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An unified formula for deriving the molecular composition of hydrocarbons

Nowy sposób wyznaczania wzorów cząsteczkowych dla wszystkich węglowodorów

Abstract

An unified method of designing molecular formulae for all types hydrocarbons is proposed in this paper. The developed formula provides the molecular composition of hydrocarbons regardless of the number of chemical bonds and bond types or the number of rings they contain. Moreover, a small modification to that formula makes it suitable for deriving the molecular composition of hydrocarbons with oxygen atoms bound to carbon atoms with single and double bonds.

Keywords: molecular formulas of hydrocarbons, hydrocarbons

Streszczenie

W artykule przedstawiono ujednolicony sposób ustalania wzorów sumarycznych dla wszystkich węglowodorów. Zaproponowano stosowanie jednego ogólnego wzoru słusznego dla wszystkich węglowodorów w miejsce oddzielnie stosowanych obecnie wzorów właściwych tylko dla jednej grupy związków. Opracowany wzór pozwala podać wzory cząsteczkowe bez względu na ilość i typ wiązań chemicznych, jak również ilość pierścieni. Ponadto niewielka modyfikacja tego wzoru pozwala podać wzory cząsteczkowe węglowodorów zawierających zarówno wiązania pojedyncze, jak i podwójne pomiędzy atomami węgla i tlenu.

Słowa kluczowe: wzory cząsteczkowe węglowodorów, węglowodory

1. Introduction

Commonly, organic chemistry textbooks present a set of three formulae for deriving the molecular compositions of one type of bond in a specific compound:

a) alkanes [1–6]

$$C_n H_{2n+2} \tag{1}$$

b) alkenes [1–3, 6]

$$C_n H_{2n} \tag{2}$$

and

c) alkynes [1, 2, 4, 6]

$$C_n H_{2n-2} \tag{3}$$

The above formulae are characterized by significant limitations. In the case of non-saturated bonds, the formulae are correct only if there is one bond of a given type in a chain. If any non-saturated hydrocarbon contains more than one bond of a given kind or mixed bonds, then formulas (2) and (3) do not allow determining molecular formula. No mathematical relationships have been found in the latest literature that enable to calculate molecular formulas for such hydrocarbons containing multiple bonds as well as mixed ones.

For cyclic and aromatic hydrocarbons, no formulae are known which take into account the number of rings and bonds as well as the diversity of these bonds and side chains. Both types of hydrocarbons require separate formulae for determining their molecular composition. In the case of saturated cyclic hydrocarbons formula (4) is used and in the case of monocyclic aromatic hydrocarbons formula (5) is used, respectively [3, 5–7]:

$$C_n H_{2n} \tag{4}$$

$$C_n H_{2n-6} \tag{5}$$

2. Results and discussion

One general formula (6) which determines the molecular composition of different types and numbers of chemical bonds is now presented.

$$C_n H_{2(n+1-D-2T-R)} \tag{6}$$

where:

- C, H – carbon and hydrogen atoms, respectively;
- n – the number of carbon atoms;
- D – the number of double bonds;
- T – the number of triple bonds;
- R – the number of rings.

This formula is also valid for alkyloaromatic hydrocarbons.

Since alkanes contain no multiple carbon – carbon bonds, hence D, T and $R = 0$, then formula (6) is reduced to well-known shape given below:

$$C_nH_{2(n+1-0-2x0-0)} = C_nH_{2n+2}$$

In alkenes with one double bond, $D = 1$, $T = 0$ and $R = 0$; therefore, formula (6) transforms as follows:

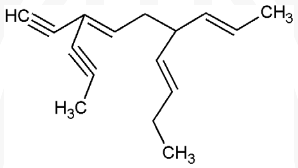
$$C_nH_{2(n+1-1-2x0-0)} = C_nH_{2n}$$

For alkynes bearing one triple bond ($D = 0$, $T = 1$ and $R = 0$) formula (6) takes the common form:

$$C_nH_{2(n+1-0-2x1-0)} = C_nH_{2n-2}$$

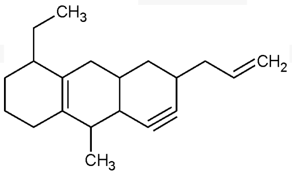
Some examples of calculations based on the proposed formula (6) are presented below.

For a structure containing sixteen carbon atoms, three double bonds and two triple ones ($D = 3$, $T = 2$, $R = 0$), the molecular formula of the below compound calculated according to the authors' formula (6) is as follows:



$$C_{16}H_{2(16+1-3-2x2-0)} = C_{16}H_{20}$$

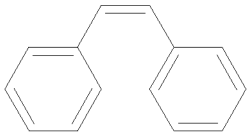
Another example shows that the proposed formula is also true for a hypothetical, complex and non-saturated cyclic hydrocarbon containing twenty carbon atoms, three rings, two double bonds, one triple bond as well as side chains. The structure of the compound is presented below:



Using the formula (6), the molecular composition of the compound is derived below:

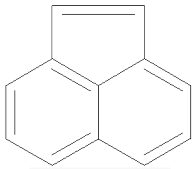
$$C_{20}H_{2(20+1-2-2x1-3)} = C_{20}H_{28}$$

In order to show an application of the proposed formula for aromatic hydrocarbons, calculations to present the molecular formula of stilbene are provided. The compound contains fourteen carbon atoms, two rings and seven double bonds. A method of calculating the molecular formula of the compound according to formula (6) is presented below:



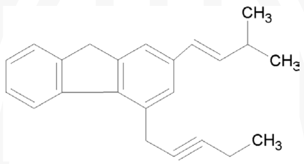
$$C_{14}H_{2(14+1-7-0-2)} = C_{14}H_{12}$$

Formula (6) is also correct for compounds of a structure such as acenaphthylene with twelve carbon atoms and three rings:



$$C_{12}H_{2(12+1-6-2x0-3)} = C_{12}H_{8}$$

Another calculation according to formula (6) has been done for a more complex, hypothetical hydrocarbon, which contains 23 carbon atoms and 24 hydrogen atoms:



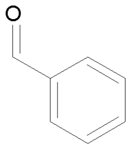
$$C_{23}H_{2(23+1-7-2x1-3)} = C_{23}H_{24}$$

A small modification to formula (6) also enables it to provide molecular formulas of hydrocarbons containing oxygen in a side chain connected with carbon by means of double bonding. If we use the formula:

$$C_n\,H_{2(n+1-D-2T-R-X)}\,O_y \qquad (7)$$

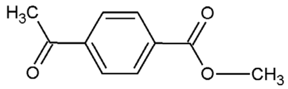
where:

- X – the number of double bonds between carbon and oxygen,
- Y – the total number of oxygen atoms, we can calculate the molecular formula of benzaldehyde:



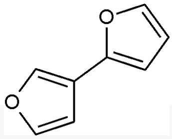
$$C_7H_{2(7+1-3-2x0-1-1)}\,O_1 = C_7H_6O$$

Formula (7) is also correct if a hydrocarbon contains both single and double bonds between carbon and oxygen atoms. For example:



$$C_{10}H_{2(10+1-3-2x0-1-2)}O_3 = C_{10}H_{10}O_3$$

If there are endocyclic oxygen atoms in the molecule, Eq. (7) is still applicable because the oxygen atoms are bound with single bonds as below:



$$C_8H_{2(8+1-4-2x0-2)}O_2 = C_8H_6O_2$$

3. Conclusions

A new, unified formula has been presented which allows the designing of molecular formulas of aliphatic and aromatic hydrocarbons. Thus far, separate relationships have been used for each homologous series and the equations have had a lot of limitations. Moreover, the formulae are not correct if the molecule contains more than one bond of a given hydrocarbon type or when there are simultaneously mixed, single, double and triple bonds. The proposed formula fits all types of hydrocarbons regardless of their structure, i.e. it takes into account the number of bonds, their diversity and in the case of cyclic and aromatic hydrocarbons, the number of rings. The formula is easy to memorise and based on it, one can readily establish the molecular formula of any hydrocarbons. Moreover, a small modification extends the approach to the molecular formulae of hydrocarbons with exocyclic oxygen atoms.

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