Tetrahedron Vol. 40, No. 11, pp. 2161 to 2164, 1984
Printed in Great Britain.

0040-4020/84 $3.00 + .00
Pergamon Press Ltd.

A NOVEL COMPACT NOMENCLATURE OF THE CONDENSED BENZENOID HYDROCARBONS

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(*Received in UK* 30 *June* 1983)

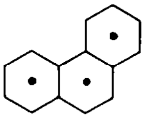
Abstract—Rules of a simplified nomenclature are formulated for condensed benzenoid hydrocarbons. They refer to all the hydrocarbons which could be treated as plane. In naming the hydrocarbon use is made of the numerator determining the number of rings and of the numeric code describing their immediate positional relationship. The proposed nomenclature enables quick and simple assignment of the name to the hydrocarbon and also provides a useful method for deriving the hydrocarbon structural formula from its name.

Nomenclature of aromatic hydrocarbons has been under intensive study for many years. The first naming system was given by Scholl,[1] and made use of the prefix benz- added to the common names of the hydrocarbons. Thus it was possible to give names to many condensed aromatic hydrocarbons, but still some could not be named. There was no clarification of the nomenclature till the naming system of Stelzner and Kuh.[2] This was accepted and modified by the IUPAC conventions, where the numbers have been exchanged on letters defining mutual positions of the structural rings.[3] In fact this system may be applied to any hydrocarbon, nevertheless, it has many apparent drawbacks. The names of compounds are lengthy, complicated and somehow sophisticated. This is the reason why the common names of many hydrocarbons are retained. Besides there are some groups of hydrocarbons where specific rules are used to name the compounds. For instance we have aromatic hydrocarbons with linearly annellated benzene rings named acenes and their "broken" analogues named phenes. Prefix circo- is needed to indicate the origin of the aromatic hydrocarbon obtained by annellation of peripheral benzene rings to the rings of a known hydrocarbon. Somewhat different nomenclature is presented in the Clar's monography on polycyclic hydrocarbons.[4] To avoid ambiguities Clar was compelled to give in addition the exact structural formula for each compound. All the above facts have been carefully examined in the papers of Balaban and Harary,[5,6] where some new nomenclature concepts for the aromatic hydrocarbons are given. Unfortunately their systematics refer only to the catacondensed hydrocarbons and the names proposed by them, in particular the numeric symbolics, are extremely complex. In general one needs to say that the naming conventions presently used by IUPAC,[7] Chemical Abstracts[8] and Ring Index[9] are inconsistent and differ in many details.

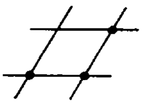
Because of the growing need in organic chemistry to accumulate and store a great deal of data it seems purposeful to devise a nomenclature for the organic compounds which would enable the name of the compound to be derived from its structural formula and *vice versa*. Many of such coding name systems have been recently proposed,[10-12] but they are important mainly for electronic processing of the data rather than for the nomenclature systematics. Therefore in this paper we present the naming system of the benzenoid hydrocarbons which is simple and easy in use and at the same time algorithmic enough to be applied to the classification of the benzenoid aromatics performed on computers.

The rules of this nomenclature are following:

(1) In the structural formula of the hydrocarbon all the benzenoic rings are replaced one by one by the points situated at their centers.



(2) The points are placed in the nodes of a plane oblique net and they determine an area for the confined parallelogram with sides parallel to the sides of the net and having as low dimensions as possible provided that the area includes all the points.

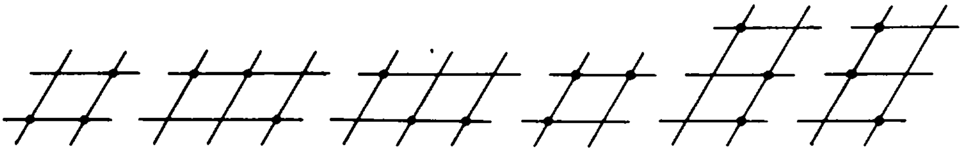


(3) In the parallelogram obtained in such a way the nodes of the net which are occupied by the benzene ring centers are characterized by 1 and the unoccupied ones by 0. Thus we get a matrix with elements 0 and 1.

$$\begin{bmatrix} 0 & 1 \\ 1 & 1 \end{bmatrix}$$

(4) There are 12 possible orientations, or less if the hydrocarbon molecule has higher symmetry, of the considered compound in the network. For each site we have a different matrix. The choice is made between them to get the matrix with minimal number of rows. Among the matrices with the same number

of rows we choose these with the lowest number of columns.



$\begin{bmatrix}0&1\\1&1\end{bmatrix}$ /1.3/

$\begin{bmatrix}1&1&0\\0&0&1\end{bmatrix}$ /6.1/

$\begin{bmatrix}1&0&0\\0&1&1\end{bmatrix}$ /4.3/

$\begin{bmatrix}1&1\\1&0\end{bmatrix}$ /3.2/

$\begin{bmatrix}1&0\\0&1\\0&1\end{bmatrix}$ /2.1.1/

$\begin{bmatrix}1&0\\1&0\\0&1\end{bmatrix}$ /2.2.1/

(5) The elements of the rows of the matrices selected according to the rule 4 generate the binary numbers which are in turn replaced by decimals. For instance a matrix

$$\begin{bmatrix}0&1&0\\1&1&0\\0&0&1\end{bmatrix}$$

with rows 010, 110, 001 is converted into a series of numbers (2.6.1) because $010_2 = 2_{10}$, $110_2 = 6_{10}$, $001_2 = 1_{10}$. This procedure goes on with the selection to get the final matrix having the lowest possible numbers in the decimal representation. At first comparison is made for the first numbers (the first rows), and if they are equal for the second and so on. For example from among two matrices:

$$\begin{bmatrix}0&1&0\\1&1&0\\0&0&1\end{bmatrix}$$

and

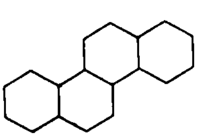
$$\begin{bmatrix}1&0&0\\0&1&1\\0&1&0\end{bmatrix}$$

the first one is chosen as it gives a series (2.6.1) while the second matrix gives a series (4.3.2) and is rejected as 4 is greater than 2.

(6) The name of the hydrocarbon consists of a series of numbers separated by dots and put in slashes and of the core word defining the number of the benzene rings in the hydrocarbon as in IUPAC convention. To each name the suffix acene is added.

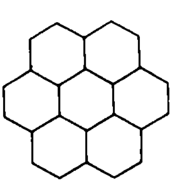
Examples

chrysene



/3.6/-tetracene

coronene

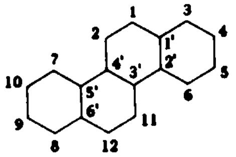


/6.7.3/-heptacene

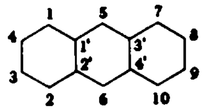
(7) The rule of numbering the C atoms is as follows: C atoms are divided into two classes (a) linked with the hydrogens, (b) internal. Arabic numerals are assigned to the first without primes, to the second with primes. Numbering in each ring has to begin on at the top and continued in clockwise manner. If we encounter the C atom once numbered its number will be retained. The priority rules for the rings are: the ring in the higher row is prior to the ring in the lower row, for the same row the numbering of the ring lying far to the left precedes the numbering of that on its right side.

Examples

chrysene



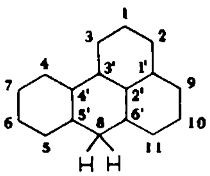
anthracene



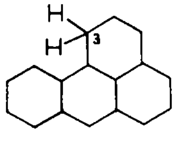
(9) The parent system of benzenoic rings in the family of hydrocarbons is recognized as that in which the C atoms are linked with single H atoms. In the case of a hydrocarbon such as perinaphthene, where the C atoms are bonded with two H atoms, the name is derived by addition of the letter H to the number describing the position of this C atom in the structural formula.

Examples

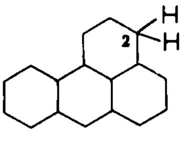
benzanthrenes



8H-/2.7/-tetracene



3H-/2.7/-tetracene



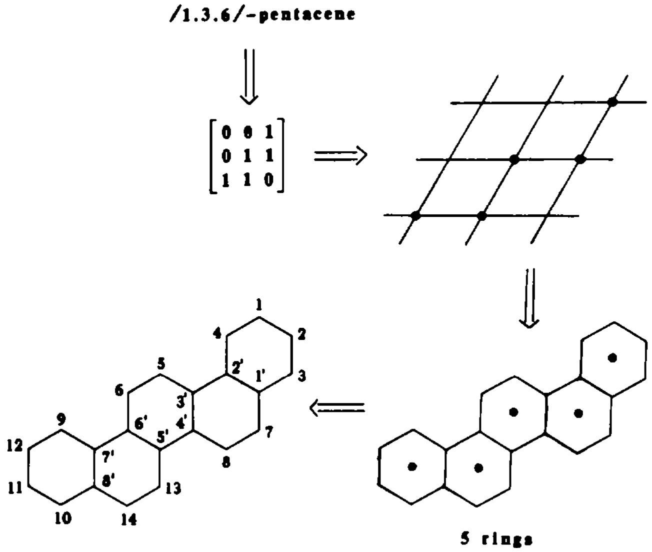
2H-/2.7/-tetracene

(10) In order to obtain the structural formula from the name of hydrocarbon the following procedure is applied: At first the zero-one matrix is generated from the normal formula. This matrix represents a set of benzene ring centers situated at the nodes of a net parallelogram. Then the centers are replaced by the benzene rings. The correctness of the above transformation can be checked by comparison of the number of obtained benzene rings with the number of benzene rings given in the normal formula. Eventually the numbering of C atoms is performed and H atoms or substituents are indicated.

Table 1. The comparison between the old and the proposed names for the benzenoid hydrocarbons

old name	new name
naphthalene	/3/-diacene
anthracene	/7/-triacene
phenanthrene	/1.3/-triacene
triphenylene	/2.6.1/-tetracene
chrysene	/3.6/-tetracene
picene	/1.3.6/-pentacene
1.2,3.4,5.6,7.8,9.10,11.12-hexabenzotriphenylene	/8.22.12.11.2/-decacene
penthaphene	/1.1.7/-pentacene
dinaphtho-(2'.1':1.2) ; (2".1":5.6)-anthracene	/3.14.24/-heptacene
perylene	/2.7.2/-pentacene
coronene	/6.7.3/-heptacene
bisanthene	/14.6.7/-octacene
ovalene	/14.15.7/-decacene
circumanthracene	/30.31.15/-tridecacene
pyrene	/3.3/-tetracene
1.2-benzopyrene	/2.6.3/-pentacene
3.4-benzopyrene	/3.7/-pentacene
dinaphtho-(2'.3':3.4) ; (2".3":8.9) -pyrene	/15.60/-octacene
anthanthrene	/7.7/-hexacene
terrylene	/2.7.14.4/-octacene
peropyrene	/3.7.6/-heptacene
quaterrylene	/2.7.14.28.8/-undecacene
triangulene	/4.6.7/-hexacene
zethrene	/2.15.4/-hexacene
heptazethrene	/2.31.8/-heptacene

Example



In Table 1 some examples of old and proposed names of chosen benzenoid hydrocarbons are listed.

The advantages of the proposed nomenclature are revealed in the simplicity of the names of hydrocarbons and in the fact that it can be applied to almost all known benzenoid hydrocarbons except for those in which benzene rings overlap (helicenes). However, this is not a serious limitation as such compounds are not numerous. In particular the advantages of the new system become clear when comparing the old names with the new ones. It is also obvious that this nomenclature can be very helpful for the accumulation and selection of the data on aromatic hydrocarbons. Application of our naming system makes the writing of a simple programme to assign the normal formula to any benzenoid hydrocarbon possible on the basis of the inputed Cartesian coordinates of its C atoms. The process of obtaining the structural formula of the compound from its normal formula can be easily performed. The programme can solve the problem of finding 12 possible orientations of the hydrocarbon molecule in the network, no matter what its initial position. A listing of such programme is available from the authors upon request.

Acknowledgement—We are grateful to Dr. A. Kolasa for kindly reading of the manuscript.

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