

Discussion of the General Formula of Arenes

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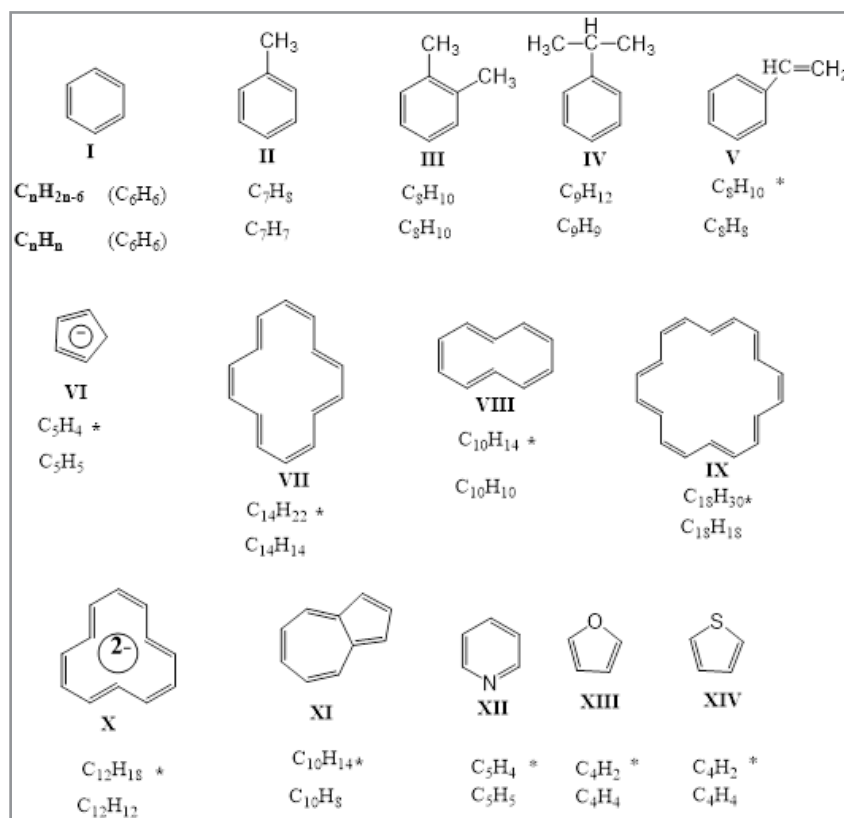
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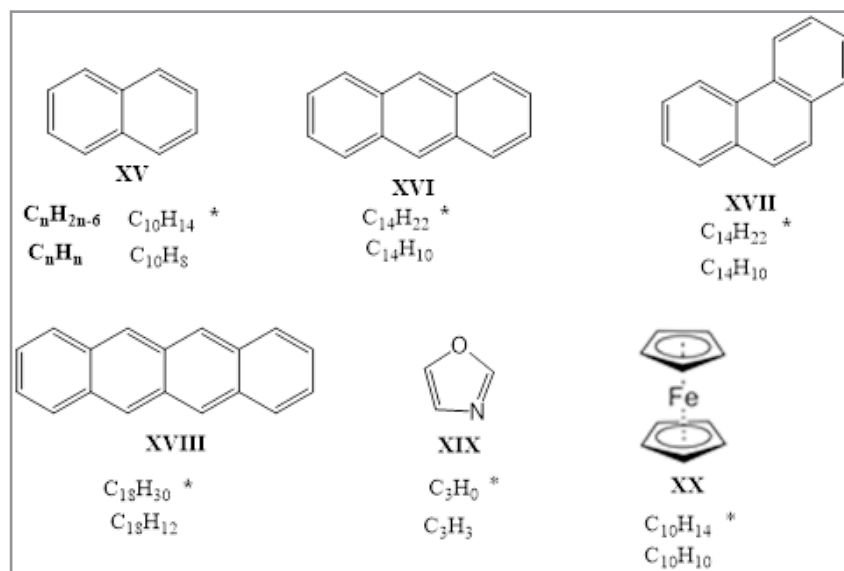
Abstract

The article discusses the general formula of aromatic hydrocarbons

Benzene, the first and simplest representative of aromatic hydrocarbons, was discovered in 1825 by the English chemist M. Faraday by liquefying illuminating gas (acetylene) under pressure and at low temperature. In 1931, the German chemist E. Hückel developed a quantum chemical approach to explaining aromaticity. This approach is still used today and is called the Hückel molecular orbital method. According to this approach, aromatic substances are cyclic compounds corresponding to the formula $4n+2$, formed by conjugated (delocalized) π - and σ -bonds with all C atoms in the plane.

By the 1860s, it was known that the ratio of carbon atoms to hydrogen atoms in the benzene molecule was similar to the ratio of C to H in acetylene, and the general formula was also assumed to be C_nH_n . Later this formula was abandoned and the formula C_nH_{2n-6} was used instead. The term "aromaticity" was introduced in 1865 by the German chemist F.A. Kekule, who determined the structure of benzene and proposed its formula (I). The general formula of arenes was adopted as follows: C_nH_{2n-6} 1-4.





* – wrong
Scheme 1.

Interestingly, the formula C_nH_{2n-6} corresponds only to benzene and its homologues (I–IV); does not describe all other aromatic compounds; for example, this formula does not work for styrene (vinyl benzene) (V). Aromatic hydrocarbons are sometimes called: “Aromatic hydrocarbons (arenes) are hydrocarbons with one or more benzene rings in their molecules.” This may not be the right approach. After all, aromatics should be understood not only as benzene and its homologues. There are other compounds that do not contain benzene that can be considered aromatic compounds. Aromatic compounds consist not only of benzene and its compounds with alkanes. As can be seen from Scheme 1, with the exception of benzene, many aromatic compounds obey Hückel's rule ($4n+2$), for which the formula C_nH_{2n-6} is incorrect. It should also be noted that if we are talking about an aromatic ring, then the expression of the alkyl side chain of benzene homologs is inappropriate in this formula. Aromatic compounds include a wide group of molecules and ions of various structures that meet the criteria of aromaticity.

The aromatic nuclei shown in Scheme 1 obey Hückel's rule ($4n+2$). However, the indicated general formula C_nH_{2n-6} does not confirm them.

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 .

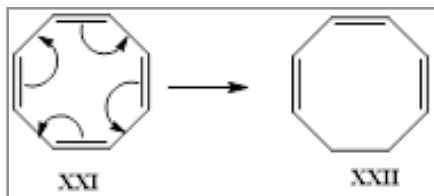
It is noteworthy that arenes such as naphthalene, anthracene and phenanthrene, tetracene partially deviate from this formula. Here, the order of naphthalene should be indicated by the formula C_nH_{n-2} , the order of anthracene and phenanthrene by the formula C_nH_{n-4} , and the order of tetracene (XVIII) by the formula C_nH_{n-6} , since this is due to the fact that there are 2 C atoms in naphthalene, 4 C atoms in anthracene and phenanthrene and 6 atoms in tetracene create additional bonds.

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 nitrogen-containing aromatic compound with 6 p-electrons, consisting of a five-membered heterocycle, belonging to the class of azoles. Although this also applies to the aromatic system, the formula C_nH_{2n-6} does not justify itself 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 [1-4].



Conclusion

After this discussion, it can be concluded that the general formula of arenes should be taken as $C_n H_n$ rather than $C_n H_{2n-6}$.

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