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Correction of the General Formula of Aromatic Hydrocarbons

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Abstract

The article discusses the general formula of aromatic hydrocarbons. The formula C_nH_{2n-6} for aromatic hydrocarbons is incorrect; the formula C_nH_n should be used inste determined.

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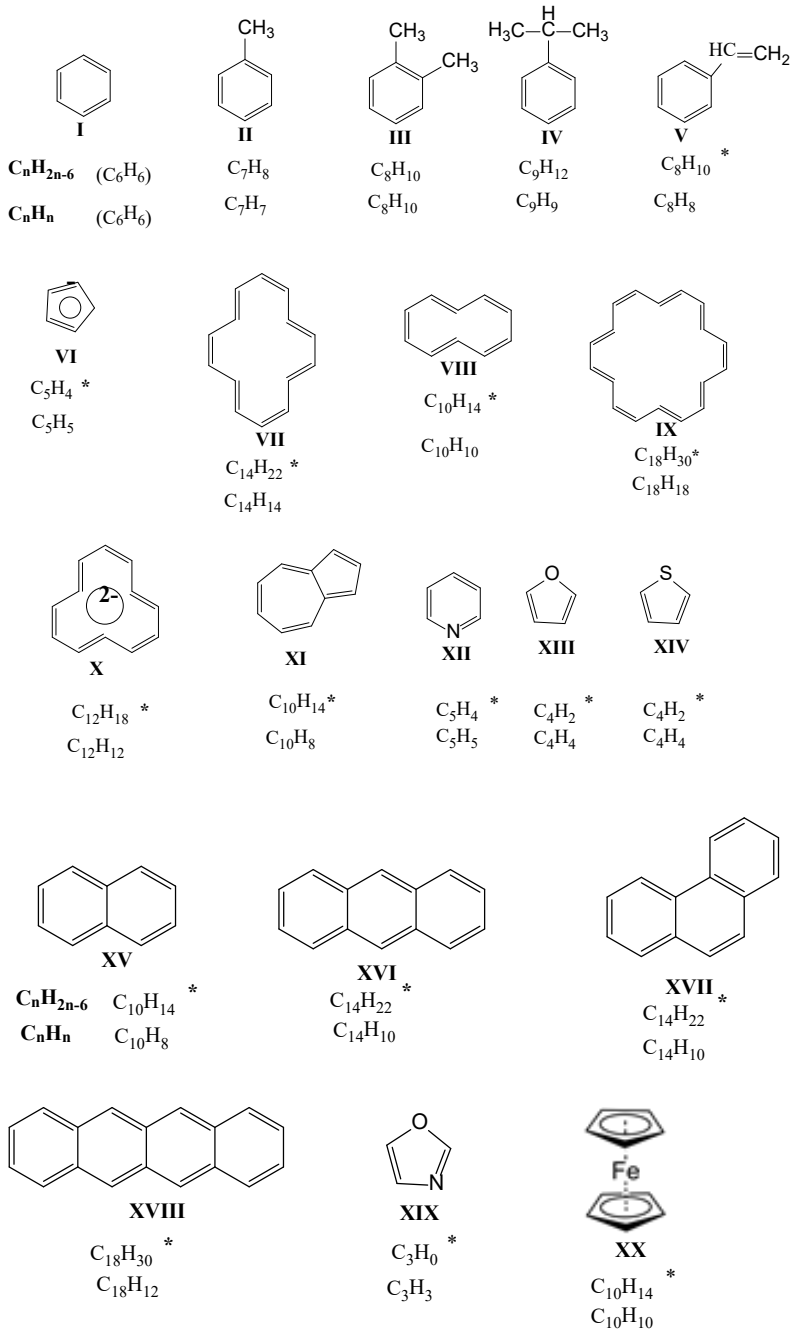
Introduction

For aromatic hydrocarbons the formula is CnH2n-6. It should be noted that this formula is completely valid for benzene and its homologs with saturated hydrocarbons (I-IV) [1-4].



* ¬ wrong Scheme 1.

Aromatic hydrocarbons are not limited to benzene and its compounds. After the discovery of the 4n+2 rule by the German chemist Hüggel, aromatic compounds can be expressed as follows:

Molecules that obey Hüggel's rule are aromatic compounds.

Interestingly, the formula C_nH_{2n-6} is only valid for benzene and its homologues (I–IV); it does not describe all other aromatic compounds; for example, this formula does not work for styrene (vinyl benzene) (V). Aromatic compounds are not only composed of benzene and its compounds with alkanes. As shown in Scheme 1, many aromatic compounds obey Hüggel's rule (4n+2), but the formula C_nH_{2n-6} does not hold. It should also be noted that if we are talking about an aromatic ring, then the expression of the alkyl side chain of the benzene homologues is inappropriate in this formula. Aromatic compounds include a wide group of molecules and ions with various structures that meet the criteria for aromaticity.

In our opinion, the general formula of arenes should be given in the form C_nH_n. This approach is noted under each arena formula and solves this problem.

The reason for the acidic properties of cyclopentadiene is the formation of a fairly stable cyclopentadienyl aromatic anion (VI) with six p-electrons.

Pyridine (XII) is an aromatic electron system that is formed by the electrons of the three double bonds of the ring. The lone pair of electrons of the nitrogen atom lies in a plane perpendicular to the plane of the ring system and does not take part in the creation of an aromatic sextet. Pyridine obeys Hückel's rule and corresponds to the general formula C_nH_n.

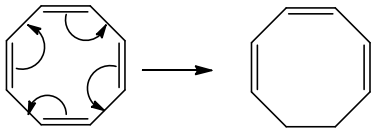
Interestingly, arenes such as naphthalene, anthracene, phenanthrene, and tetracene deviate slightly from this formula. Here, the naphthalene sequence should be represented by the formula C_nH_{n-2}, the anthracene and phenanthrene sequences by the formula C_nH_{n-4}, and the tetracene (XVIII) sequence by the formula $C_nH_{n-6.}$

Azulene (XI), consisting of fused seven-membered and five-membered rings of aromatic character (10e), corresponds to the formula C_nH_{n-2}, like naphthalene.

Oxazole (XIX) is a five-membered heterocycle, 6-p-electron nitrogen-containing aromatic compound belonging to the azole class. Although it belongs to this aromatic system, the formula C_nH_{2n-6} does not hold true here either.

In ferrocene (XX), the single and double bonds of the C_5H_5 rings are averaged, as in benzene, which is indicated by a ring symbol within the ring. The peculiarity of the structure of ferrocene is that the metal atom interacts not with one specific carbon atom, but with all the carbon atoms of two organic molecules at once. The orbitals of the p-electrons belonging to the cycles overlap with each other and with the unoccupied d-orbitals. A complex compound arises where all p-electrons of the cyclopentadienyl rings take part in the formation of a bond with the iron atom, forming coordination bonds with the metal. This is an independent type of chemical bond, called a p-complex bond. In terms of chemical properties, it resembles benzene: hydrogen atoms can be easily replaced by various organic groups. The ferrocene molecule clearly obeys the general formula C_nH_n.

It is known that cyclooctatetraene (XXI) is not an aromatic compound, although it has conjugate electrons, since it contains 8 p-electrons. Let's say we reduce its 2 electrons to 6 (XXII). At this point, the 6-electron system should be aromatic, but it is not considered aromatic because these electrons do not undergo cyclic delocalization as in benzene.



XXI XXII

Conclusion: After this discussion, it can be concluded that the general formula of arenes should be taken as CnHn rather than C_nH_{2n-6}.

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