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Atommetrics: Another View of Atomic Structure Based on Electron Orbital Geometry Part 2

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Abstract. This paper along with the original one (*Forma*, **17**, 293–308, 2002) offers a simple model of the atom as a structural balance of tension (attractive) and compression (repulsive) members which helps to explain three-dimensionally and effectively the workings of the atom independently as well as in bonds as molecules. In this model, the structure of the atom is composed of invisible "struts" of attractive, nuclear forces on the electrons in tension and of repulsive, electron forces on each other in compression.

1. Introduction

As can be seen in Fig. 1 (next page), the model is a cube with 2 interpenetrating tetrahedra (black and white) interlocked by the peripheral edges of the cube (gray). Diagonal force lines piercing through the nucleus are in tension, as the nucleus attracts and pulls on the electrons, while all others are in compression, as the electrons repel and push against each other.

The author knows well that the electron behavior is described based on quantum mechanics and the electron orbits are obtained by solving the Schroedinger equation. The purpose of this paper is to point out a similarity between atomic structure and polyhedra and to propose another way of understanding it by a new model. This kind of a model is expected to have its own role, i.e. to provoke a flexible mind for research and development in the material sciences. While Heisenberg's Principle of Uncertainty dictates that the position and the speed of an electron cannot be accurately *measured* simultaneously, it does not imply that there is no orderly structure and motion of electrons in the atom. The model may be able to not only predict certain molecular configurations but also, in reverse, design and engineer artificial atoms and molecules of perhaps immense applicational potential.

The following is the basic model of the atom for those atoms with from 1 to 8 valence electrons.

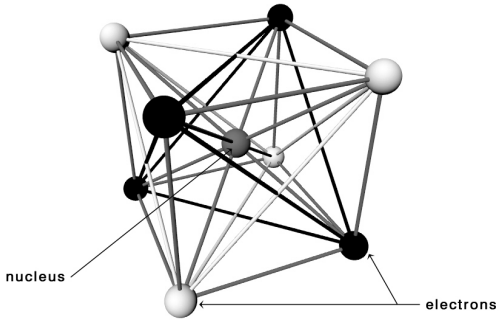


Fig. 1. Basic atom model. Diagonal lines piercing through the nucleus are in tension; all others are in compression.

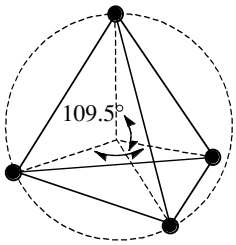


Fig. 2. 4 orbits with 1 electron each constituting a tetrahedron.

2. Electron Configurations and Orbits

The present model begins with a model of the Carbon atom. In order to minimize electron repulsion and to form the simplest, symmetrically balanced configuration, the Carbon atom is assumed to have the tetrahedral configuration shown in Fig. 2.

This tetrahedral configuration is the simplest and the most stable three-dimensional relationship that can exist among four electrons. This tetrahedral relationship might explain how atoms with half-filled valence shells are stable just as atoms with their shells completely full. The vital role of the Carbon atom in organic life might be explained by such structural integrity as well as by its capacity to bond with other elements, being only half full, as shall be demonstrated henceforth.

Evidence to support this postulate that Carbon has four orbits with one electron each may be identified in the way it bonds with, for instance, Hydrogen to create methane. Since each orbit is half full, there is an empty slot at the opposite side of the orbital where an external electron could occupy. Since these slots are all at the opposite ends of the tetrahedral vertices, they in turn create another tetrahedral configuration. These are where

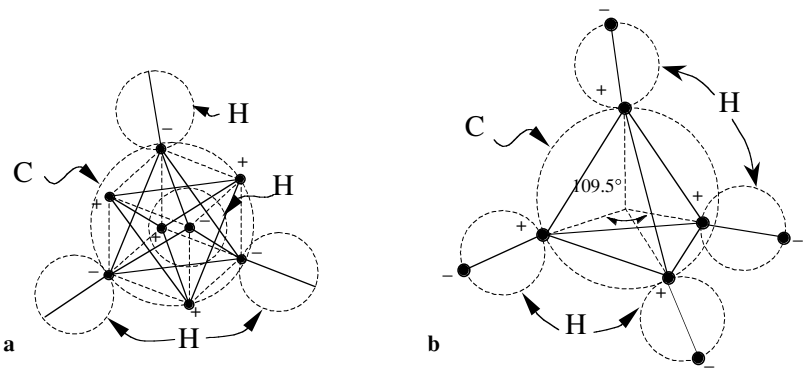


Fig. 3. a) Molecular structure of methane (with Carbon electrons paired. Atoms not to scale). b) Molecular structure of methane (with Hydrogen electrons paired, as seen from a different angle. Atoms not to scale).

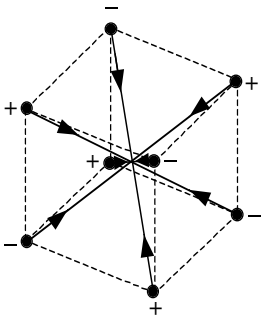


Fig. 4. Four diagonal "bracings" through the center of Carbon in methane. "Plus" and "minus" signs indicate pairing of electrons of opposite spins. Arrows indicate tensile, attractive forces.

the Hydrogen atoms bond. Thus, this could be the reason that the molecular structure of methane is tetrahedral.

When all the electrons in Fig. 3(a) make half a revolution around their respective orbits, the resulting configuration is as in Fig. 3(b).

When the single electrons of each of the four Hydrogen atoms occupy the four empty slots of the Carbon atom, the Hydrogen electrons create another tetrahedron crisscrossing the original tetrahedron of the Carbon electrons. Therefore, in effect, there are two interlocking tetrahedra, one comprised of Carbon electrons, and the other of Hydrogen electrons.

The cube, comprised of the peripheral, right-angled edges, is a shape but not looked upon as a structure. In the proposed model, only when braced by the diagonals that constitute the edges of either of the tetrahedra, the cube is considered to acquire a structure.

Moreover, each electron of one atom is directly related to that of the other atom by the line that links the opposite end of each orbit. A molecule such as methane is not only doubly braced by two tetrahedra but also reinforced by these four diagonals of the orbital lines that pierce through the center of the host (in case of methane, Carbon) atom. These bracings might constitute the structural integrity for the principle of the "octet rule" (Fig. 4).

Needless to say, these internal bracings pierce through the nucleus of the atom. Effectively, they are the tensile forces of the positively charged nucleus pulling on the negatively charged electrons, counterbalancing the compressional, repulsive forces of the electrons working on each other. Simply, these electric, invisible "struts" are arranged in orderly geometry while electrons orbit around the atomic nucleus to render atoms and molecules their definite and regular patterns.

These internal bracings in tension, piercing through the nucleus, constitute the so-called "lone pairs" in atoms and "bonding pairs" in molecules. In both cases of pairing, the positively charged nucleus acts as "the glue" to bond the negatively charged electrons.

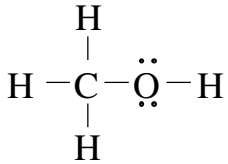
Since the publication of the original paper, the author has discovered the "Cubic Model" of the atom advocated by LEWIS (1916). While the models appear very similar there is a subtle difference in that Atommetrics deals with structural geometry of electron relationships. In Atommetrics the cube, which by itself is not a structure, is actually comprised of two interlocking tetrahedra, the simplest three-dimensional structural system, inscribed within the cube and thus constitutes a structure. In Lewis' model the cube is treated as a shape rather than as a structure, although in essence the shape is derived from the structure. The basic concept of Atommetrics lies in the fact that electrons form the simplest, symmetrically balanced (ideally triangular to tetrahedral) geometric configurations in order to acquire and maintain stable relationships amongst each other.

From experience, it is known that atoms with eight valence electrons, or half that, i.e. four electrons, are stable (octet rule). It is evident from this model that the reason for the stability is the tetrahedroning of the cube, either singly or doubly. To simplify, though, the tetrahedral configuration shall henceforth be omitted to show just the cube. However, it should be remembered that the tetrahedral configuration is actually there to account for the structural stability.

3. Molecular Structure Based on Atommetrics.

3.1. Methanol (CH_3OH)

Methanol is a polyatomic molecule without a central atom. The Lewis structure for methanol is:



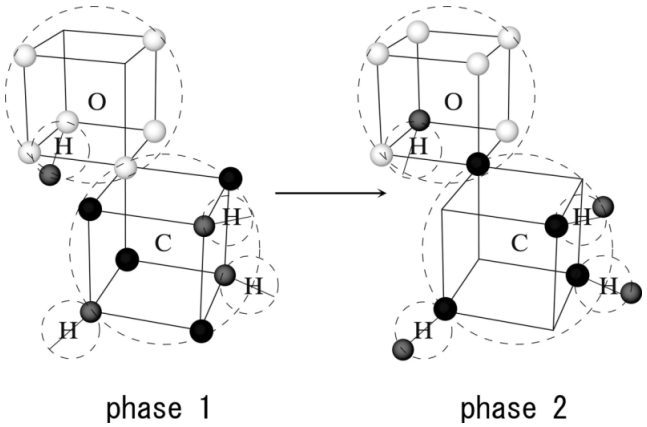
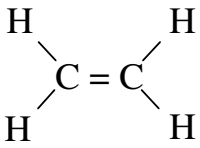


Fig. 5. Two phases of the molecular structure of methanol (with all electrons paired).

Since Carbon has four valence electrons with a tetrahedral arrangement, the one Oxygen and three Hydrogen atoms will occupy the four empty slots to complete the orbits of Carbon (see Fig. 5: Phase 1). At this time the Oxygen atom would have only its original electrons arranged in an octahedral configuration. One Hydrogen attached to the Oxygen would have its electron paired with one of Oxygen electrons. In another phase (Phase 2) one Hydrogen electron and one Carbon electron would pair with those of Oxygen respectively to complete all the orbits of Oxygen. At this time the three other Carbon electrons would pair with those of the three Hydrogen atoms attached to Carbon to complete their orbits.

3.2. Ethylene (C_2H_4)

The Lewis Structure for ethylene is:



Atoms lie in a plane and electron arrangement of individual atoms is thus:

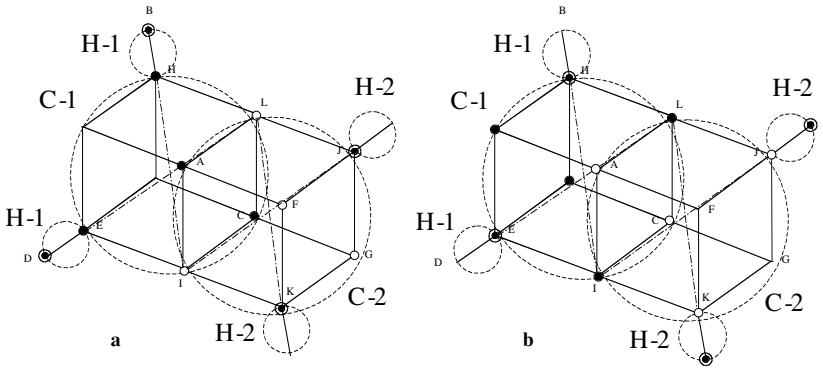


Fig. 6. Molecular structure of ethylene (C_2H_4). a) Phase 1: All of C-2 and H-1 atoms are paired (atoms not to scale). b) Phase 2: All of C-1 and H-2 atoms are paired (atoms not to scale).

When all the electrons make half a revolution within their respective orbits, all of Carbon-1 and Hydrogen-2 atoms' electrons become paired (see Fig. 6: Phase 2). Since there is a Carbon-Carbon double bond, which is considered as one effective pair, it is generally believed that each Carbon is surrounded by 3 effective pairs and therefore the bond is trigonal planar and the angles 120 degrees each. Each Carbon actually has 6 bonding pairs (see Fig. 6(a)): for C-1, 2 Hydrogen-Carbon (B-H, D-E) and 4 Carbon-Carbon (E-L, H-I, A-G, C-F). As is evident in the above figures, the two Carbons are basically two tetrahedra-based spheres interpenetrating each other. How the pairs of Hydrogen atoms on either end respectively attach to the Carbon atoms is similar to those in methane (CH^4), but since the pair of Hydrogen atoms attached to the adjacent Carbon atom is now further apart and electron repulsion less, and also since the center of mass of the molecule shifts from the respective centers of each Carbon to their bonded center, the regular Carbon orbits shift to displace the position where Hydrogen atoms would normally attach at 109.5 degrees, which is the angle in a regular tetrahedral configuration (as in methane). Hence, the resulting bond angle between 2 Hydrogen atoms on each end is greater than 109.5 degrees but not necessarily 120 degrees. In fact, observational evidence indicates this angle to be 116.7 degrees.

3.3. Ethylene (C_2H_4): Alternative

While the proposed model satisfies the planar arrangement of atoms in the ethylene molecule, it also suggests a non-planar version. This fact had for some time been puzzling the author as well as receiving criticism from reviewers of the paper. The author is happy to relate that evidence for this occurrence had been reported in a paper written in 1974 by FOO and INNES (1974). Accordingly, it had been observed that when energy is applied to ethylene the planar arrangement of the atoms change. It is postulated here that the new arrangement is as follows (Fig. 7):

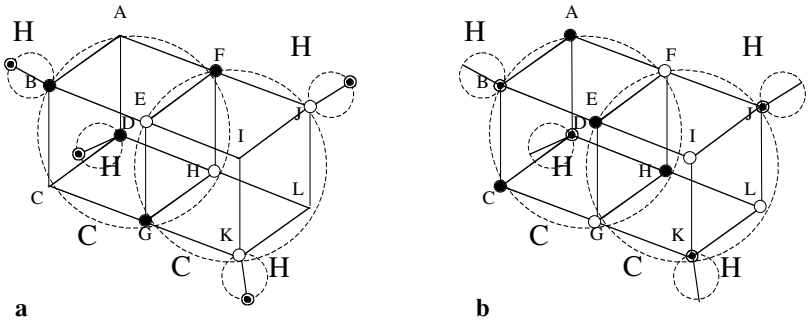


Fig. 7. Molecular structure of ethylene (C_2H_4)—alternative: a) Phase 1: All of Hydrogen atoms paired in their respective orbits (atoms not to scale); b) Phase 2: All of C atoms paired in their respective orbits (atoms not to scale).

As shown, the new arrangement has a pair of Hydrogen atoms rotated 90 degrees in relation to the other pair. It is thought that when energy is applied to the Hydrogen atoms, their electrons respectively jump to the next larger shell such that electron repulsion is increased between those Hydrogen atoms on either side of the 2 Carbon atoms. Therefore, one pair of Hydrogen atoms rotate 90 degrees such that internuclear distance is increased and hence electron repulsion minimized.

3.4. Benzine

Benzine consists of six Carbon atoms in a hexagonal ring with a Hydrogen atom attached to each Carbon. It is known that all six C-C bonds are equivalent. The molecular structure for benzene in two forms are (Fig. 8):

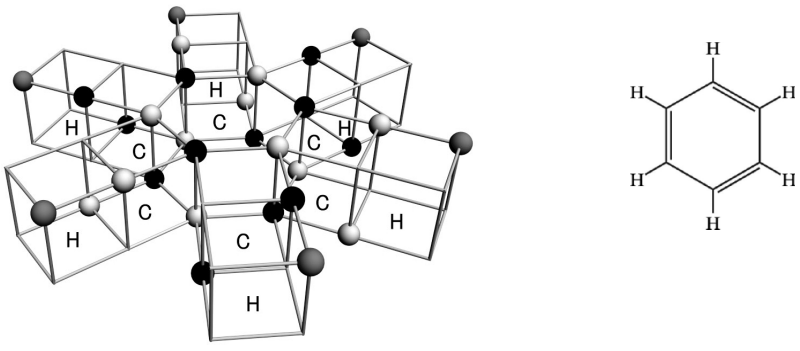


Fig. 8. Molecular structures of benzine.

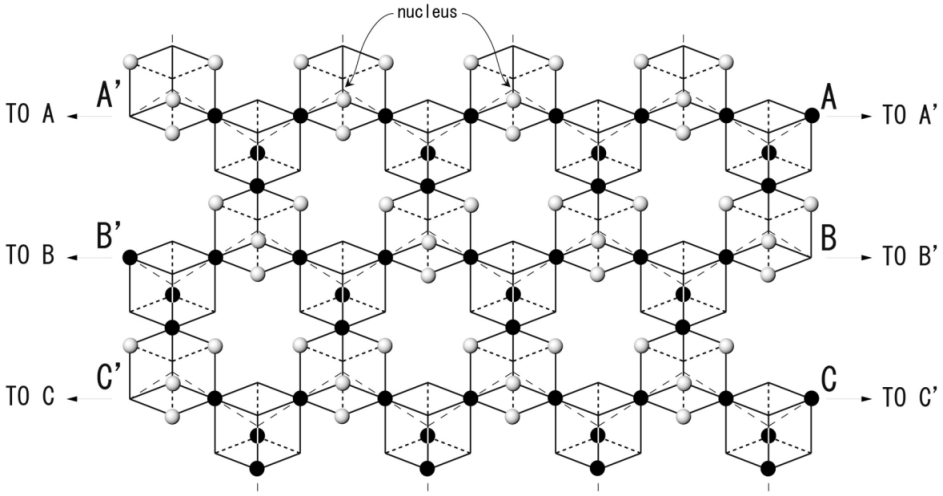


Fig. 9. Carbon nanotube: flattened typical segment—when such segments are multiplied and the resulting plane is folded cylindrically, a nanotube is created.

As is evident here, all the adjacent Carbons are doubly bonded to each other in an equivalent fashion without the need of resonance structures.

3.5. Carbon nanotube

A Carbon nanotube is basically graphite's two-dimensional plane closing in three-dimensionally to form a cylinder (Fig. 9). Three of the four electrons of each Carbon form bonding pairs with those of the adjacent Carbon atoms, leaving one electron free. This free electron could account for the conductivity of Carbon nanotubes. Nanotube Carbons form the hexagonal web of electrons and nuclei (long dotted lines) such that the tension (attractive force) exerted by the nucleus on and through the bonding electrons is very strong to render the entire web of Carbon nanotubes a very high tensile-strength material.

3.6. Buckminsterfullerene (C-60)

Buckminsterfullerene, or C-60, is comprised of 60 Carbon atoms arranged in R. Buckminster Fuller's geodesic system; hence, the name. The molecular configuration is of 12 pentagons and 20 hexagons (Fig. 10).

Pairs of Carbon atoms joined along the edges of the hexagons are doubly bonded, while those along the edges of the pentagons are singly bonded (ALDERSEY-WILLIAMS, 1995).

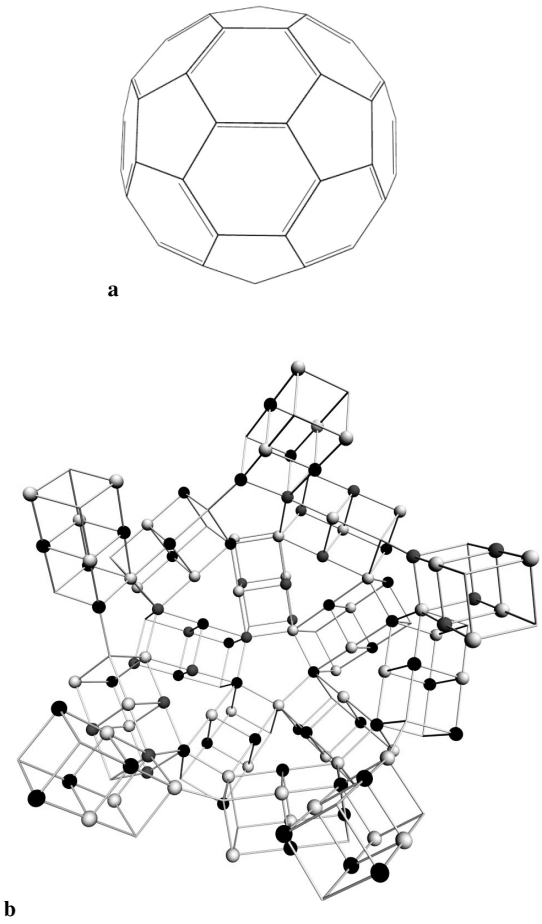


Fig. 10. a) Single and double bonds in C-60. b) 1/2 molecular structure of C-60 (as seen from inside the molecule).

4. New Forms of Carbon Suggested by Atommetrics

The following are some forms of Carbon that seem to be theoretically possible as suggested by Atommetrics. If and when discovered naturally or produced artificially, one or more of these molecules could substantiate the validity of Atommetrics.

4.1. C_N-Carbon needle (Fig. 11)

This is a series of Carbon quadruply bonded in a linear fashion, theoretically ad infinitum. The ends of the molecule perhaps need to be bonded by pairs of Hydrogen in order to render it stable.

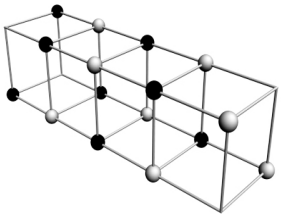


Fig. 11. C_N-Carbon needle.

4.2. C_3/C_6-Trigonal hexagonal Carbon sheets (Fig. 12)

This is a molecule of Carbon where three Carbons doubly bonded to each other propagate bonding to form an array of triangles and hexagons quite similar to benzene. In place of Hydrogen attaching linearly to Carbon, as in benzene, here Carbon attaches to two other Carbons to form a triangle amongst each other.

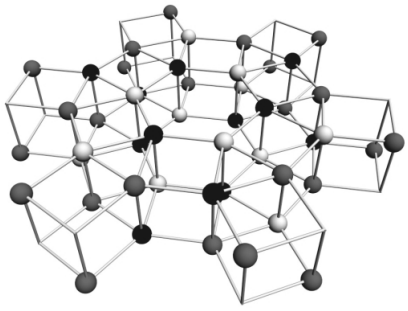


Fig. 12. C_3/C_6-Trigonal hexagonal Carbon sheets.

4.3. C_6-Octahedron (Fig. 13)

This is a molecule of six Carbons arranged in an octahedral configuration. Each Carbon is singly bonded to four Carbons. This may be the smallest three-dimensional polyhedron available in Carbon.

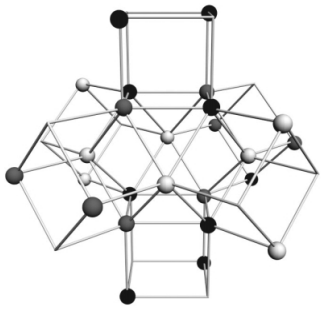


Fig. 13. C_6-Octahedron.

4.4. C_{12}-Carbon vector equilibrium or cubo octahedron (Fig. 14)

This is a molecule of twelve Carbons in vector equilibrium or cubo octahedral configuration. Each Carbon is singly bonded to four other Carbons.

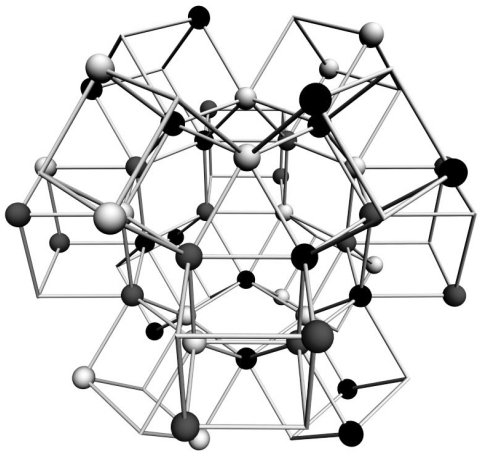


Fig. 14. C_{12}-Carbon vector equilibrium or cubo octahedron.

4.5. Carbon lattice (Fig. 15)

This is a planar molecule of Carbon where each Carbon is doubly bonded to four others in a lattice.

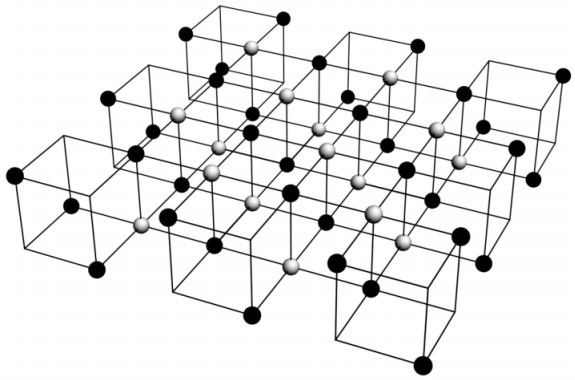


Fig. 15. Carbon lattice.

5. Concluding Remarks

Based on the atomic model proposed in this paper, some observations can be made as to the nature of atomic and molecular structure.

1) Each shell appears to possess a definite set of orbits characteristic to itself.

2) Electrons assume positions of least repulsion among themselves, assuming independent orbits, if necessary, continually joggling each other in order to find the most comfortable position of good, symmetric balance.

3) In general, each electron assumes an independent orbit first to complete a structure, after which it pairs to complete the orbit.

4) The above item 3) may be due to allow external electrons to fill in to form molecules.

5) In molecular bonding, atoms first attach to orbits with unpaired electrons, after which they attach to orbits with paired electrons, if necessary, to complete their own orbits.

While this paper is concerned with only electron orbits, it is regarded with optimism that along similar lines a comprehensive description of the atom including the proton and the neutron could be worked on. It is hoped that the model could help not only to thoroughly understand atomic and molecular structures but also, as a consequence, to lead into research and development of artificial atoms and molecules. It would be ideal for it to be able to eventually pioneer the development of creative engineering and design of immense applicational potential, such as of superconductivity, to better our physical environment.

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