# Enumeration of Chemical Isomers of Polycyclic Conjugated Hydrocarbons with Six-Membered and Five-Membered Rings

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Z. Naturforsch. **51a,** 1073–1078 (1996); received April 4, 1996

Polygonal systems P consist of exclusively hexagons and pentagons. They correspond (as chemical graphs) to a certain class of polycyclic conjugated hydrocarbons. This class includes proto-fullerenes. General formulations for the maximum numbers of internal vertices for P systems with $p \leq 6$ are derived; here $p$ is the number of pentagons. The $C_nH_s$ chemical formulas of P systems are studied with special emphasis on the semibuckminsterfullerene ($C_{30}H_{12}$), circum-semibuckminsterfullerene ($C_{58}H_{16}$) and corannulene ($C_{20}H_{10}$) isomers. Numbers of all $C_nH_s$ isomers for P systems with $r \leq 6$ are computed; here $r$ is the total number of polygons.

## Introduction

In the present work, certain classes of polycyclic conjugated hydrocarbons are considered. As chemical graphs [1] they are represented by polygonal systems. Benzenoid systems, which correspond to molecules with six-membered rings exclusively, have been studied most extensively with regard to their isomer enumerations [2–6]. However, many polygonal systems with different ring sizes [7, 8] are realized chemically. Polygonal systems with hexagons and pentagons are especially of great interest in view of the current investigations of $C_{60}$ buckminsterfullerene [9, 10] and other fullerenes [11, 12]. Many of the conjugated hydrocarbons under consideration are fragments of buckminsterfullerene supplied with hydrogens [13] and sometimes referred to as proto-fullerenes [14, 15].

Some systematic studies have been conducted on polygonal systems with a fixed number of pentagons and otherwise hexagons. Fluorenoids and fluoranthenoids [16–20] are systems with one pentagon each; $C_9H_7$ indenyl and $C_{16}H_{10}$ fluoranthene are chemical prototypes. Indacenoids [21] have two pentagons each and otherwise only hexagons; $C_{12}H_8$ *s*-indacene and *as*-indacene are prototypes. Finally, many classes of catacondensed systems with hexagons and pentagons have been enumerated [22–24].

In the present work, the $C_nH_s$ chemical formulas of polygonal systems with hexagons and pentagons are considered. The $C_{30}H_{12}$ and $C_{58}H_{16}$ isomers of the relevant conjugated hydrocarbons are used to exemplify the need of some general formulations for the pertinent extremal systems. Furthermore, a substantial amount of new isomer numbers are reported in order to fill the gaps of the existing data, which so far have been rather incomplete, even for relatively small systems.

## Basic Concepts

A chemical graph P is defined as a simply connected polygonal system possessing $p$ pentagons and otherwise only hexagons (if any), so that the total number of polygons is $r$. The definition implies that P has no holes, but helicenic systems (with overlapping edges when drawn in a prescribed way) are tolerated. The number of internal vertices is identified by the symbol $n_i$. An internal vertex is by definition shared by three polygons. The system P is pericondensed or catacondensed, depending on whether $n_i > 0$ or $n_i = 0$, respectively.

Assume that P has $s$ vertices of degree two and $n$ vertices in total. Then the formula $C_nH_s$ is associated with P. The following relations are easily deduced:

$$r = \frac{1}{2}(n-s)+1, \quad n_i = n-2s+6-p. \tag{1}$$

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Conversely,

$$n=4r-n_i+2-p, \quad s=2r-n_i+4-p. \tag{2}$$

Let $P(n;s)$ symbolize that P has the formula $C_nH_s$, and consider (circum-P) $(n_1;s_1)$, assuming that P can be circumscribed by hexagons. Then

$$n_1=n+2s+6-p, \quad s_1=s+6-p. \tag{3}$$

In general for ($k$-circum-P) $(n_k;s_k)$, which pertains to $k$-fold circumscribing by hexagons, the following was found:

$$n_k=n+2ks+(6-p)k^2, \quad s_k=s+(6-p)k. \tag{4}$$

## Isomers of Semibuckminsterfullerene and Circum-Semibuckminsterfullerene

Semibuckminsterfullerene, $C_{30}H_{12}$, or circumfulvalene (circum-$C_{10}H_8$) [25] is a typical proto-fullerene, which recently has been synthesized [26]; see **I** of Figure 1. It is a P system with $p=2$. The total number of $C_{30}H_{12}$ isomers of this category is known to be 45 [15, 25]. According to *ab initio* calculation, the most stable of these isomers is represented by **II** of Fig. 1 [14, 15]. Fowler et al. [15] reported also the numbers of $C_{30}H_{12}$ P isomers with $p=3$, 4 and 5 (but not $p=1$); their results are 752, 3872 and 8825, respectively.

Now the following question arises naturally: – How can we ascertain that $C_{30}H_{12}$ P isomers can be constructed for $p=2$, 3, 4 and 5, but not for $p=1$? All these isomers are associated with $r=10$ in accordance with (1). In Table 1 all the chemical formulas which are compatible with $r=10$ P systems are listed for $p \leq 6$, including $p=0$ for benzenoids. Here the top row pertains to catacondensed systems ($n_i=0$). At the bottom of each column one finds the formula for the appropriate extremal system, which is characterized by $n_i=(n_i)_{\max}$. A representative of each of the extremal systems may be found by the principle of spiral walk [18, 27, 28], as is illustrated in Figure 2. In conclusion, P systems with the formula $C_{30}H_{12}$ (boldface in Table 1) are possible for $2 \leq p \leq 10$. Here the upper bound pertains to $p=r$ (only pentagons), which of course is the absolute upper limit. It was verified by examples that this $p$ value, which is associated with the minimum number of internal vertices, $(n_i)_{\min}=2$, actually is realized for $C_{30}H_{12}$. Similarly, all the $p$ values in the given range were verified.

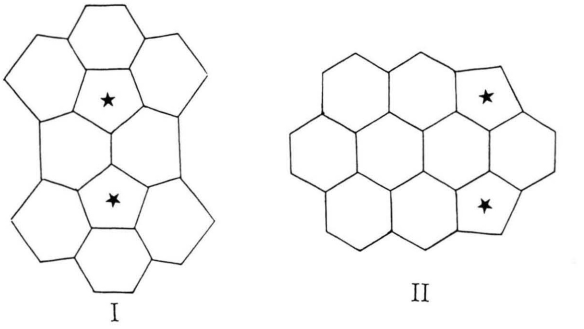

Fig. 1. Semibuckminsterfullerene (**I**) and another $C_{30}H_{12}$ isomer (**II**). Pentagons are indicated by asterisks.

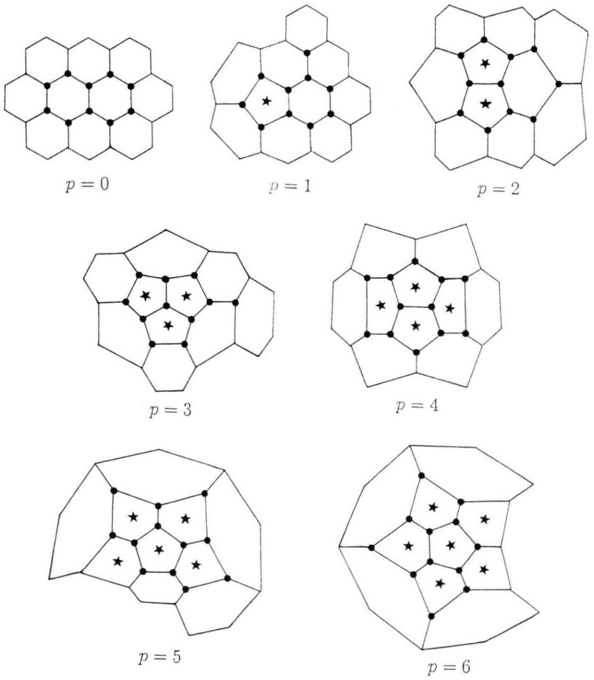

Fig. 2. Representatives of $r=10$ extremal P systems for $0 \leq p \leq 6$.

The isomers of $C_{58}H_{16}$ semibuckminsterfullerene were treated in the same way as described above. Notice that $C_{58}H_{16}$=circum-$C_{30}H_{12}$, in consistency with (3). In this case $r=22$, and Table 2 was deduced. The number of $C_{58}H_{16}$ P isomers for $p=2$ is known to be 51 [15, 25]. In conclusion, P systems with the formula $C_{58}H_{16}$ are possible for $2 \leq p \leq 22$. Here again the upper bound pertains to $p=r$, and in this case, $n_i=(n_i)_{\min}=10$. All the $p$ values in the given range were again found to be realized by inspection.

Table 1. Formulas for P systems with $r=10$.

| $n_i$ | $p$ 0 | 1 | 2 | 3 | 4 | 5 | 6 |
|---|---|---|---|---|---|---|---|
| 0 | $C_{42}H_{24}$ | $C_{41}H_{23}$ | $C_{40}H_{22}$ | $C_{39}H_{21}$ | $C_{38}H_{20}$ | $C_{37}H_{19}$ | $C_{36}H_{18}$ |
| 1 | $C_{41}H_{23}$ | $C_{40}H_{22}$ | $C_{39}H_{21}$ | $C_{38}H_{20}$ | $C_{37}H_{19}$ | $C_{36}H_{18}$ | $C_{35}H_{17}$ |
| 2 | $C_{40}H_{22}$ | $C_{39}H_{21}$ | $C_{38}H_{20}$ | $C_{37}H_{19}$ | $C_{36}H_{18}$ | $C_{35}H_{17}$ | $C_{34}H_{16}$ |
| 3 | $C_{39}H_{21}$ | $C_{38}H_{20}$ | $C_{37}H_{19}$ | $C_{36}H_{18}$ | $C_{35}H_{17}$ | $C_{34}H_{16}$ | $C_{33}H_{15}$ |
| 4 | $C_{38}H_{20}$ | $C_{37}H_{19}$ | $C_{36}H_{18}$ | $C_{35}H_{17}$ | $C_{34}H_{16}$ | $C_{33}H_{15}$ | $C_{32}H_{14}$ |
| 5 | $C_{37}H_{19}$ | $C_{36}H_{18}$ | $C_{35}H_{17}$ | $C_{34}H_{16}$ | $C_{33}H_{15}$ | $C_{32}H_{14}$ | $C_{31}H_{13}$ |
| 6 | $C_{36}H_{18}$ | $C_{35}H_{17}$ | $C_{34}H_{16}$ | $C_{33}H_{15}$ | $C_{32}H_{14}$ | $C_{31}H_{13}$ | $\mathbf{C_{30}H_{12}}$ |
| 7 | $C_{35}H_{17}$ | $C_{34}H_{16}$ | $C_{33}H_{15}$ | $C_{32}H_{14}$ | $C_{31}H_{13}$ | $\mathbf{C_{30}H_{12}}$ | $C_{29}H_{11}$ |
| 8 | $C_{34}H_{16}$ | $C_{33}H_{15}$ | $C_{32}H_{14}$ | $C_{31}H_{13}$ | $\mathbf{C_{30}H_{12}}$ | $C_{29}H_{11}$ | $C_{28}H_{10}$ |
| 9 | $C_{33}H_{15}$ | $C_{32}H_{14}$ | $C_{31}H_{13}$ | $\mathbf{C_{30}H_{12}}$ | $C_{29}H_{11}$ | $C_{28}H_{10}$ | $C_{27}H_{9}$ |
| 10 | $C_{32}H_{14}$ | $C_{31}H_{13}$ | $\mathbf{C_{30}H_{12}}$ | $C_{29}H_{11}$ | $C_{28}H_{10}$ | $C_{27}H_{9}$ | $C_{26}H_{8}$ |
| 11 |  |  | $C_{29}H_{11}$ | $C_{28}H_{10}$ | $C_{27}H_{9}$ | $C_{26}H_{8}$ | $C_{25}H_{7}$ |
| 12 |  |  |  |  | $C_{26}H_{8}$ | $C_{25}H_{7}$ | $C_{24}H_{6}$ |

Table 2. Formulas for P systems with $r=22$.

| $n_i$ | $p$ 0 | 1 | 2 | 3 | 4 | 5 | 6 |
|---|---|---|---|---|---|---|---|
| 0 | $C_{90}H_{48}$ | $C_{89}H_{47}$ | $C_{88}H_{46}$ | $C_{87}H_{45}$ | $C_{86}H_{44}$ | $C_{85}H_{43}$ | $C_{84}H_{42}$ |
| ⋮ | ⋮ | ⋮ | ⋮ | ⋮ | ⋮ | ⋮ | ⋮ |
| 28 | $C_{62}H_{20}$ | $C_{61}H_{19}$ | $C_{60}H_{18}$ | $C_{59}H_{17}$ | $\mathbf{C_{58}H_{16}}$ | $C_{57}H_{15}$ | $C_{56}H_{14}$ |
| 29 |  | $C_{60}H_{18}$ | $C_{59}H_{17}$ | $\mathbf{C_{58}H_{16}}$ | $C_{57}H_{15}$ | $C_{56}H_{14}$ | $C_{55}H_{13}$ |
| 30 |  |  | $\mathbf{C_{58}H_{16}}$ | $C_{57}H_{15}$ | $C_{56}H_{14}$ | $C_{55}H_{13}$ | $C_{54}H_{12}$ |
| 31 |  |  |  | $C_{56}H_{14}$ | $C_{55}H_{13}$ | $C_{54}H_{12}$ | $C_{53}H_{11}$ |
| 32 |  |  |  |  | $C_{54}H_{12}$ | $C_{53}H_{11}$ | $C_{52}H_{10}$ |
| 33 |  |  |  |  | $C_{53}H_{11}$ | $C_{52}H_{10}$ | $C_{51}H_{9}$ |
| 34 |  |  |  |  |  | $C_{51}H_{9}$ | $C_{50}H_{8}$ |

## General Formulations

Each column of formulas in Tables 1 and 2 start at the top with the catacondensed P formula, viz. $C_{4r+2-p}H_{2r+4-p}$. In contrast, it is a nontrivial task to find algebraic expressions for the extremal P formulas at the bottom of each column. Nevertheless, much has been done in this area for related systems.

Firstly, for $p=0$ (benzenoids) the following formula is known [27, 29]:

$$(n_i)_{\max}=2r+1-\lceil\sqrt{12r-3}\rceil, \quad (p=0). \qquad (5)$$

Secondly, for $p=1$ [30–32]:

$$(n_i)_{\max}=2r-\left\lceil\frac{1}{2}\sqrt{40r-15}-\frac{1}{2}\right\rceil, \quad (p=1). \qquad (6)$$

A new formula for $p=2, 3, 4$ was derived here on the basis of the principles of circumscribing and the spiral walk. It has been shown that for $p\leq 6$ and arbitrary $r\geq p$ the spiral starting with $p$ pentagons exists and that it maximizes the number of internal vertices. The new formula reads

$$(n_i)_{\max} = 2r - 1 - \left\lceil \frac{1}{2}\sqrt{8(r-p)(6-p) + (6+p)^2} + \frac{1}{2}p \right\rceil,$$
$$(p = 2,\ 3,\ 4). \qquad (7)$$

The special case of $p = 2$ is consistent with a previous analysis [33]. In addition,

$$(n_i)_{\max} = 2r - 1 - \left\lceil \frac{1}{2}\sqrt{8r + 73} + \frac{1}{2} \right\rceil, \ (p = 5) \qquad (8)$$

and finally:

$$(n_i)_{\max} = 2r - 7 - \left\lceil \frac{r-1}{5} \right\rceil + \left\lfloor \frac{r-1}{5} \right\rfloor, \quad (p = 6). \qquad (9)$$

It was not attempted to deduce the corresponding expressions for $p > 6$. Already for $p = 6$ it is seen that the expression (9) has a quite different form from those of $p < 6$, viz. (5)–(8). The simplicity of (9) stems from the fact that the system of one pentagon circumscribed by five pentagons ($C_{15}H_5$), when circumscribed by hexagons indefinitely, leaves five hexagons in each layer while the number of hydrogens is constantly five. It is a complicating feature that the closest packing of pentagons for $p > 6$ starts to close into itself and ends up with a $C_{20}$ dodecahedron graph (for $p = 12$) [34]. At least, for all (finitely many) values of $r$ for which the spiral exists in the case of $6 < p < 12$, it is again associated with maximal $n_i$. Using the Euler formula, the following upper bound valid for all $p$ can easily be deduced:

$$(n_i)_{\max} \leq 2r - p + 4. \qquad (10)$$

It becomes an equation for a P with $s = 0$. Such a P exists for example for $p = r = 11$ (dodecahedron graph without the outer face) and can also be constructed for $18 \leq p \leq r - 6$.

## Spectrum of Formulas

The benzenoid $C_nH_s$ formulas are known to be restricted with respect to the allowed ranges for $n$ and $s$ [4, 6]. A polygonal system P may or may not be associated with a benzenoid formula. In the former case this means that at least one benzenoid among the isomers of P can be constructed. In Table 1 the benzenoid formulas are recognized as those above the indicated staircase line.

In general, the benzenoid formulas for a given $r$ span from a catabenzenoid (e.g. $C_{42}H_{24}$ in Table 1) to the appropriate extremalbenzenoid formula (e.g. $C_{32}H_{14}$). The infrabenzenoid and ultrabenzenoid formulas are found outside these boundaries, specifically at the relatively hydrogen-rich and hydrogen-poor sides, respectively. A spectrum of formulas has emerged. The position of a $C_nH_s$ formula on this spectrum is determined most directly by the following criteria:

$$s > \frac{1}{2}n + 3; \quad \text{infrabenzenoid,}$$

$$s = \frac{1}{2}n + 3; \quad \text{catabenzenoid,}$$

$$3 + \lceil\sqrt{6n - 6s + 9}\rceil \leq s \leq \frac{1}{2}n + 3; \quad \text{benzenoid,}$$

$$s = 3 + \lceil\sqrt{6n - 6s + 9}\rceil; \quad \text{extremalbenzenoid,}$$

$$s < 3 + \lceil\sqrt{6n - 6s + 9}\rceil; \quad \text{ultrabenzenoid.}$$

It is inferred that any $C_nH_s$ formula of P (polygonal system with pentagons and hexagons) is either a benzenoid formula (but not catabenzenoid for $p > 0$) or ultrabenzenoid.

## Basic Numerical Values

A basic material of the numbers of isomers for the smallest P systems has not been published previously. Table 3 shows the relevant $C_nH_s$ formulas for $p \leq 6$, and in Table 4 the corresponding numbers of isomers are reported. Where comparison is possible, agreement with previously published data (cf. Introduction) is found.

The numbers reported in Table 4 were obtained by a computer program that exploits the property of the spiral to maximize the number of internal vertices in order to decide the construction methods (circumscribing, gluing together fragments or constructing the system polygon by polygon) for every given formula individually and recursively. Every system has its own way how it must be constructed, and using the spiral property it can be determined *a priori* which combinations occur.

## Corannulene

The important proto-fullerene called corannulene, $C_{20}H_{10}$ (Fig. 3) is included in the present enumerations. It is an extremal fluoranthenoid ($p = 1$), and its

Table 3. Formulas for the smallest P systems.

| $r$ | $n_i$ | $p$ | | | | | | |
|---|---|---|---|---|---|---|---|---|
| | | 0 | 1 | 2 | 3 | 4 | 5 | 6 |
| 1 | 0 | $C_6H_6$ | $C_5H_5$ | | | | | |
| 2 | 0 | $C_{10}H_8$ | $C_9H_7$ | $C_8H_6$ | | | | |
| 3 | 0 | $C_{14}H_{10}$ | $C_{13}H_9$ | $C_{12}H_8$ | $C_{11}H_7$ | | | |
| | 1 | $C_{13}H_9$ | $C_{12}H_8$ | $C_{11}H_7$ | $C_{10}H_6$ | | | |
| 4 | 0 | $C_{18}H_{12}$ | $C_{17}H_{11}$ | $C_{16}H_{10}$ | $C_{15}H_9$ | $C_{14}H_8$ | | |
| | 1 | $C_{17}H_{11}$ | $C_{16}H_{10}$ | $C_{15}H_9$ | $C_{14}H_8$ | $C_{13}H_7$ | | |
| | 2 | $C_{16}H_{10}$ | $C_{15}H_9$ | $C_{14}H_8$ | $C_{13}H_7$ | $C_{12}H_6$ | | |
| 5 | 0 | $C_{22}H_{14}$ | $C_{21}H_{13}$ | $C_{20}H_{12}$ | $C_{19}H_{11}$ | $C_{18}H_{10}$ | $C_{17}H_9$ | |
| | 1 | $C_{21}H_{13}$ | $C_{20}H_{12}$ | $C_{19}H_{11}$ | $C_{18}H_{10}$ | $C_{17}H_9$ | $C_{16}H_8$ | |
| | 2 | $C_{20}H_{12}$ | $C_{19}H_{11}$ | $C_{18}H_{10}$ | $C_{17}H_9$ | $C_{16}H_8$ | $C_{15}H_7$ | |
| | 3 | $C_{19}H_{11}$ | $C_{18}H_{10}$ | $C_{17}H_9$ | $C_{16}H_8$ | $C_{15}H_7$ | $C_{14}H_6$ | |
| 6 | 0 | $C_{26}H_{16}$ | $C_{25}H_{15}$ | $C_{24}H_{14}$ | $C_{23}H_{13}$ | $C_{22}H_{12}$ | $C_{21}H_{11}$ | $\mathbf{C_{20}H_{10}}$ |
| | 1 | $C_{25}H_{15}$ | $C_{24}H_{14}$ | $C_{23}H_{13}$ | $C_{22}H_{12}$ | $C_{21}H_{11}$ | $\mathbf{C_{20}H_{10}}$ | $C_{19}H_9$ |
| | 2 | $C_{24}H_{14}$ | $C_{23}H_{13}$ | $C_{22}H_{12}$ | $C_{21}H_{11}$ | $\mathbf{C_{20}H_{10}}$ | $C_{19}H_9$ | $C_{18}H_8$ |
| | 3 | $C_{23}H_{13}$ | $C_{22}H_{12}$ | $C_{21}H_{11}$ | $\mathbf{C_{20}H_{10}}$ | $C_{19}H_9$ | $C_{18}H_8$ | $C_{17}H_7$ |
| | 4 | $C_{22}H_{12}$ | $C_{21}H_{11}$ | $\mathbf{C_{20}H_{10}}$ | $C_{19}H_9$ | $C_{18}H_8$ | $C_{17}H_7$ | $C_{16}H_6$ |
| | 5 | | $\mathbf{C_{20}H_{10}}$ | $C_{19}H_9$ | $C_{18}H_8$ | $C_{17}H_7$ | $C_{16}H_6$ | $C_{15}H_5$ |

Table 4. Numbers of isomers for the smallest P systems.

| $r$ | $n_i$ | $p$ | | | | | | |
|---|---|---|---|---|---|---|---|---|
| | | 0 | 1 | 2 | 3 | 4 | 5 | 6 |
| 1 | 0 | 1 | 1 | | | | | |
| 2 | 0 | 1 | 1 | 1 | | | | |
| 3 | 0 | 2 | 3 | 3 | 1 | | | |
| | 1 | 1 | 1 | 1 | 1 | | | |
| 4 | 0 | 5 | 9 | 13 | 6 | 2 | | |
| | 1 | 1 | 4 | 5 | 3 | 1 | | |
| | 2 | 1 | 2 | 3 | 2 | 1 | | |
| 5 | 0 | 12 | 35 | 56 | 41 | 16 | 3 | |
| | 1 | 6 | 22 | 35 | 28 | 11 | 2 | |
| | 2 | 3 | 9 | 16 | 12 | 6 | 1 | |
| | 3 | 1 | 3 | 6 | 6 | 3 | 1 | |
| 6 | 0 | 37 | 137 | 266 | 247 | 140 | 37 | 6 |
| | 1 | 24 | 112 | 214 | 219 | 122 | 36 | 5 |
| | 2 | 14 | 55 | 109 | 105 | 61 | 16 | 3 |
| | 3 | 4 | 19 | 41 | 46 | 28 | 9 | 1 |
| | 4 | 3 | 8 | 19 | 22 | 16 | 6 | 2 |
| | 5 | | 1 | 1 | 2 | 2 | 1 | 1 |

formula (boldface in Table 3) is ultrabenzenoid. Corannulene was synthesized for the first time by Barth and Lawton [35, 36]. The crystal and molecular structures of corannulene have been investigated [37], and calculated electronic spectra are available [38, 39]. Corannulene has recently attracted new interest among organic chemists, and two new syntheses of it have been reported [40, 41]. The infrared and Raman active frequencies of corannulene from a normal coordinate analysis are available [42], as well as these vibrational frequencies from an ab initio study [43].

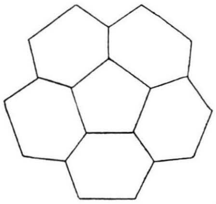

Fig. 3. Corannulene.

As a result of the present work, we find that P systems with the corannulene formula ($C_{20}H_{10}$) can be constructed exactly for $1 \leq p \leq 6$ (cf. Table 3). The total number of P systems with this formula is 169, and the distribution over the different $p$ values is found in Table 4.

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