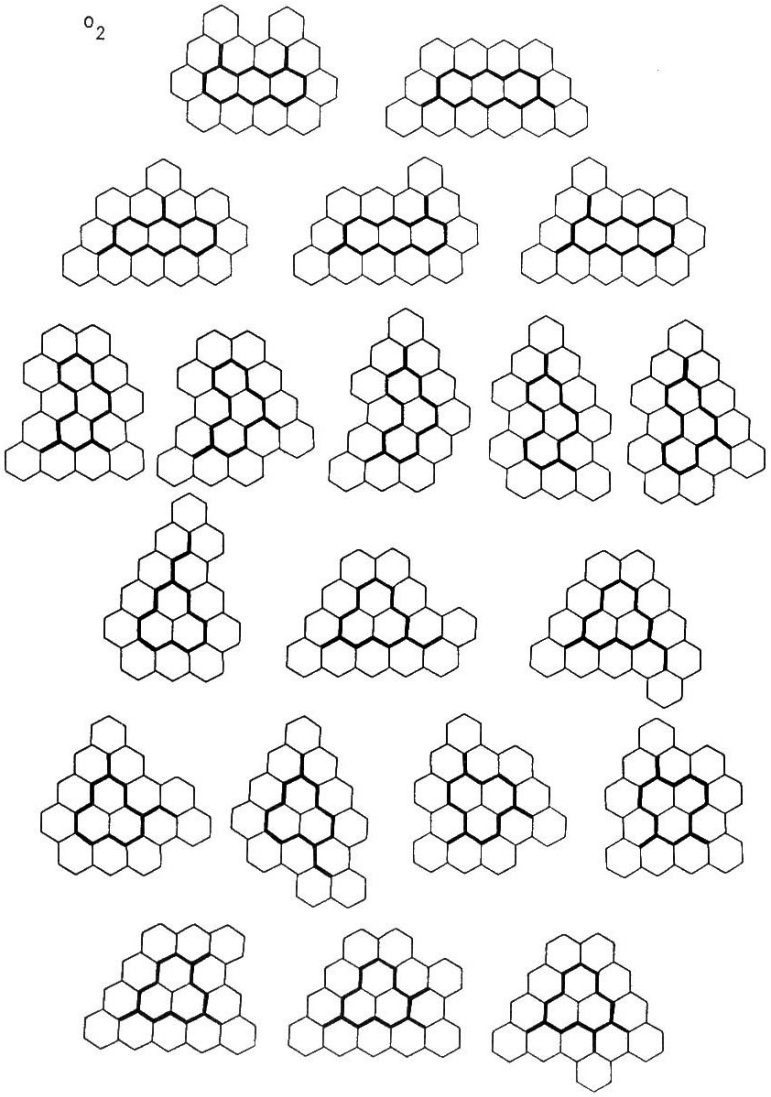

O_2

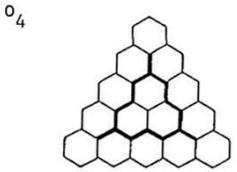
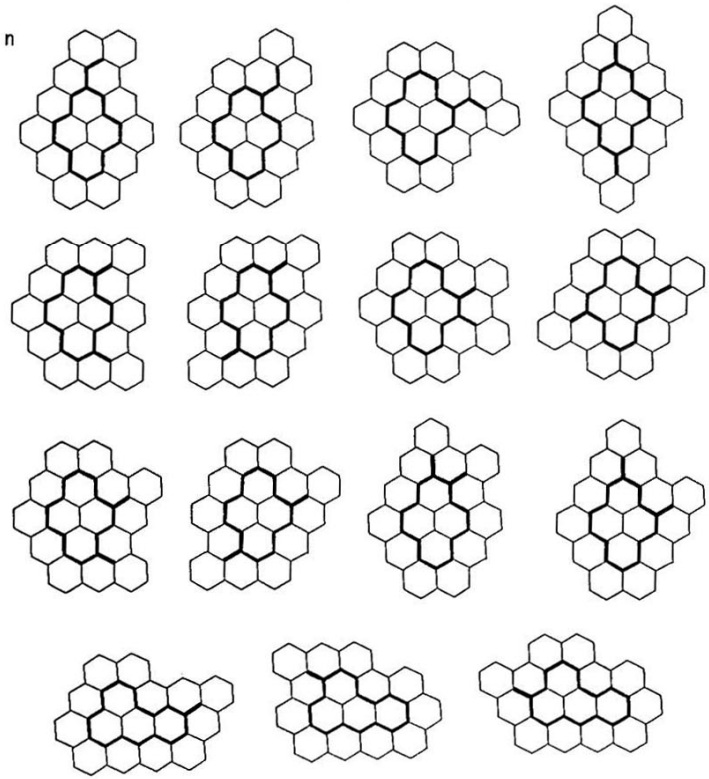


Fig. 11. The 70 $C_{46}H_{18}(47n+2e+20o_2+o_4)$ isomers (h = 15) The last two of the n benzenoids are not strictly pericondensed.



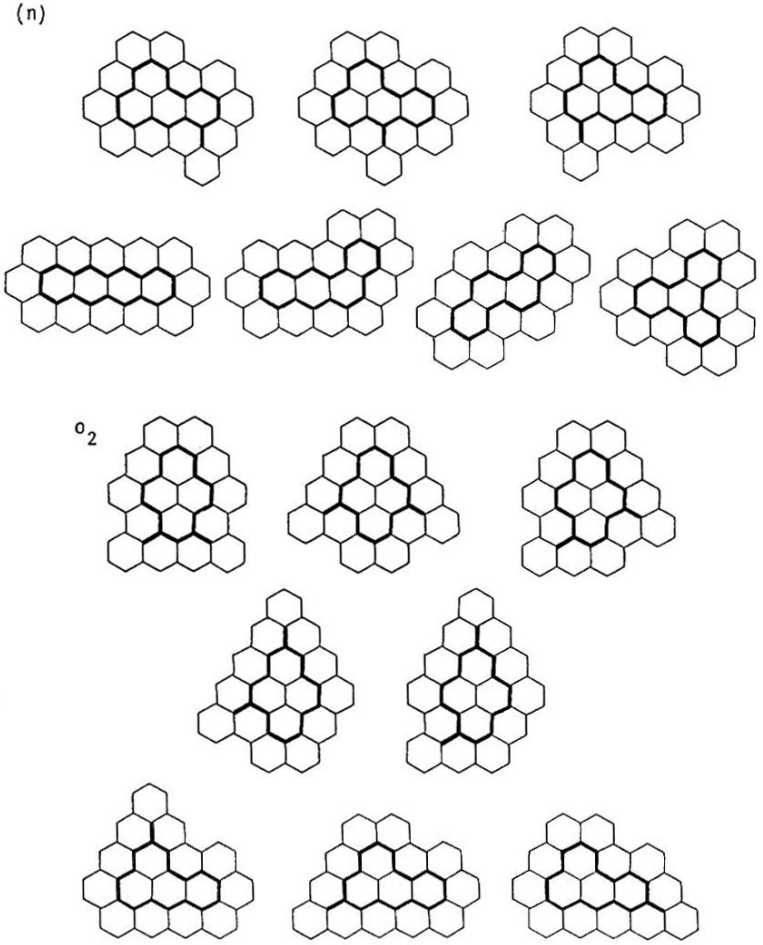


Fig. 12. The 30 $C_{48}H_{18}(22n+8o_2)$ isomers ($h = 16$).

$C_{50}H_{18}$ ($h = 17$) and $C_{52}H_{18}$ ($h = 18$)

The $C_{50}H_{18}(7n+2o_2)$ isomers consist of 7 Kekuléan [4,6,12] and 2 non–Kekuléan [9] benzenoids, which all were identified by Dias. They are the ground forms of a nine–isomer series [6]. The forms in question are reproduced in Fig. 13.

The two Kekuléan benzenoids from $C_{52}H_{18}(2n+o_2)$ have been depicted, with or without the excised internal structures, several times by Dias [4–7,9–12]. For the sake of completeness they are also reproduced in Fig. 14. Dias [6] identified the pertinent three–isomer series, of which the ground forms are the $h = 6$ benzenoids appearing as the excised internal structures of Fig. 14.

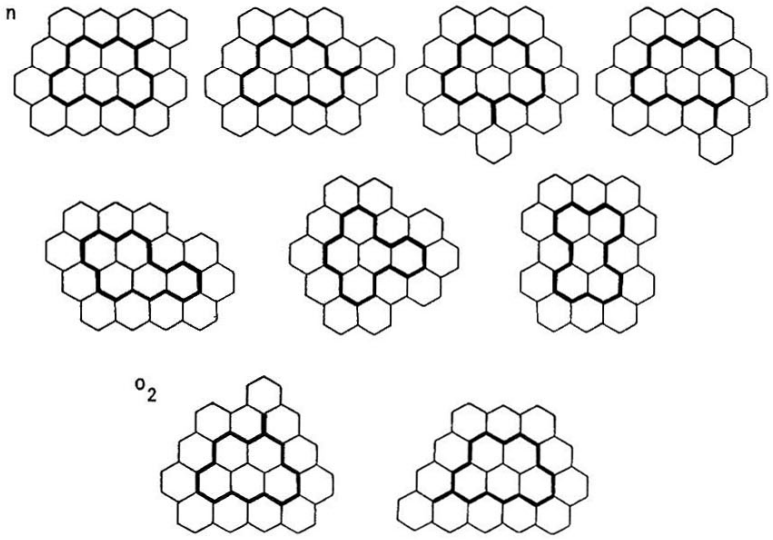


Fig. 13. The 9 $C_{50}H_{18}(7n+2o_2)$ isomers ($h = 17$): ground forms for a nine–isomer series.

Fig. 14. The 3 $C_{52}H_{18}(2n+o_2)$ isomers ($h = 18$): the excised internal structures are the ground forms for a three–isomer series.

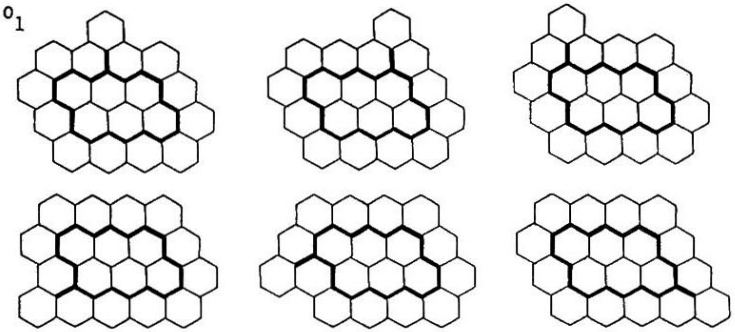
$C_{54}H_{18}$ and $C_{55}H_{19}$ ($h = 19$)

$C_{54}H_{18}(n)$ is circumcoronene [1].

For $C_{55}H_{19}(17o_1+o_3)$ Dias [9] reported 15 isomers (without figures), while we have arrived at the 18 forms of Fig. 15.

$C_{57}H_{19}$ ($h = 20$)

The $C_{57}H_{19}(4o_1)$ isomers were enumerated by Dias [9] without indicating the forms. They are depicted in Fig. 16 and are the ground forms of a four–isomer series.



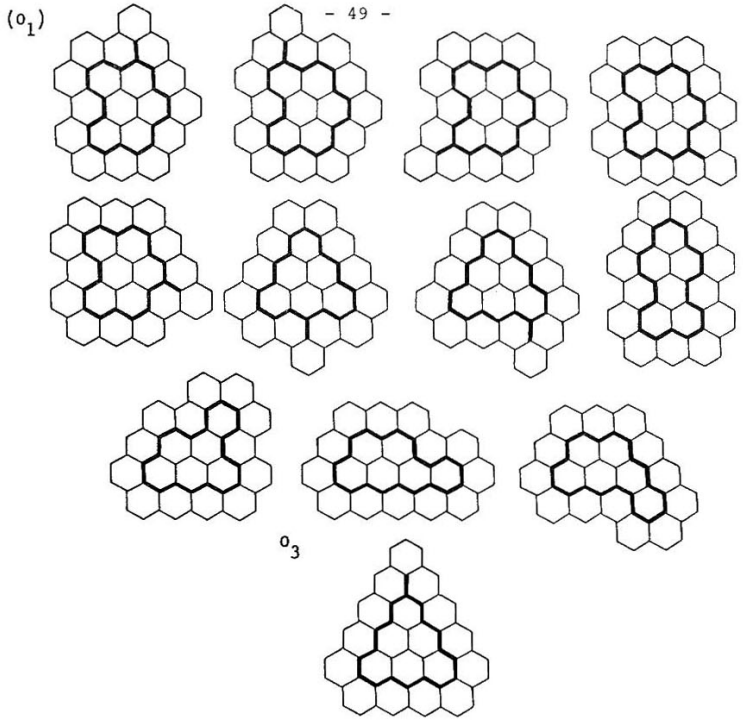


Fig. 15. The 18 $C_{55}H_{19}(17o_1+o_3)$ isomers ($h = 19$).

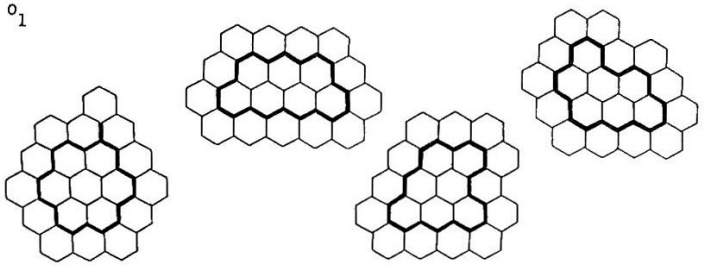
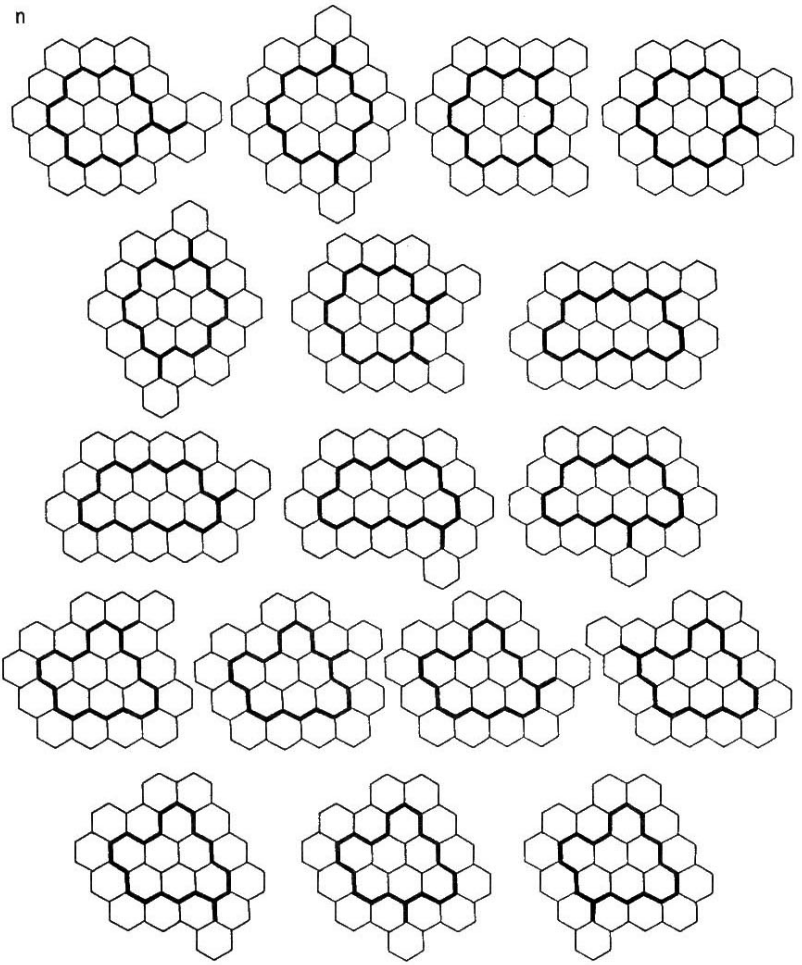


Fig. 16. The 4 $C_{57}H_{19}(4o_1)$ isomers ($h = 20$): ground forms for a four–isomer series.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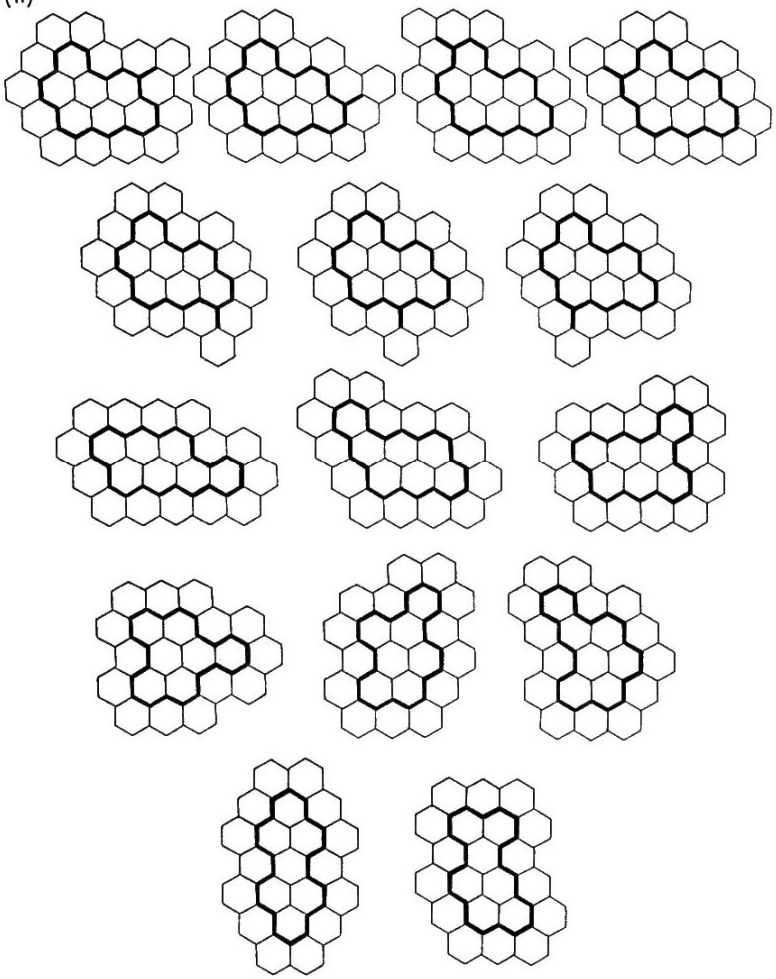

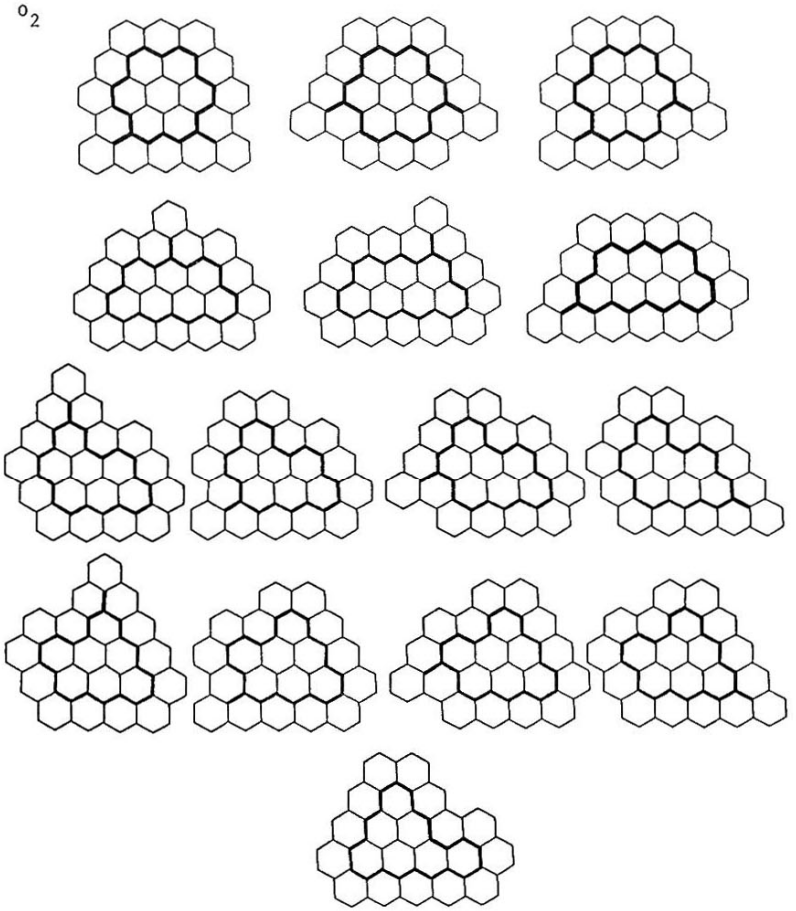

Fig. 17. The 47 $C_{60}H_{20}(32n+15o_2)$ isomers ($h = 21$).

$C_{59}H_{19}$ and $C_{60}H_{20}$ ($h = 21$)

$C_{59}H_{19}(o_1)$, a member of a one–isomer series [9], is circumbenzo[*bc*]coronene.

The forms of the $C_{60}H_{20}(32n+15o_2)$ isomers are displayed in Fig. 17. Our analysis of this set was originally prompted by the special treatment of C_{60} benzenoids published by Dias [14]. In a previous note [17] we have pointed out the significant errors which Dias had committed on this point.

$C_{62}H_{20}$ ($h = 22$)

For the $C_{62}H_{20}(12n+4o_2)$ Dias [6] gave the right number 12 (without illustrations) when the Kekuléan benzenoids are concerned. For the non–Kekuléan benzenoids on the other hand, he missed one form [9]. The case is important inasmuch as these benzenoids are basic forms of a sixteen–isomer series. The forms are depicted in Fig. 18.

$C_{64}H_{20}$ ($h = 23$), $C_{66}H_{20}$ ($h = 24$) and $C_{69}H_{21}$ ($h = 25$)

The three Kekuléan benzenoids from $C_{64}H_{20}(3n+o_2)$ have been depicted several times by Dias [5–7,12]. He has also given the number of non–Kekuléans [6,9] and identified the four–isomer series [6] to which these benzenoids belong. It is referred to Fig. 19, where the ground forms are the $h = 9$ excised internal structures.

$C_{66}H_{20}(n)$ is circumovalene or dicircumnaphthalene [4,6], a member of a one–isomer series.

For the $C_{69}H_{21}(12o_1+o_3)$ benzenoids we shall introduce an abbreviation in their specification. It is sufficient to state that 9 forms $(8o_1+o_3)$ are obtained by circumscribing the benzenoids of Fig. 2. The additional 4 forms $(4o_1)$ are depicted in Fig. 20.

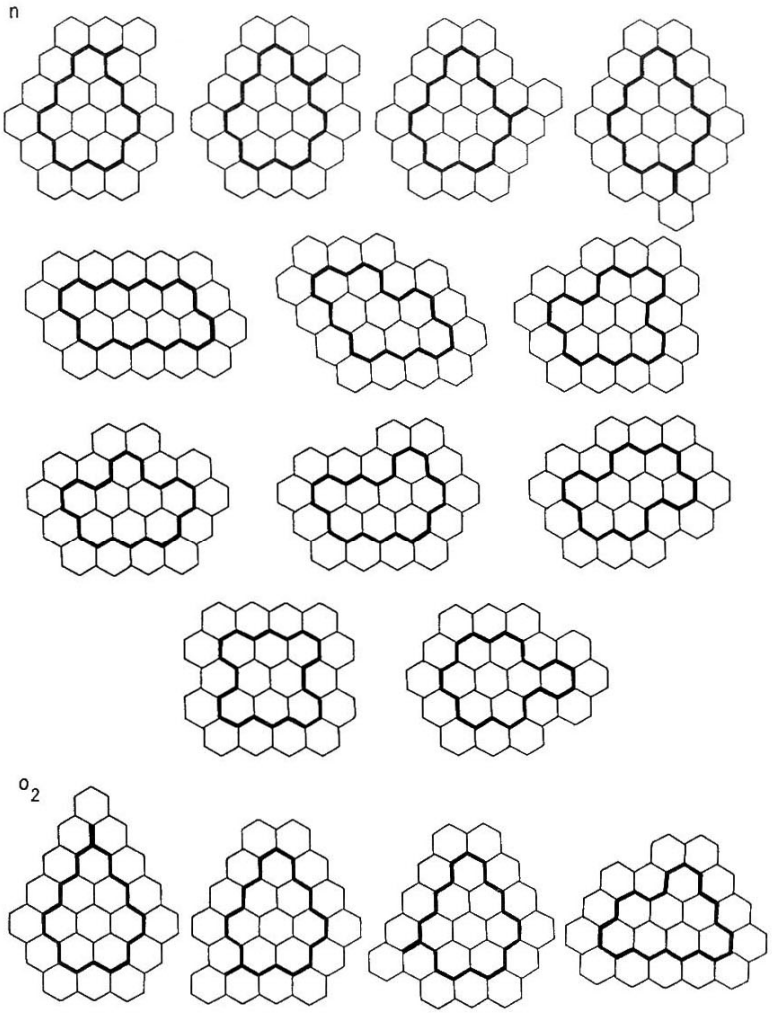

Fig. 18. The 16 $C_{62}H_{20}(12n+4o_2)$ isomers (h = 22): ground forms for a sixteen-isomer series.

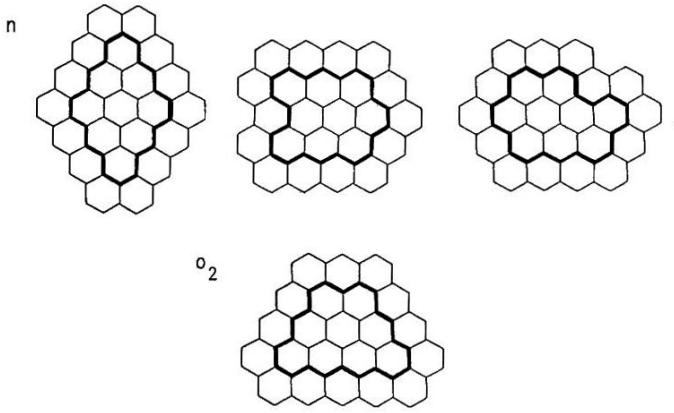

Fig. 19. The 4 $C_{64}H_{20}(3n+o_2)$ isomers ($h = 23$): the excised internal structures are the ground forms for a four–isomer series.

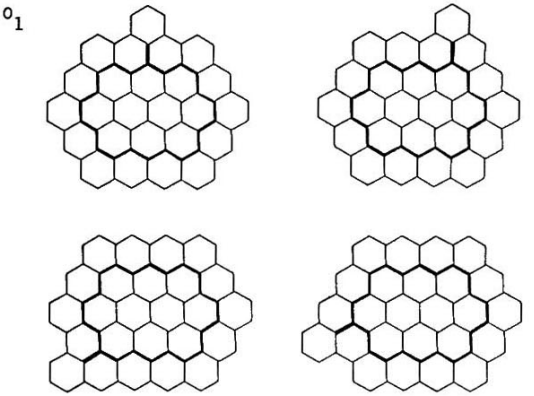

Fig. 20. The 4 $C_{69}H_{21}(4o_1)$ isomers ($h = 25$) which supplement the 9 forms $(8o_1+o_3)$ obtained by circumscribing the benzenoids of Fig. 2.

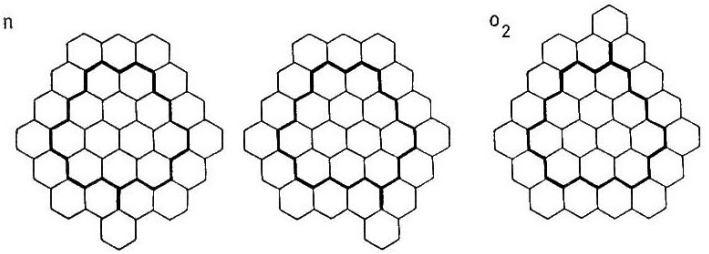

Fig. 21. The 3 $C_{76}H_{22}(2n+o_2)$ isomers (h = 28) which supplement the 13 forms $(10n+3o_2)$ obtained by circumscribing the benzenoids of Fig. 6.

$C_{71}H_{21}$ (h = 26), $C_{73}H_{21}$ (h = 27) and $C_{76}H_{22}$ (h = 28)

The $C_{71}H_{21}(2o_1)$ benzenoids belong to a two–isomer series and are obtained by circumscribing those of Fig. 4.

$C_{73}H_{21}(o_1)$ is dicircumphenalene [9].

The set of $C_{76}H_{22}(12n+4o_2)$ is again specified in an abbreviated form: 13 forms $(10n+3o_2)$ are obtained by circumscribing the benzenoids of Fig. 6, and the additional 3 forms $(2n+o_2)$ are given in Fig. 21.

$C_{78}H_{22}$ (h = 29), $C_{80}H_{22}$ (h = 30) and $C_{83}H_{23}$ (h = 31)

The $C_{78}H_{22}(3n+o_2)$ benzenoids belong to a four–isomer series [6] and are obtained by circumscribing the forms of Fig. 7.

$C_{80}H_{22}(n)$ is dicircumpyrene [4,6].

The set of $C_{83}H_{23}(19o_1+o_3)$ is obtained by circumscribing the 16 forms $(15o_1+o_3)$ of Fig.9 and taking the 4 forms $(4o_1)$ of Fig. 22 in addition.

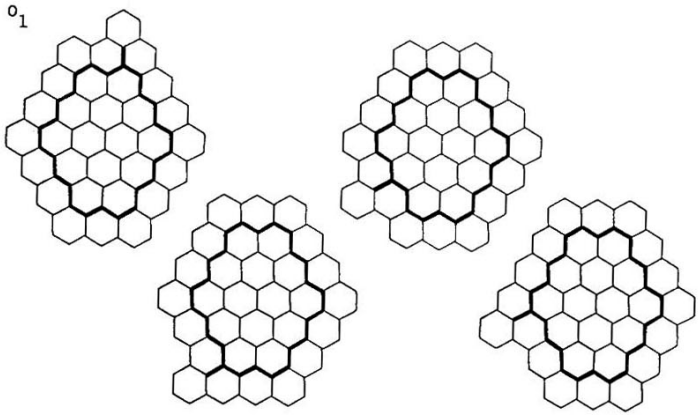

Fig. 22. The 4 $C_{83}H_{23}(4o_1)$ isomers ($h = 31$) which supplement the 16 forms ($15o_1+o_3$) obtained by circumscribing the benzenoids of Fig. 9.

$C_{85}H_{23}$ ($h = 32$), $C_{87}H_{23}$ ($h = 33$) and $C_{90}H_{24}$ ($h = 34$)

$C_{85}H_{23}(4o_1)$ are members of a four–isomer series, and are obtained by circumscribing the forms of Fig. 10.

$C_{87}H_{23}(o_1)$ is dicircumnaphthanthrene [9].

The $C_{90}H_{24}(27n+12o_2)$ forms are obtained by circumscribing the 30 benzenoids ($22n+8o_2$) of Fig. 12 and taking the 9 forms ($5n+4o_2$) of Fig. 23 in addition.

$C_{92}H_{24}$ ($h = 35$), $C_{94}H_{24}$ ($h = 36$), $C_{96}H_{24}$ ($h = 37$) and $C_{99}H_{25}$ ($h = 38$)

The $C_{92}H_{24}(7n+2o_2)$ benzenoids belong to a nine–isomer series [6] and are obtained by circumscribing the forms of Fig. 13.

$C_{94}H_{24}(2n+o_2)$ represents a three–isomer series [6]. The forms are obtained by circumscribing the benzenoids of Fig. 14.

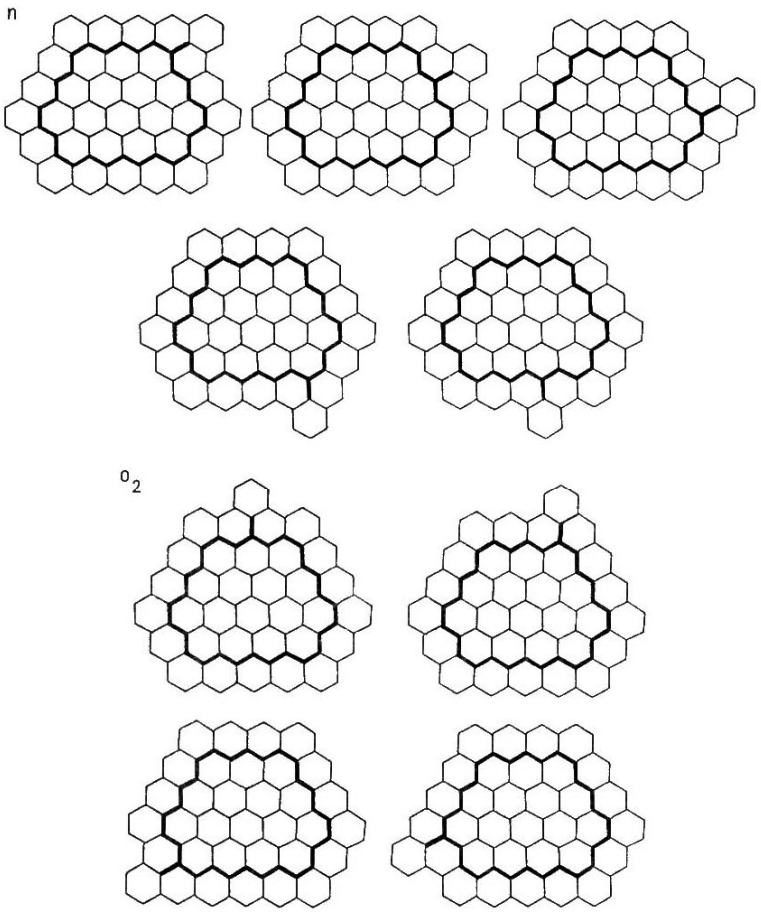

Fig. 23. The 9 $C_{90}H_{24}(5n+4o_2)$ isomers (h = 34) which supplement the 30 forms $(22n+8o_2)$ obtained by circumscribing the benzenoids of Fig. 12.

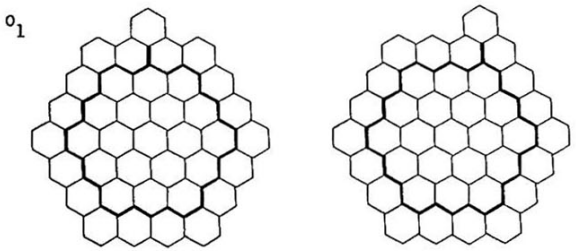

Fig. 24. The 2 $C_{99}H_{25}(2o_1)$ isomers ($h = 38$) which supplement the 18 forms ($17o_1+o_3$) obtained by circumscribing the benzenoids of Fig. 15.

$C_{96}H_{24}$(n) is dicircumcoronene [1].

The forms of $C_{99}H_{25}(19o_1+o_3)$ are: the 18 benzenoids ($17o_1+o_3$) of Fig. 15 circumscribed, in addition to the 2 forms ($2o_1$) of Fig. 24.

Benzenoids with $39 \leq h \leq 44$

The set of $C_{101}H_{25}(4o_1)$ forms belongs to a four–isomer series of benzenoids with $h = 39$. They emerge by circumscribing the forms of Fig. 16.

$C_{103}H_{25}(o_1)$ is dicircumbenzo[*bc*]coronene [9], a benzenoid with $h = 40$.

The benzenoids of $C_{106}H_{26}(38n+19o_2)$ with $h = 41$ are obtained by: circumscribing the 47 forms ($32n+15o_2$) of Fig. 17 and adding the 10 forms ($6n+4o_2$) of Fig. 25.

The $C_{108}H_{26}(12n+4o_2)$ forms for these benzenoids with $h = 42$ are obtained by circumscribing the forms of Fig. 18.

The $C_{110}H_{26}(3n+o_2)$ benzenoids with $h = 43$ emerge by circumscribing the forms of Fig. 19 [6].

$C_{112}H_{26}$(n) is tricircumnaphthalene [4,6], a benzenoid with $h = 44$.

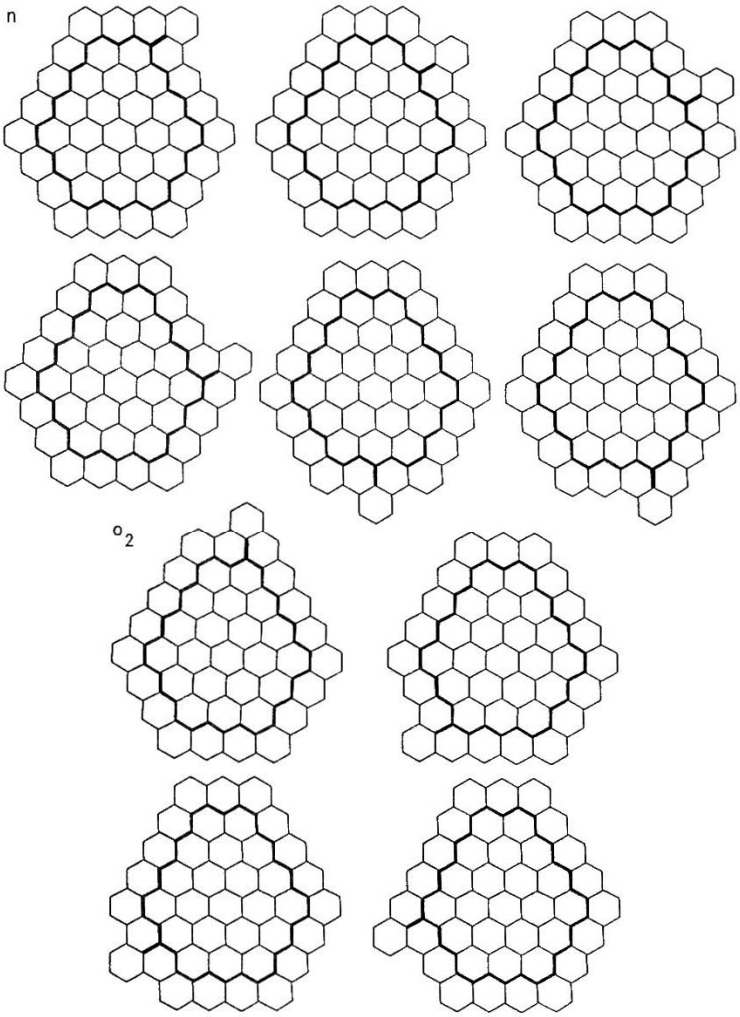

Fig. 25. The 10 $C_{106}H_{26}(6n+4o_2)$ isomers ($h = 41$) which supplement the 47 forms $(32n+15o_2)$ obtained by circumscribing the benzenoids of Fig. 17.

CONCLUSION

The theoretically possible numbers of isomers for different chemical formulas has always been considered as important information in organic chemistry. The traditions of isomer enumeration goes more than hundred years back [24] when we think of the C_NH_{2N+2} alkanes. The story of their enumeration has been vividly described by Knop et al. [16].

The myriads of chemical formulas of benzenoid hydrocarbons was a chaos until Dias (see above) started their systematization. He collected the formulas in a periodic table and devised useful methods of isomer enumerations. We understand the importance of listing the numbers of benzenoid isomers, but of course the published numbers should be correct. As it has been demonstrated above the Dias numbers are in general not reliable. We have recently produced extensive listings of revised numbers [18]. The present work deals with the benzenoid isomers of relatively few numbers, for which it is practically feasible to specify the forms.

Painstaking precautions have been taken in order to avoid errors in the present material. Yet if anybody should detect one or more errors the authors would be grateful for a notice.

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