

Experimental confirmation of the existence of
the three-electron bond and theoretical basis of its existence.

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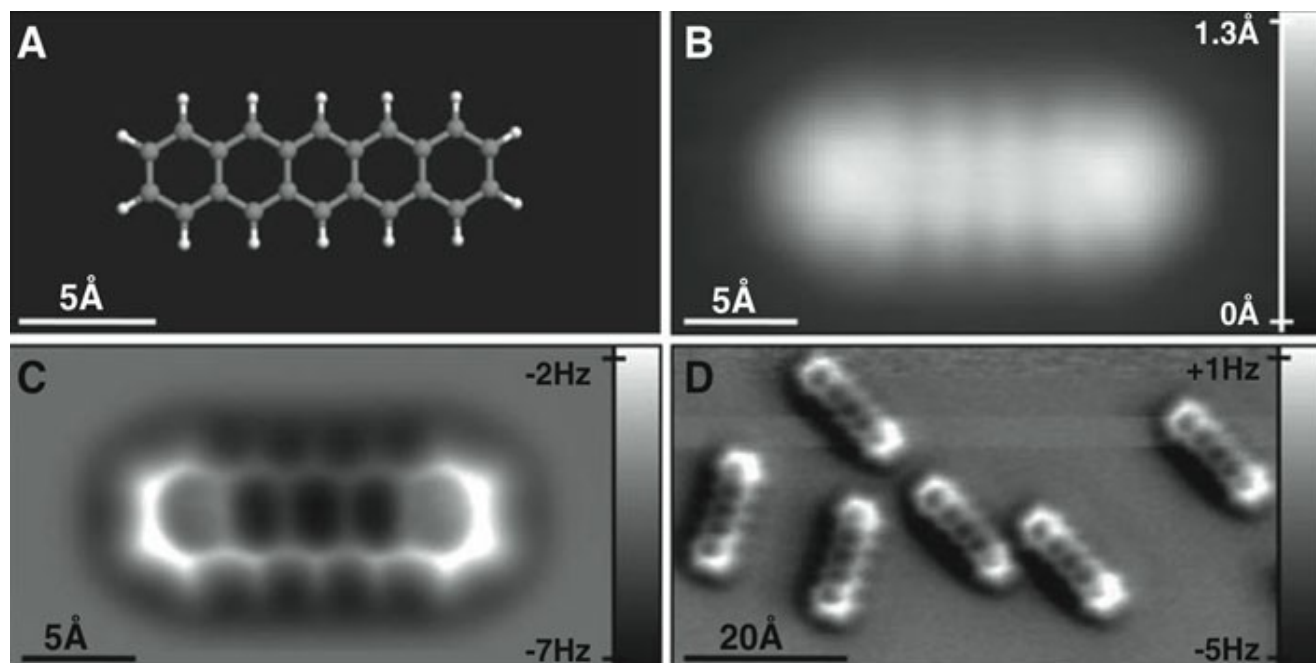
Abstract: Analysis of images made in techniques of atomic force microscopy (AFM) of high resolution in pentacene and other aromatic systems shows that according to predictions, aromatic three-electron bond is deflected to the centre of aromatic nuclei, which clearly confirms the fact of existence of three-electron bond in benzene, pentacene and other aromatic systems. It also confirms the existence of this bond in carboxylate anions and other similar ions and molecules.

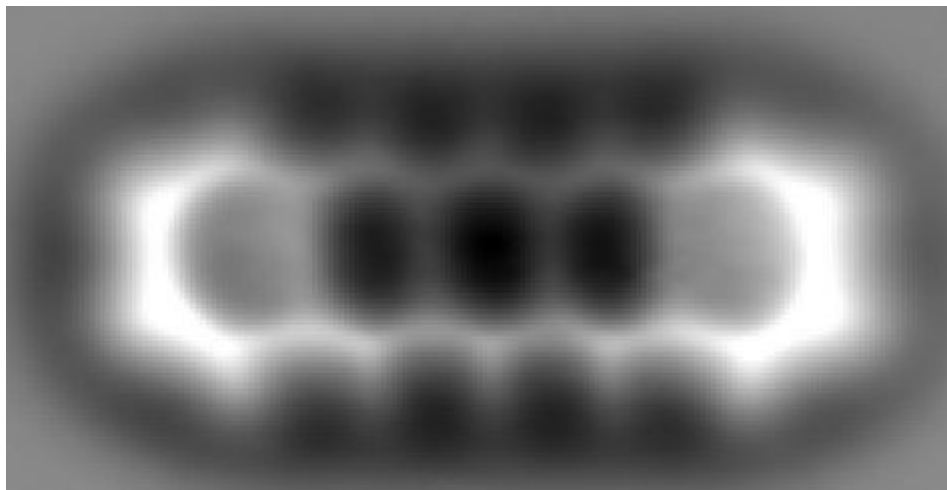
Keywords: three-electron bond, spin, semi-virtual particle, fermion, pentacene, AFM.

INTRODUCTION

Three-electron bond in benzene is classic, "direct", along the axis of the bond, but not in the form of "banana bond" [1]. Due to real interaction through the cycle the bond should deviate slightly from the axis, possibly by $0.1 \text{ \AA} - 0.2 \text{ \AA}$, somewhat shift a little to the centre of the cycle. This shift is very slight as compared to "banana bond".

Let us consider the picture of the molecule of pentacene [2]:

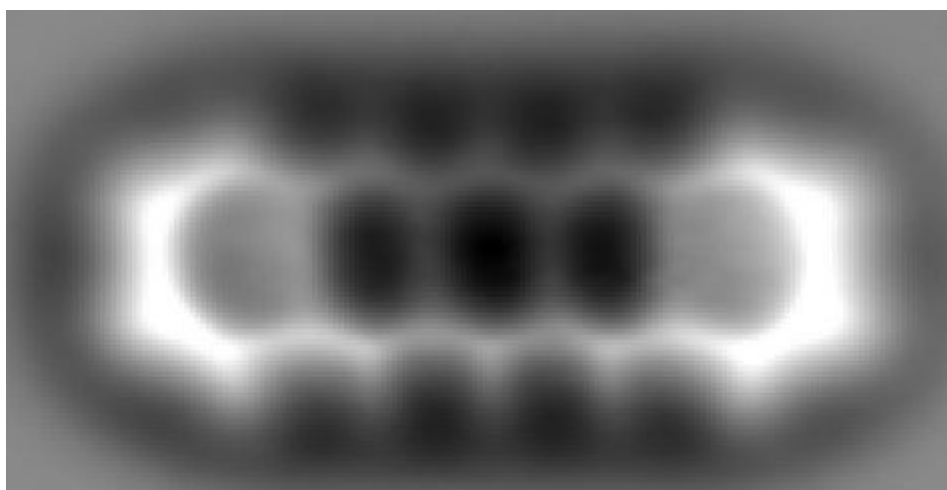




Using an atomic force microscope (AFM), it is possible to obtain such photos of molecules and actually to study individual molecules and their bonds; and this particular is needed to determine the presence of the three-electron bond.

RESULTS AND DISCUSSION.

Molecule of pentacene is the most representative, see photos



where the displacement of the chemical bond (or rather the bond path) to the centre of the extreme cycles is clearly shown, which should be observed according to the three-electron bond theory (TBT) and the interaction through the cycle.

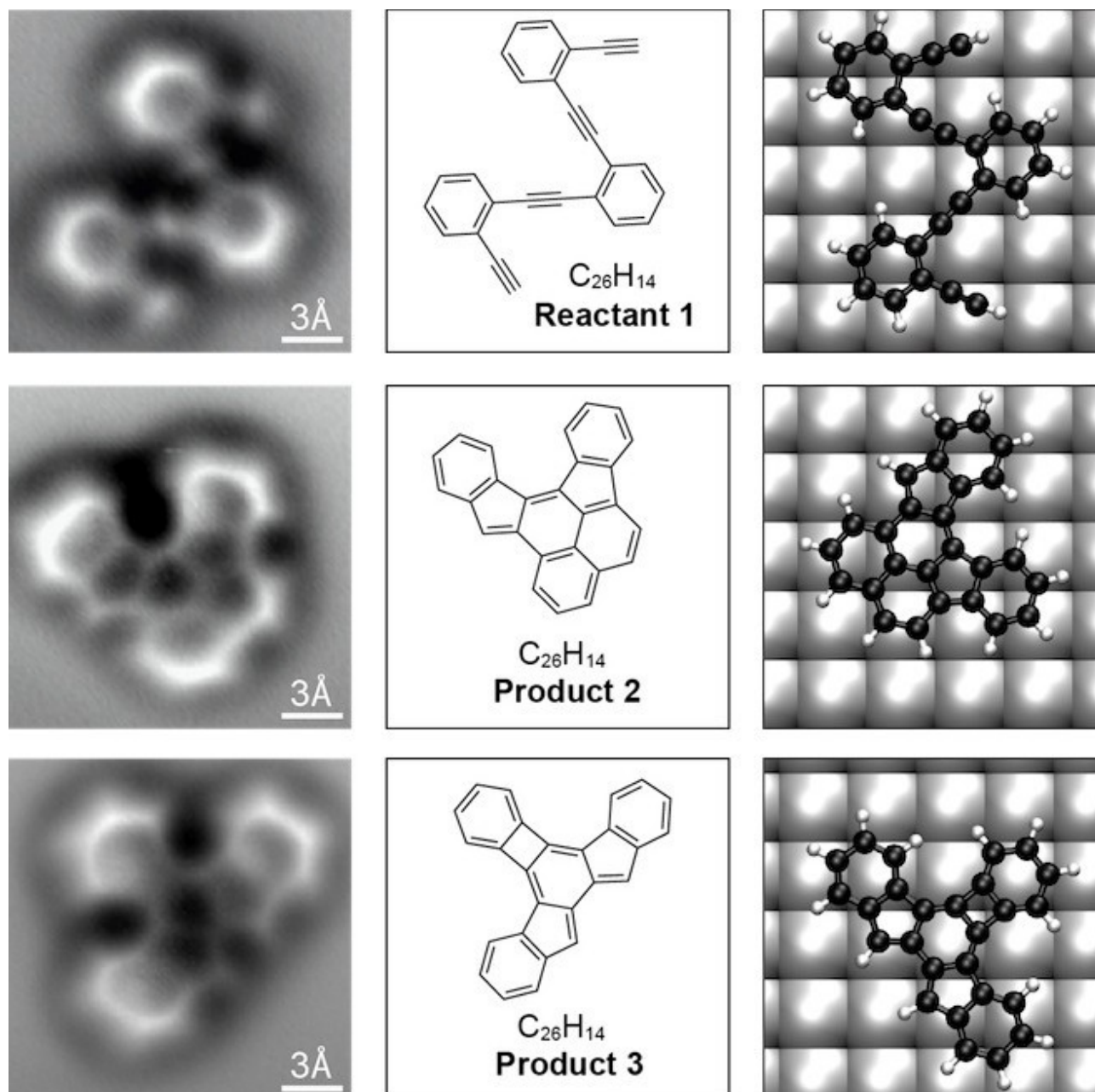
Formulae of naphthalene and anthracene are presented at p. 19 [1] according to the TBT. The molecule of pentacene will have a similar structure according to the three-electron bond theory.

Displacement of the chemical bond in the inner cycles of pentacene cannot be detected at the photo, which is logical taking into account the interaction of central electrons of the three-electron bond of inner cycles, because neighbouring central electrons act in opposite directions; so the shift to the centre of cycles is minimal or absent.

Distribution of the intensity of chemical bond in pentacene visible in the photo can be logically explained by addition of electron densities, or broadly speaking by addition of the number of electrons involved in chemical bond. Electron density near the carbon atom is not less than in the centre of the chemical bond, so there is no protrusion of the centre of the chemical bond to the centre of the cycle (regardless of the presence of three-electron bond), which is understandable considering two three-electron bonds near the carbon atom, and therefore two neighbouring electrons with opposite spins will interact with each other.

We shall see no protrusion of the centre of the chemical bond to the centre of the cycle in similar photos of antiaromatic systems. The whole image should be similar to the image of pentacene but with a shift of the chemical bond "out of the cycle".

If one consider the following molecules



the following conclusions can be drawn [3]:

See photo Reactant 1 – it is clearly shown how the triple acceptor bond pulls electron density from the benzene ring, and thus the chemical bonds of the corresponding carbon atoms will not be (or too much lesser extent will not be) drawn to the centre of the benzene cycle or so to speak "will neither bend no strain", as we can see in the photo.

See photo Product 2 - it is clearly shown two benzene nuclei and one naphthalene nucleus. The situation is repeated where the displacement of chemical bonds (three-electron bonds) to the centre of cycles is possible; it occurs and can be clearly seen in the photo. Where interaction (pumping) of electron density occurs in the result of conjugation with double bonds, we shall see no shift of the chemical bond to the centre of the cycle. Therefore, the displacement of chemical bonds of outer sides of benzene and naphthalene is clearly visible, however this effect is not observed for inner sides.

See photo Product 3 - it is similar to the Product 2, we just have three benzene nuclei, and the shift of chemical bonds of outer sides of benzene rings is clearly visible, however this effect is not observed for inner sides involved in conjugation.

Analysis of images made in techniques of atomic force microscopy (AFM) of high resolution in pentacene and other aromatic systems shows that aromatic three-electron bond is deflected to the centre of aromatic nuclei, which clearly confirms the fact of existence of three-electron bond in benzene, pentacene and other aromatic systems. It also confirms the existence of this bond in carboxylate anions and other similar ions and molecules.

AFM images of benzene can be presented on the basis of pentacene image, and if it exists, or if it is received at the appropriate resolution, it will be another confirmation of real existence of the three-electron bond.

There is no doubt that AFM images of cyclobutadiene (planar) and cyclooctatetraene (planar) or of any other planar antiaromatic system, when received at the appropriate resolution, will be another confirmation of the interaction through the cycle in aromatic and antiaromatic systems. It should be noted that the deviation of chemical bond in antiaromatic systems will be "from the cycle", similarly to pentacene, but in the opposite direction.

But there is a nuance as for antiaromatic systems: an antiaromatic system (system of nuclei) should be planar in order to have the interaction through cycle [1, p. 5 – 6]. If the system is not planar, it will be a transition into the "bath" in cyclooctatetraenyl (four double bonds), a transition into the diradical in cyclobutadiene (double bond and two unpaired electron, the nuclei system shall be planar and not a square). Then the AFM image shall show the appropriate structure, ie double bonds plus unpaired electrons in cyclooctatetraene and cyclobutadiene.

Therefore, to obtain AFM images of antiaromatic cyclobutadiene and cyclooctatetraene, it is necessary to consolidate their atoms on a special matrix for achieving a perfect planarity of the system, and only then to pick AFM images of appropriate resolution, if it is possible. Undoubtedly, this AFM image will confirm the interaction of three-electron bonds through the cycle.

Now the question is how to explain the existence of the three-electron bond in benzene and other molecules and ions from the point of view of quantum theory. It stands to reason that any placement of three electrons on the same atomic or molecular orbital is out of the question. Therefore it is necessary to lay the existence of three-electron bond in molecules in reality as an axiom. In this case the three-electron bond in benzene can be actually considered a semi-virtual particle. A real particle, such as an electron, exists in the real world for indefinitely long time. Virtual particles exist for the time which is insufficient for experimental registration (strong interactions in atomic nuclei). So we shall call the three-electron bond which really exists for indefinitely long time only in molecules and ions a semi-virtual particle.

The three-electron bond as a semi-virtual particle has certain characteristics:
its mass is equal to three electronic masses,
its charge is equal to three electronic charges,
it has half-integer spin (plus, minus 1/2)
and a real spatial extension.

That is, our semi-virtual particle (the three-electron bond) is a typical fermion. Fermions are particles with half-integer spin; they follow the Fermi-Dirac statistics, and have appropriate consequences, such as the Pauli exclusion principle etc. An electron is a typical fermion, and therefore such distribution in atomic and molecular orbitals is accepted (calculated).

It follows that the three-electron bond in benzene is a real fermion in benzene, so quantum calculations can be extended to the molecule of benzene (and other systems) with the use of corresponding fermion (i.e. three- electron bond as a particle) instead of the electron in calculations. Then everything shall be made as usual: the Pauli exclusion principle, distribution in MO, binding and disintegrating MO, etc.

Then, there will be three fundamental interactions (between fermions) in chemistry:
electron - electron;
electron - fermion-three-electron bond;
fermion-three-electron bond - fermion-three-electron bond;
the calculation of which should ideally lead to the calculation of any system.

Following from the above, interaction of two three-electron bonds in benzene (or rather interaction of three pairs) through the cycle is a typical interaction between two fermions in a molecule at a distance of 2.4 Å which is similar to the interaction of two electrons at the chemical bond formation.

By the way, two-electron bonds, four-electron bonds and six-electron bonds can be studied as typical bosons following the Bose-Einstein statistics.

Hückel rule ($4n + 2$) for aromatic systems can be written in a different form, in the form of $2n$ where n - unpaired number. So, we have: 2, 6, 10, 14, 18, etc. This is also true for the electron shells in the atom and aromatic systems. The principle of the interaction of fermions always one, everywhere. And now, need to remember J.W. Linnett with Double Quartet Theory [4]. J.W. Linnett was right. Just need take to the point, that chemical bond is interaction of fermions (here they are doublets) with oppositely directed spins, and the fact, that octet (single atom, and, in general, the atoms form a chemical bond) consists of the sum of the electrons on the different levels s-, p-, d- (for a single atom), etc.

Consider an atom: then in the s-levels of interaction two fermions (1 (+) and 1 (-)), on the p-levels are also interacting two fermions (3 (+, -, +) and 3 (-, +, -)) two fermions (5 (+, -, +, -, +) and 5 (-, +, -, +, -)) to similarly interact d-level. But all these fermions are composed of different number of electrons for the s-levels are 1 (+) electron, p-level is 3 electrons (+, -, +) for the d-level is 5 electrons (+, -, +, -, +). Huckel rule clearly defines the number of electrons is to always get a fermion (so n -unpaired number, $2n$). Given the number of electrons at different levels (s-, p-, d-) we obtain the total number of electrons corresponding to the octet rule (2, 8, etc.). What is particularly important to minimize the repulsion between the electrons needed to separate fermion consisted of electrons whose spins have a different direction (ie neighboring electrons have opposite spins, for example, for fermions composed of three electrons, we have: 1 (+), 2 (-), 3 (+). Naturally, the two interacting fermions are oppositely directed back 1 (+) and 2 (-).

Now consider the benzene. As it was shown in [1] in benzene exists between carbon atoms three-electron bond (a fermion), which interacts with the other through a series of three-electron bond (with another fermion). If we apply the idea of Linnett six of p-electrons in benzene, then benzene will be the spirit of the interaction of fermions (or two doublets): (3 (+, -, +) and 3 (-, +, -)). If we take the more general case, all the 18 electrons of benzene and then we have two interaction fermions, each of which consists of 9 electrons (9 (+) and 9 (-)). Naturally, these two fermions placed in a field of six carbon nuclei.

We now turn to the chemical bonds of different multiplicity.

Consider a single two-electron bond: we have interaction between two fermions, ie, two electrons (1 (+) and 2 (-)).

Dual four-electron bond should be considered as a combination of two single two-electron bonds. And here it is impossible not to recall the idea of Pauling on the description of multiple bonds by means of bent bonds [5]. Consider the double bond as the interaction between two fermions prohibits that two electrons with opposite spins (curved bond) is a boson. In principle, the double bond can be viewed as the interaction of two bosons, which are due to the repulsive give two equivalent curved bonds (bosons tend to occupy one energy level).

Triple six-electron bond can be described by Pauling as a combination of three curved single bonds, and using ideas Linnet (which in our opinion is more true) as the interaction between two fermions (two three-electron bonds, two doublets) which have opposite spins (3 (+, - +) and 3 (-, +, -)). Here, as in the benzene six electrons interact, but now they are placed between two carbon atoms (benzene between six carbon atoms). This description is supported by its triple bond less "unsaturated" and more specific properties as compared with a double bond.

From the above it should be clear that the formation of octet, aromatic systems in general and chemical bonds is the interaction of fermions in various different environments, which leads to a variety of chemical systems.

CONCLUSION

Construction of diagrams showing how electrons gravitate (in explaining the interaction through the cycle, etc.) is an attempt to explain the Quantum interaction of electrons by using methods of classical chemistry [1 p. 4 – 5]. It is clear that electrons do not gravitate towards each other (gravitational interaction is neglected), but on the contrary, if they gravitate, a force should exist, as well as an equation for the calculation of this force. In nature, there are only four fundamental interactions:

1. Gravity.
2. Electromagnetic.
3. Strong.
4. Weak.

With neglect of gravitational interaction, it is only electromagnetic interaction and broadly speaking, Coulomb attraction and repulsion in the molecule (or rather between electrons and nuclei).

Quantum mechanics defines what such a chemical bond. Without quantum mechanics it is impossible. Classical concepts to explain what the chemical bond is impossible (and this despite the existence of four fundamental interactions). It is obvious that when the chemical bond formation quantum effects are important. That is, to form a chemical bond is not enough to have two specific atoms with unpaired electrons and the four fundamental interactions, but still need these two atoms placed at a certain distance where quantum effects "help" form a chemical bond. Without quantum

effects these baselines (atoms and fundamental interactions) is not enough to form a chemical bond. It is obvious that when the chemical bonds forming, important not only the properties of atoms and fundamental interactions but also the structure of the space-time at distances of several angstroms (scale chemical bond). Quantum effects of the space-time begin to affect the interaction of atoms (the house begins to affect the interaction between residents), without it, explaining the formation of a chemical bond is impossible.

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