Supplement to the theoretical justification of existence of the three-electron bond.

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Abstract: The existence of large aromatic monocycles has been proved impossible based on interaction of three-electron bonds through the cycle at distances between the bonds (through the cycle) greater than 3.5 Å due to the lack of energy interaction (the length of chemical bonds is in the range of distances 0.74 Å – 3.5 Å). The chemical bond (two-electron and three-electron) is considered on the assumption that the electrons in a chemical bond can be regarded as being in an entangled quantum state, that is, the chemical bond is seen as a new "indivisible" particle. There has been provided an algorithm for calculating the two-electron chemical bond "on the tip of the pen". An attempt was made to explain the mechanism of interaction of particles in an entangled quantum state on the basis of a new model of the Interfering Universe.

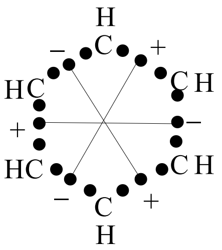
Keywords: three-electron bond, fermion, spin, semi-virtual particle, entangled quantum state, Interfering Universe.

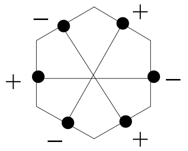
INTRODUCTION.

Consider and try to explain the interaction scheme of chemical bonds in the benzene molecule [1, p. 2-5, 10-11]. The interaction of two three-electron bonds in a molecule of benzene at a distance of 2.42 Å (on opposite sides) can be explained if we consider these two three-electron bonds as two particles (two fermions) in an entangled quantum state. That is, these two fermions are in an entangled quantum state. Quantum entanglement is a quantum mechanical phenomenon, in which the quantum states of two or more fermions or bosons prove to be interconnected [2-6]. And surprisingly, this interconnection remains at virtually any distance between the particles (when there are no other known interactions). It should be realized that the entangled quantum system is in fact an "indivisible" object, a new particle with certain properties (and the particles of which it is composed should meet certain criteria). And most importantly, when measuring the spin (or other property) of the first particle we will automatically unambiguously know the spin (property) of the second particle (let's say we get a positive spin of the first particle, then the spin of the second particle will always be negative, and vice versa). Two particles in an entangled state prove to be bound by an "invisible thread", that is, in fact, they form a new "indivisible" object, a new particle. And this is an experimental fact.

RESULTS AND DISCUSSION.

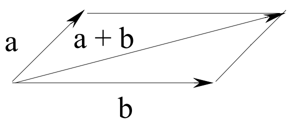
As for the benzene molecule [1, p. 2-11], if we consider the interaction of all six three-electron bonds as an entangled quantum state of six fermions (three-electron bonds), then the definition of the spin of one of the fermions automatically implies the knowledge of all the spins of the other five fermions, and in closer inspection it means the knowledge of the spins of all 18 benzene electrons that form all the six C-C bonds. In fact, on this basis, the benzene molecule can be used to study the entangled quantum states of electrons (fermions).

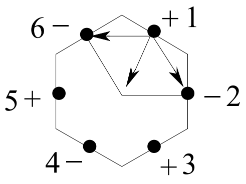


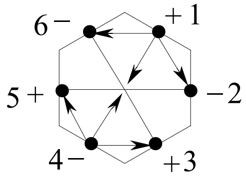


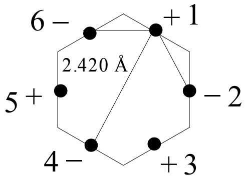
"+" - the spin directed up
"−" - the spin directed down

One can realize that the interaction of three-electron bonds in a molecule of benzene at a distance of 2.42 Å is significant on the basis of the fact that the bond length in a molecule of iodine (I-I) is about 2.66 Å. Therefore, it is reasonable to assume that the energy interaction of the three-electron bonds (or central electrons) at distances between them of 2.42 Å will be significant.









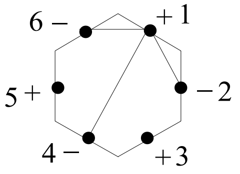
$L_{1-2} = L_{1-6} = 1.210$ Å

$L_{1-4} = 2.420$ Å

In addition, the length of chemical bonds in the general case is in the approximate range of 0.74 Å – 3.5 Å.

The value of 3.5 Å, in principle, restricts the existence of large monocyclic aromatic systems such as of cyclodecapentaene.

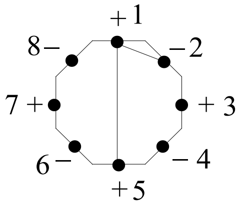
$L_{c\text{-}c}$ = 1.397 Å



$L_{1-2} = L_{6-1} = 1.210$ Å

$L_{1-4} = 2.420$ Å

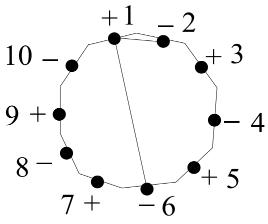
$L_{c\text{-}c}$ = 1.410 Å



$L_{1-2} = L_{8-1} = 1.303$ Å

$L_{1-5} = 3.404$ Å

$L_{c\text{-}c}$ = 1.400 Å

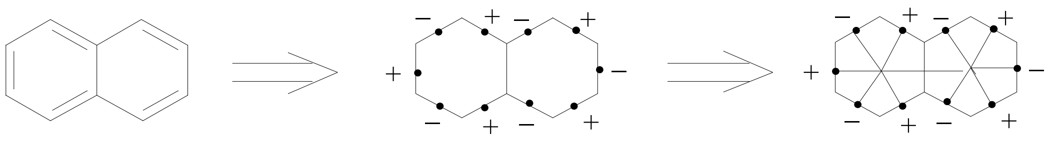


$L_{1-2} = L_{10-1} = 1.331$ Å

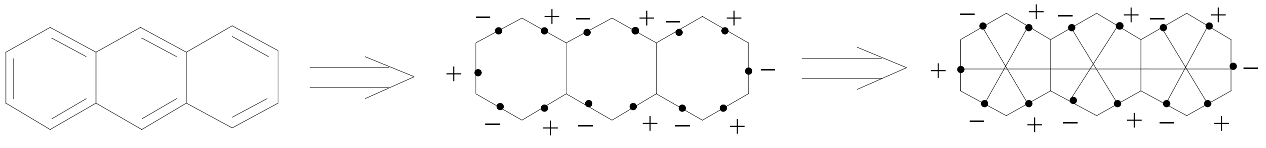
$L_{1-6} = 4.309$ Å

Since the distance between the opposite bonds is equal to 4.31 Å, i.e., there is no significant interaction between the three-electron bonds (or electrons located on opposite sides of the cycle) and thus there won't be stabilization of the cycle because the distance is more than 3.5 Å, that is longer than the "longest chemical bond". Without this interaction energy, it will be impossible to stabilize a large monocyclic aromatic system, in which the cyclic strain will substantially increase.

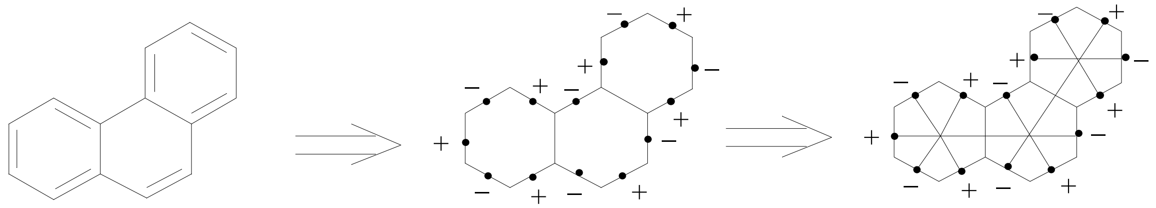
In other systems such as naphthalene, anthracene, tetracene, pentacene, and the like, the longest interaction between two three-electron bonds of different cycles (longer than 3.5 Å) will also be insignificant in terms of formation of a chemical bond [1, p. 19-20].



Naphthalene



Anthracene



Phenanthrene

Three-electron bonds will exist in such systems (system stabilization due to of the core of six-membered rings), but there will be no significant interaction between specific bonds over long distances (in energy terms). But this does not mean that these three-electron bonds will not interact in any way. Quite the contrary, they will certainly interact, and this interaction will lead to the formation of an entangled quantum state, which in fact will determine the type of the electron spin (or the three-electron bond). Moreover, in general, in the two-electron chemical bond, the electrons can also be regarded as being in an entangled quantum state, which actually determines their spins.

The fact that electrons during the formation of chemical bonds are in an entangled quantum state, is very important for chemistry and quantum mechanical bond calculations. For example, when calculating the two-electron chemical bond of a hydrogen molecule, it will no longer be necessary to consider the movement of two electrons in general, i.e. as independent and virtually any relative to one another.

And we will know for sure that in an entangled quantum state, these two electrons can be considered actually bound by an "invisible thread" with a certain length, that is, two electrons are connected and form a new "indivisible" particle. That is, the movement of two electrons in the field of cores can be described by the movement of a point located in the middle of the "invisible thread" (or in the center of a new particle, or in the center of mass, and so on), what should greatly simplify the quantum mechanical calculations.

The length of the "invisible thread" will definitely be much less than the sum of the covalent radii of hydrogen atoms, and it is this length that will determine the Coulomb repulsion between the two electrons. The length of the "invisible thread" between electrons in various chemical bonds should not greatly differ, and perhaps it will be a constant for all, without exception, chemical bonds (meaning two-electron bonds), maybe it will be another constant.

The three-electron bond can also be seen as an entangled quantum state in which there are three electrons. Then the length of the "invisible thread" between electrons will be different from that of the two-electron bond. You can also expect that for all, without exception, three-electron bonds the distance between electrons will be the same that is constant.

All types of chemical bonds (two-electron, three-electron, four-electron, five-electron, six-electron, and so on) can be seen as an entangled quantum state, in which there are electrons involved in chemical bonding. And interestingly, all entangled particles behave as they should according to the quantum theory, that is, their characteristics remain uncertain until the moment of measurement. From this point of view (the quantum mechanical point), it becomes clear the cause of failure to calculate chemical bonds "on the tip of the pen" with attempts to calculate the speed and energy of electrons and other characteristics. But these characteristics of electrons of the chemical bond (a chemical bond is a quantum entangled system, which contains electrons of the bond) cannot be determined in principle, because it is so constituted the quantum world. Logically, that what is impossible to determine is impossible to calculate in principle, what is confirmed by the history of quantum chemical calculations. That is, all attempts to calculate characteristics of electron chemical bond (speed, power, and so on) were doomed to failure from the beginning. Therefore, in our opinion, it would be more correct to consider the chemical bond as a certain new "indivisible" particle, with well-defined characteristics and spatial extension, which we called a "semi-virtual particle" [14, p. 5-8]. In particular chemical substance the chemical bond is really indivisible. In addition, such semi-virtual particle is a fermion for the three-electron bond and other bonds with an unpaired number of electrons and total half-integral spin. And the semi-virtual particle will be a boson for the two-electron bonds and other bonds with a paired number of electrons and total integral or zero spin. And the characteristics of a semi-virtual particle (as an integral), we can calculate. These are the characteristics of a semi-virtual particle, such as energy, spatial extension, length, and so on, that are very important for chemistry.

Calculations of a hydrogen molecule will actually come to the solution of the movement of one point in the field of two protons, which is similar to the solution of a task for the hydrogen molecular ion H_2 + [7-13]. And we can expect that finally the two-electron chemical bond will be calculated "on the tip of the pen”.

Besides that, an entangled quantum state clearly demonstrates that the chemical bond is real and that it is neither an abstraction, nor a convenient concept used to describe and explain. Two electrons indeed form a chemical bond (which is a new particle), and they really "know each other's spins", and are in an entangled quantum state. This means that these two electrons forming a chemical bond and connected by an "invisible thread" have their own well-defined characteristics. And this bond (or this thread) is real, but not in terms of energy (if the energy of such bond really exists and is not equal to zero, then its value cannot be compared with the energies of chemical bonds).

Now, let's try to explain the possibility of interaction of electrons and other particles, which are in an entangled quantum state, what presupposes the existence of any distance between them, for example, 1 m, or 1000 km, it is not essential, the distance can be arbitrarily long. And this distance does not affect the entangled quantum system, the particles of which miraculously know the characteristics of each other. To do this we'll have to simulate our Universe. So, let's imagine our infinite Universe as a finite (for convenience of description) object, such as an ordinary cube. Now let's imagine this cube empty of matter, space-time, and in general of any fields and other characteristics, there is no matter, and, in principle, anything. Now, let's "insert" an electron in the cube, and at once in the Universe there will appear space-time, weight, variety of fields (gravitational, electromagnetic, and so on), energy and other characteristics. After the electron appeared in the Universe, it came to life, and was born in principle. And now let's specify that the electron is not simply located in the Universe and has specific location and spot size, and its fields (electromagnetic, gravitational, and other existing and unknown) occupy and fill the whole Universe, the entire space-time continuum, our whole infinite Universe. Now let's step by step fill our cube (our Universe) with all elementary particles that exist in the Universe. And there is one condition that must be followed: each elementary particle occupies entirely and completely the whole Universe by its fields, energy and other characteristics, that is each particle completely fills (literally) all the infinite Universe, but at the same time it has certain coordinates (the most probable place of elementary particle detection).

With this description, our Universe, which is infinite in all senses (spatial, energy, time, etc.), will represent a giant interference of any and all elementary particles, a model of the "Interfering Universe".

And now the main thing: since each elementary particle occupies (fills) the whole Universe (and at the same time is in a particular place with certain coordinates (its most probabilistic definition in this point, or more precisely in this region of space)), then there is nothing unusual in the fact that when forming an entangled quantum state each elementary particle "knows" the characteristics of its partner in a quantum state. Elementary particles "know" everything about all the other elementary particles since they fill the same Universe (it is their common home). They (elementary particles) constantly interact, interfere, but depending on their characteristics and the characteristics of their partners (coordinates, mass, energy, field, distances between the peak densities of detection, wave characteristics, etc.) form stable bonds (most varied and not only energy) only with certain partner particles.

CONCLUSION.

Based on the foregoing, we can conclude that our Universe, our world more precisely, is an interference pattern of each and every particle in the Universe. Now the wave-particle duality of particles, probabilistic interpretation of quantum mechanical phenomena and other quantum effects of the microcosm become intuitively clear. For example, why there is a non-zero probability of finding an electron, which rotates in a specific hydrogen atom (which is in a particular laboratory), for example, on the Moon. And it is both on the Moon and on the Sun, as well as anywhere in the space of our Universe, it really fills (takes) the whole Universe. But its presence in a particular area, "the density of presence", so to speak (probability of detection), is different at different points of the space.

In the Interfering Universe, all elementary particles "know everything" about all the other elementary particles (since they are in the same Universe), but not all of them are suitable for all in terms of formation of various bonds (in energy and other senses). Therefore, only those particles interact, which have a well-defined set of characteristics for each other and for specific types of interactions. And our world forms as a result of such interactions.

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