ATOMMETRICS: ANOTHER VIEW OF ATOMIC STRUCTURE BASED ON ELECTRON ORBITAL GEOMETRY

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Abstract.

This paper 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. 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 model defines specific valence electron geometries for atoms and helps to explain the principle behind the "octet rule," how single and multiple bonds work, and the operational meaning of "resonance structures," amongst others.

Keywords: Atommetry; Electron Orbital; Vector Equilibrium; Tension; Compression

1. INTRODUCTION

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. If the nucleus and the electrons are looked upon as "compression" particles, then they are held in their respective and relative positions by electromagnetism, the "tension" counterpart.

In essence, the atom is a "tensegrity." Tensegrity is short for "tension integrity." It denotes a type of structure whose compression members are discontinuous, held in respective positions by a continuous thread of tension members (Fuller, 1975).

While Heisenberg's Principle of Uncertainty dictates that the position and the speed of an electron cannot be accurately <u>measured</u> simultaneously, it does not imply that there is no orderly structure and motion of electrons in the atom.

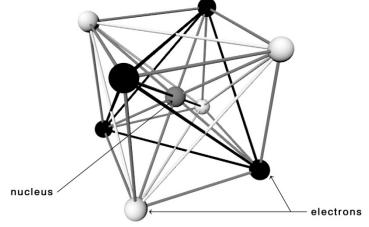


Figure 1. Basic atom model. Diagonal lines piercing through the nucleus are in tension; all others are in compression.

As can be seen in Figure 1, 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. The model eliminates the need of "resonance" structures, for example, as a result of being able to explain electron relationships simply and effectively in three-dimensional and dynamic (i.e. delocalized) form, in contrast to current models. Although the model may appear similar to that of VSEPR (Valence Shell Electron Pair Repulsion), it is different in that while in the VSEPR it is "pairs" of "localized" electrons in molecular configurations that are kept as far apart as possible to minimize repulsion, in the proposed model it is instead "single, delocalized" electrons in individual atomic configurations that are kept at symmetrically maximum distances. As distinct from VSEPR, electrons in this model are free to move about the entire region of the atom's "electron cloud," always maintaining the relative distance of least repulsion between each other. In this way, electrons maintain symmetric, geometric relationships, introduced here as "atommetry," not only in molecular configurations, as do the "pairs" of electrons in VSEPR, but also in individual atoms. The model is based on an Archimedean polyhedron (Figure 3) which is known as the vector equilibrium (cubo-octohedron), because all of its inner radial and outer edge lengths are equal. This polyhedron is unique also in that it contains within itself the 5 Platonic configurations, some of which would correspond to the stable geometry of electrons in the atom. The polyhedron has 25 axes of spin which are symmetric to its configuration. The planes perpendicular to and pierced by these axes define 25 great circles (FULLER, 1975). The model employs some of these great circles to represent orbitals where electrons are to be found in their relative positions.

1.1 Orbit and Orbital.

An "orbital," in common atomic terminology, refers to a region of space where an electron is most likely to be found, as distinct from an "orbit," or path generally defined mathematically by a circle or an ellipse. In this paper, a great circle orbit represents an orbital and should not be taken as a path of an electron. Such electron routes are unknown, and the seemingly rigid orbits of the great circles are thus arbitrary and illusive. The orbits are nonetheless used to only and clearly indicate respective orbitals and "pairing" of electrons in such.

Since Pauli's exclusion principle stipulates that an orbital, or orbit in this paper, can carry only 2 electrons, an orbit is assumed to be a "line" between the positive-spin and the negative-spin electrons paired at opposite ends, where electrons always move in unison at 180-degree angle of maximum separation with greatest probability, minimizing electron repulsion and expending least energy (Figure 2).

180°

Figure 2. Paired electrons in an orbit (orbital) as a "line" relationship.

The model postulates that orbitals are "hybridized" in individual atoms to begin with and treats orbitals of different sublevels of a level as degenerate. Hund's rule, therefore, applies to all orbitals, and the model assumes that "the lowest energy configuration for an atom is the one having the maximum number of unpaired electrons...(with) parallel spins" (ZUMDAHL, 1989) throughout the different sublevels.

ELECTRON CONFIGURATIONS AND ORBITS 2.

Level 1: 1 orbit, 1-2 electrons.

Figure 3. Hydrogen as a point and helium as a line.

The Hydrogen has 1 orbit with 1 electron (1s¹). The Helium has 1 orbit with 2 electrons (1s²). While the great circle orbits of the vector equilibrium diagrams seem to represent electron routes, it should be remembered henceforth that they actually represent "orbitals" and indicate "pairing" of electrons.

The vector equilibrium is shown both in the polygon as well as in the inflated, spherical shapes for clarity of the 25 great circles. All the electrons and only the orbits in the foreground are drawn solid, while in the background the orbits are dotted. Arrows arbitrarily indicate orbital direction only to show that paired electrons maintain their relative positions.

While the electron orbital shell here is represented by level 1 of Hydrogen and Helium, it may apply to any other valence shell with the same number of electrons. The same applies to the shells henceforth presented.

Level 2: 3 orbits with 3 electrons and 2.2 4 orbits with 4-8 electrons

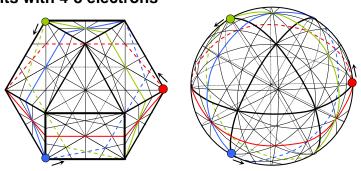


Figure 4. Trigonal planar for Boron atom.

The Boron has 3 orbits with 3 electrons (2s¹2p² instead of 2s²2p¹). It is generally accepted that Boron and other atoms with three valence electrons are in the s²p¹ form. It is postulated here that instead the form is of s¹p² to indicate that there are three orbits instead of two, because if there were only two orbits there would be two electron separation angles of 180 degrees and 90 degrees (Figure 5).

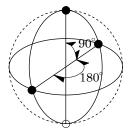


Figure 5.

However, if there were three orbits, the configuration could be of trigonal planar with common separation angles of 120 degrees to minimize electron repulsion evenly (Figure 6).

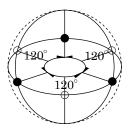


Figure 6.

Again, for the Carbon atom, in order to minimize electron repulsion and to form the simplest, symmetrically balanced configuration, a 4-orbit system, rather than 3, is postulated.

The Carbon has 4 orbits with 4 electrons $(2s^12p^3 \text{ instead of } 2s^22p^2)$.

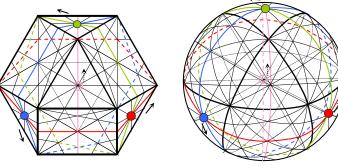


Figure 7. Tetrahedral for Carbon.

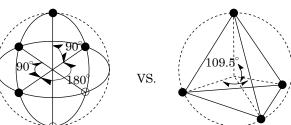


Figure 8. 3 orbits vs. 4 orbits

This tetrahedral configuration included in Figure 7 is the simplest and the most stable three-dimensional relationship that can exist among four electrons (Figure 8). 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 end (side) of the orbit (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 the Hydrogen atoms bond. Thus, this could be the reason that the molecular structure of methane is tetrahedral.

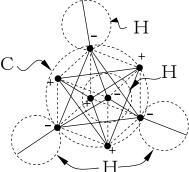


Figure 9. Molecular structure of methane (with Carbon electrons paired. Atoms not to scale).

When all the electrons in Figure 9 make half a revolution (<u>in terms of the great circle and not necessarily in actuality</u>) around their respective orbits, the resulting configuration is thus:

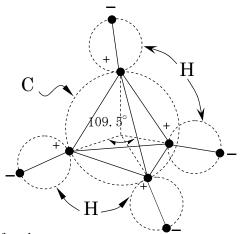


Figure 10. Molecular structure of methane

(with Hydrogen electrons paired, as seen from a different angle. Atoms not to scale).

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 ends 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" (Figure 11).

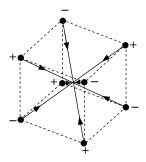


Figure 11. Four diagonal "bracings" through the center of Carbon in methane.

"Plus" and "minus" signs indicate pairing of electrons of opposite spins. Arrows indicate tensile, attractive forces.

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.

While the Atommetrics model appears very similar to the "Cubic Model" of the atom advocated by G. N. Lewis (Lewis, 1916), 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.

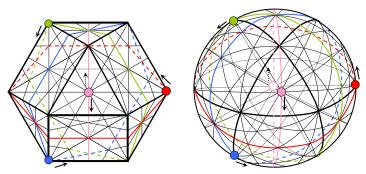


Figure 12. Trigonal bipyramidal for Nitrogen.

The Nitrogen has 4 orbits with 5 electrons (2s²2p³). The four orbits are the same as those of the previous 4-electron arrangement (Figure 12). The opposite ends of one orbit is now filled, and the 3 electrons of the 3 other orbits previously on the triangular faces, or tetrahedral vertices, move to three of the six equatorial vertices in order to balance electron repulsion.

Evidence to substantiate this configuration may be found in the way Nitrogen bonds with three Hydrogen atoms to form ammonia (Figure 13).

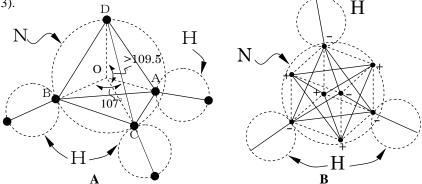


Figure 13, A, B. Bonding angles and pairing of ammonia (atoms not to scale. The 1 electron that pairs with D to form a lone pair is not drawn in the left diagram.)

pairs of circumferential electrons move back to fill the six respective triangular faces, or tetrahedral vertices, in order to minimize electron repulsion by forming two intersecting tetrahedra as a whole. In essence, the Hydrogen atoms are bonded to Nitrogen at three of the four tetrahedral vertices. The bond angles, however, are not 109.5 degrees, as were the case with methane. As different from the common belief that the so-called "lone pair," supposedly occupying the remaining vertex of the tetrahedral arrangement, takes up more space than the bonding pairs and thus compresses the bond angles to 107 degrees, the reason that the normal angle of 109.5 degrees is not maintained could be that either 1) one of the electrons that forms a lone pair and closer to the 3 Hydrogen atoms could attract their nuclei and pull them in respectively to reduce the bond angles, or 2) the lopsided proximity of the three Hydrogen atoms shifts the center of mass of the ammonia molecule such that the regular vector equilibral orbits of Nitrogen become elliptical and shift themselves such as to reduce the bond angle to 107 degrees, or 3) combination of both 1 and 2. This shift forces AB, BC, and CA to shorten, while it forces AD, BD, CD to elongate. As a result, angle AOB is reduced from 109.5 degrees to 107 degrees, while angle COD is expanded to become greater than 109.5 degrees (Figure 13, A). The paired electrons (DE) in Fig. 14 in the Nitrogen atom are what is generally called "the lone pair." When the vacant slots of the unpaired ones (A, B, C) are filled by electrons of bonding atoms, in this case Hydrogen, "bonding pairs" (AH, BG, CF) are formed (Figure 14).

F D E C

Figure 14. "Lone pair" and "bonding pairs" of ammonia (atoms not to scale).

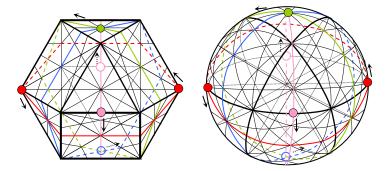


Figure 15. Octahedral for Oxygen

The Oxygen has 4 orbits with 6 electrons (2s²2p⁴). To the previous Nitrogen configuration an electron is added to fill one of the unfilled orbits. Since there are now 6 electrons and in order to minimize electron repulsion, the 2 originally paired electrons in Nitrogen move from the triangular faces to their respective positions on the circumference of the vector equilibrium, while the other unpaired electrons move respectively to the adjacent triangular faces at opposite sides. As a result, the new configuration is octahedral (Figure 15).

One may wonder why there are 4 orbits instead of 3, as they would suffice to pair the 6 electrons octahedrally. The reason may be in that otherwise an atom such as Oxygen would not be able to accommodate any other electron to form molecules, as in the following example.

It is evident that while four of the electrons are paired respectively and their orbits complete, the remaining two are not. When Oxygen combines with Hydrogen to form water, the 2 hydrogen atoms attach to the empty slots of the unfilled orbits. When this happens, all the Oxygen electrons as well as the 2 Hydrogen atoms' electrons occupy the 8 vertices to form 2 interlocking tetrahedra, or cube. The molecular structure is thus modeled as shown in Figure 16.

Figure 16. Two interlocking tetrahedra in the Oxygen of H₂O (with Oxygen electrons paired. Atoms not to scale).

When all the electrons rotate 180 degrees, the molecular structure is thus, as in Figure 17.

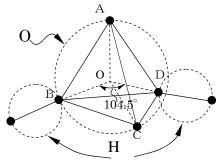


Figure 17. Molecular structure of H_2O (with Hydrogen electrons paired . Atoms not to scale. The 2 electrons that pair with A and C to form lone pairs are not drawn.)

As was the case with ammonia, either 1) two of the electrons that respectively form lone pairs and closer to the 2 Hydrogen atoms could attract their nuclei and pull them in respectively to reduce the bond angles (by a greater margin than in the case of ammonia on account of the double electrons), or 2) the lopsided proximity of the Hydrogen atoms shifts the center of mass of the resulting molecule from the center of Oxygen to cause a shift in the regular vector equilibral orbits to reduce the bond angles (more so than in ammonia, since there are only two atoms this time and no third atom, the shift being increased in one direction), or 3) combination of 1 and 2. Therefore a bond angle BOD of 104.5 degrees results.

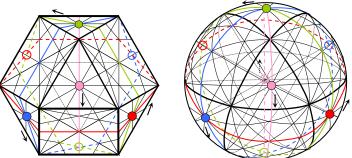


Figure 18. Two interlocking tetrahedra (cube) for Neon.

Fluorine has 4 orbits with 7 electrons $(2s^22p^5)$. The Neon has 4 orbits with 8 electrons $(2s^22p^6)$ as in Fig.18. This arrangement is the same as that of the water molecule, but in place of the 2 Hydrogen atoms' electrons are the 2 new electrons.

Evidently, the stability of neon and other so-called inert gases might owe to the structural integrity of the two interlocking tetrahedra.

While only those configurations up to 4 orbits with 8 electrons are here presented, those up to 16 orbits with 32 electrons, such as Ytterbium (Yb) with the maximum number of orbits and electrons in a single shell, are believed to be operable following similar electron arrangements and great circle orbits of the vector equilibrium. Except for atoms such as Hydrogen and Helium, which have 1 orbit each, and atoms such as Boron, which has 3 orbits, atoms with up to 8 valence electrons have 4 orbits. Electrons occupy each empty orbit first before pairing in a singly occupied orbit. This might be the reason that 2 Hydrogen atoms bond to oxygen at an angle of 104.5 degrees, rather than 180 degrees, and that 3 Hydrogen atoms bond to Nitrogen at angles of 107 degrees, rather than planar 120 degrees.

3. MOLECULAR STRUCTURE BASED ON THE FOREGOING ATOMIC STRUCTURE

3.1 Phosphorous pentachloride(PCl₅):

Phosphorous $(3s^23p^3)$ has a total of 5 electrons and Chlorine $(3s^23p^5)$ has 7 in their respective outer shells. The structure of Phosphorous is trigonal bipyramidal and the molecular structure of PCl₅ is considered to be as shown in Figure 19.

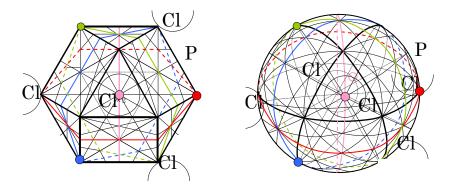


Figure 19. Molecular structure of PCl₅ (atoms not to scale).

The 3 Chlorine atoms attach to the empty slots of Phosphorous' 3 orbits, thus completing them. The 2 remaining Chlorine atoms attach to the opposite ends of the already filled fourth orbit.

Until the early 1960's, it was believed that the noble gases, with s and p valence orbitals filled, were not chemically reactive and were hence called "inert" gases. However, several compounds of Krypton, Xenon, and Radon were synthesized to show that these gases were capable of reacting chemically (ZUMDAHL, 1989). The reason for this phenomenon is similar to that of Phosphorous and Chlorine electrons as follows. In Phase 2, the paired electrons of phosphorous can no longer remain in their original orbit and move into those of the bonding Chlorine atoms in order to make room for the pairing Chlorine electrons. Thus, the unpaired electrons of the two Chlorine atoms are able to each bond to the paired electrons of the one complete orbit of Phosphorous.

As has been demonstrated with examples of atoms and molecules, other atoms and molecules follow similar pattern of development from rearrangement of vector equilibrium geometry and great circle orbits. A simpler, albeit often approximate and sometimes crude, method of analysis and synthesis of atoms and molecules will now be presented to facilitate a three-dimensional visualization thereof. It has already been demonstrated with 8-electron configurations and is the double tetrahedra. However, in order to facilitate viewing electron as well as molecular arrangements of atoms, each atom shall henceforth be presented not as part of double tetrahedra but simply of cube, as follows:

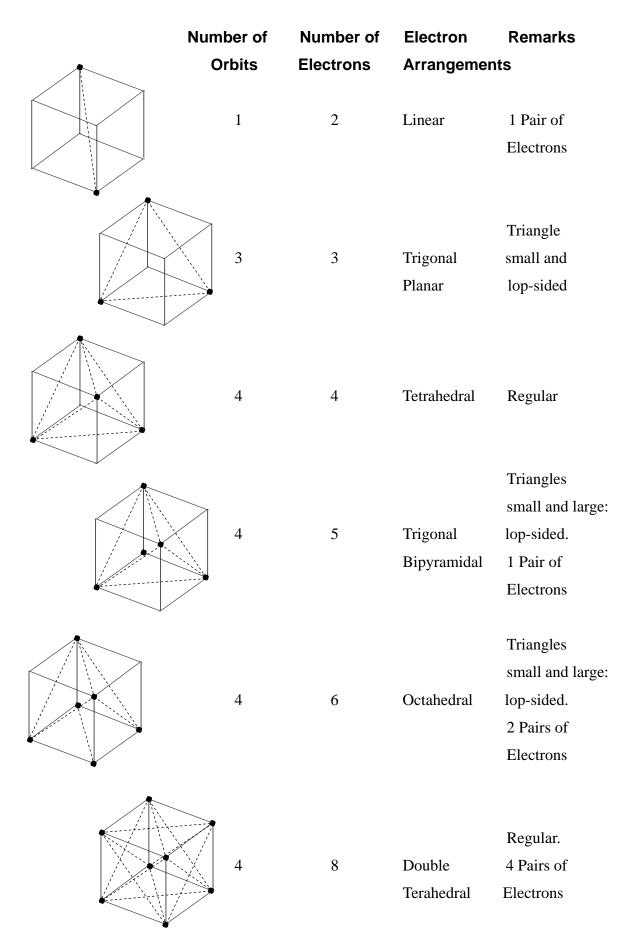


Figure 20. Regular arrangements of electrons in "cubes."

For sake of brevity, only the cube arrangements without the vector equilibral orbits shall henceforth be used to explain molecular structures. While they are often not exact representations of the actual configurations, they are nonetheless complete and simple.

3.2 NO₃ lon:

All of the molecules thus far presented had tangential bonding, that is, they were merely touching each other at the shell surfaces. An example will now be presented where the bonding atoms interpenetrate each other. Nitrogen has 4 orbits with 5 electrons $(2s^22p^3)$ and Oxygen has 4 orbits with 6 electrons $(2s^22p^4)$. With an electron added, all the atoms have 6 valence electrons each.

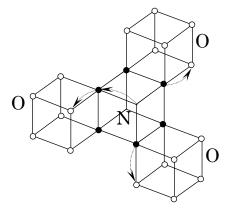


Figure 21. Molecular structure of NO₃ with 3 double bonds. Phase 1: All electrons paired.

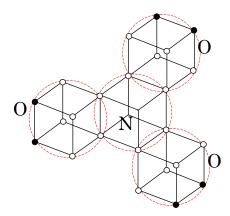


Figure 22. Molecular structure of NO_3 . Phase 2: All electrons paired with Nitrogen electrons in Oxygen orbits (ionic bonding). Spheres around the cubes show how the atoms interpenetrate each other.

As is evident from the diagrams, the bond angles are 120 degrees. Again, it should be noted that Nitrogen and Oxygen have 4 orbits each, but with the addition of an electron to the molecule they have rearranged their electrons from their original tetrahedral configurations to those that fit the molecular structure (dotted jumps in Figure 21).

Structures such as NO_3^- are generally known as "resonance" structures and are basically a superposition of the possible Lewis structures. In case of NO_3^- , the molecular structure is expressed as follows:

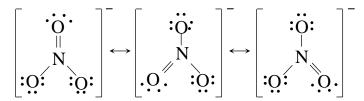


Figure 23. Lewis structure for NO_3 .

The localized electron (LE) model postulates that electrons are localized between a given pair of atoms. In reality, however, electrons are delocalized, and so the concept of resonance has to be applied to compensate for the defective assumption of this model (ZUMDAHL, 1989). In the Atommetrics model herein presented, atomic electrons are delocalized to begin with and therefore move about the entire molecule three-dimensionally when bonded to perhaps present a direct and more accurate picture of reality.

3.3 Carbon dioxide (CO₂):

Carbon dioxide has two sets of Oxygen-Carbon double bond.

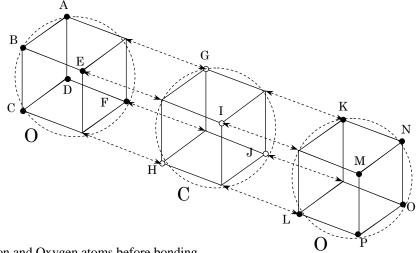


Figure 24. Carbon and Oxygen atoms before bonding.

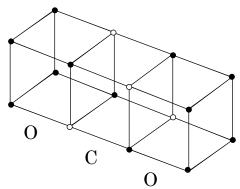


Figure 25. CO₂ molecule. Phase 1: All electrons in their respective atomic orbits (covalent bonding).

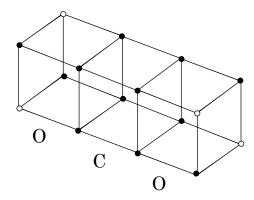


Figure 26. CO₂ molecule. Phase 2: All Carbon electrons in their respective Oxygen orbits (ionic bonding).

As is evident in the 2-phase diagrams of the CO₂ molecule (Figures 25, 26), here is a case where a combination of covalent and ionic bonding occurs. In phase 2, the Carbon electrons are not able to navigate along their own orbits, as the adjacent Oxygen atoms respectively fill the empty slots of Carbon when their electrons make half a revolution around their orbits. Hence, the Carbon electrons at locations G and H, and at I and J trade places with those of Oxygen at locations C and A, and at O and M, respectively. Carbon dioxide is thus linear with a bond angle of 180 degrees. Simple calculation of x, the depth of interpenetration for the atoms, assuming Carbon and Oxygen radii equal and disregarding forces of electron repulsion and nuclear attraction, indicates x to be roughly 42.5% of atomic diameter.

Atomic radii differ that the geometric relationships thus far presented are hence not exact. However, atomic radii are approximate to begin with, and in molecules, where electrons are often shared by all atoms involved, the atomic sizes ought to be more closely evened than when they are on their own, even though their atomic numbers differ.

3.4. Methanol (CH3OH):

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

$$\begin{matrix} H \\ H - \overset{\mid}{C} - \overset{\mid}{O} - H \\ \overset{\mid}{H} \end{matrix}$$

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 (Figure 27: 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 orbitals 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.

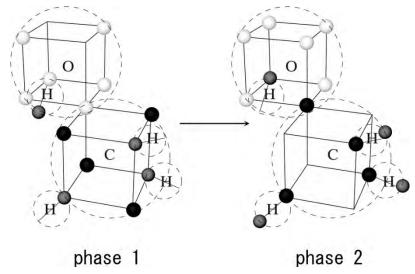


Figure 27. Two phases of the molecular structure of methanol (with all electrons paired).

3.5. Ethylene (C2H4)

The Lewis Structure for ethylene is:

$$H$$
 $C = C$ H

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

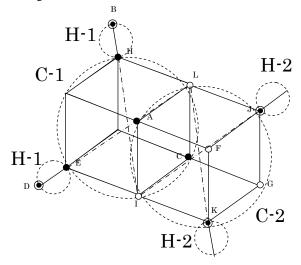


Figure 28. Molecular structure of ethylene (C_2H_4). Phase1: All of C-2 and H-1atoms are paired (atoms not to scale).

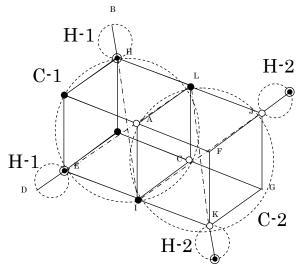


Figure 29. Molecular structure of ethylene (C_2H_4).

Phase 2: All of C-1 and H-2 atoms are paired (atoms not to scale).

When all the electrons make half a revolution around their respective orbits, all of Carbon-1 and Hydrogen-2 atoms' electrons become paired (Figure 29: 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 (Figure 28): 2 Hydrogen-Carbon (B-H, D-E and I-J, L-K) 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 (CH⁴), 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.

3.6. Ethylene (C2H4): Alternative

While the proposed model satisfies the planar arrangement of atoms in the ethylene molecule, it also predicts 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 (Foo & 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:

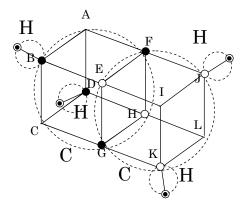


Figure 30. Molecular structure of ethylene (C_2H_4): alternative.

Phase 1: All of Hydrogen atoms paired (atoms not to scale).

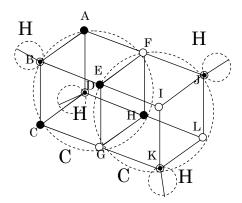


Figure 31. Molecular structure of ethylene (C_2H_4): alternative

Phase 2: All of C atoms paired (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.

3.7. Benzine

Benzine consists of six Carbon atoms in a hexagonal ring with a Hydrogen atom attached to each Carbon thus:

It is known that all six C-C bonds are equivalent. The resonance structures for benzene are:

In Atommetrics, the structure is thus:

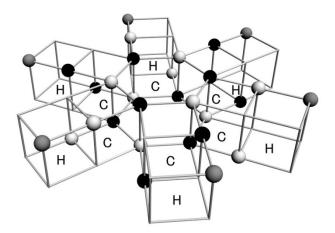


Figure 32. Molecular structure of benzene.

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

3.8. Carbon Nanotube

A Carbon nanotube is basically graphite's two-dimensional plane closing in three-dimensionally to form a cylinder. 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 as well as of graphite. 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.

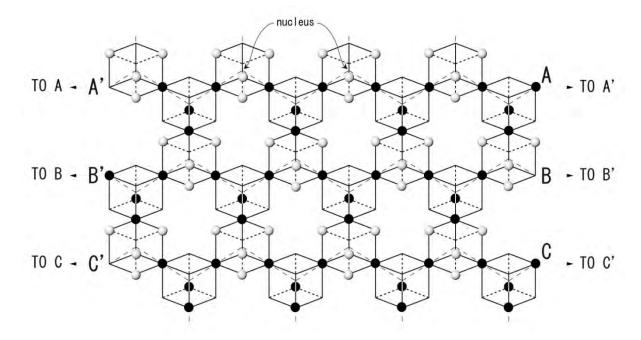
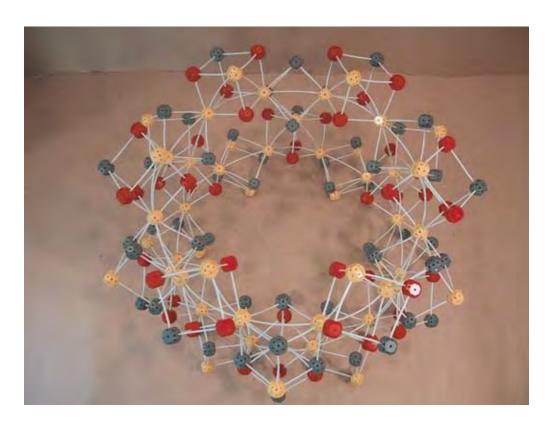


Figure 33. Carbon nanotube: typical segment (when such segments are multiplied and the resulting plane is folded cylindrically, a nanotube is created).



Model photo of Carbon Nanotube.

3.9. 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 as shown below:

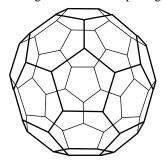


Figure 34. Molecular structure of buckminsterfullerene (C-60).

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).

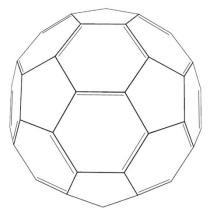


Figure 35. Single and double bonds in C-60.

With the cubes, the molecular arrangement is:

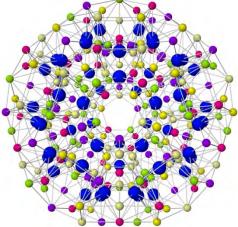


Figure 36-A. Molecular structure of C-60.

Large blue balls represent atomic nuclei, while the smaller balls represent electrons.

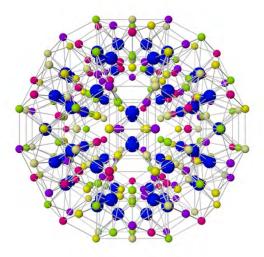


Figure 36-B. Molecular structure of C-60 (as seen from a different angle).

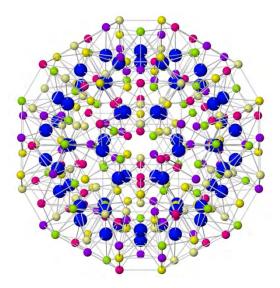


Figure 36-C. Molecular structure of C-60 (as seen from a different angle).



Model (made by Dennis Dreher) photo of C-60.

4. NEW FORMS OF CARBON PREDICTED BY ATOMMETRICS.

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

4. 1. CN-Carbon Needle

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.

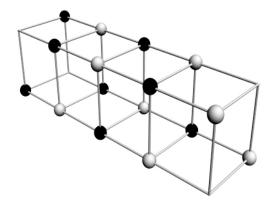


Figure 37. C_N-Carbon Needle.

4. 2. C3/C6- Trigonal Hexagonal Carbon Sheets

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.

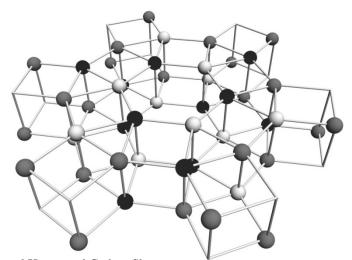


Figure 38. C₃/C₆- Trigonal Hexagonal Carbon Sheets.

4.3. C6-Octahedron

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.

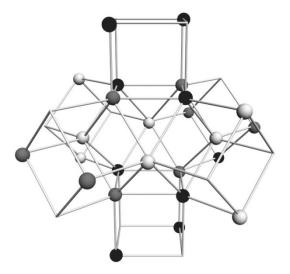


Figure 39. C₆-Octahedron

4. 4. C12- Carbon Vector Equilibrium or Cubo Octahedron

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

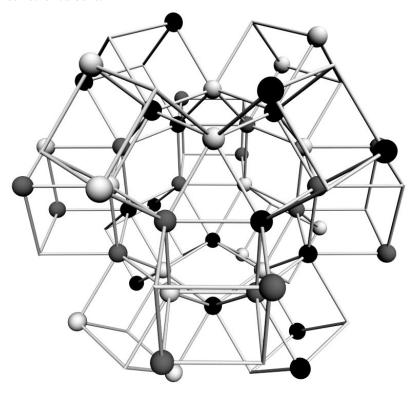


Figure 40. C_{12} - Carbon vector equilibrium or cubo octahedron.

4.5. Super Diamond

It is well known that each Carbon in diamond is surrounded by four Carbons bonded at the tetrahedral vertices. While Atommetrics meets this condition it also predicts another that the author calls Super Diamond. In Atommetrics, each Carbon can be surrounded by not just four but eight Carbons bonded at each of the two tetrahedral vertices. Each electron of each Carbon is covalently bonded with that of the adjacent Carbon. A basic model of Super Diamond is thus:

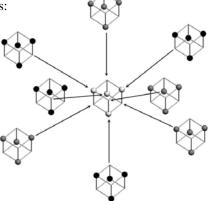


Figure 41. Basic model of Super Diamond: before bonding

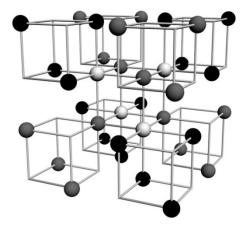


Figure 42. Basic model of Super Diamond: after bonding.



Model photo of Super Diamond showing 8 Carbons around 1 Carbon (not shown).

4. 6. Carbon Lattice

This is a planar molecule of Carbon where each Carbon is doubly bonded to four others in a lattice. Since it resembles the three-dimensional lattice of diamond compressed into a two-dimensional one, the molecule should have the rigid characteristics of Super Diamond (Figure 42).

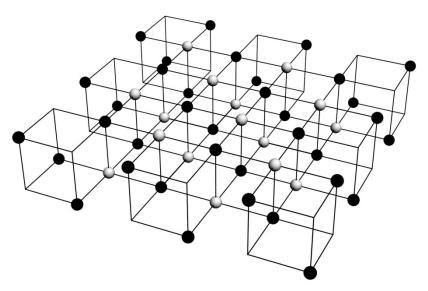


Figure 43. Carbon Lattice.

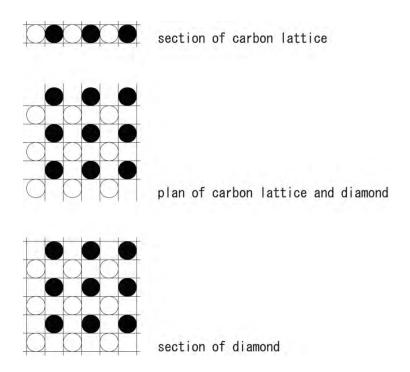


Figure 44. Plan and Sections of Carbon Lattice and Super Diamond.

5. CONCLUSION.

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 orbitals characteristic to itself.
- 2) Electrons assume positions of least repulsion among themselves, assuming independent orbitals, 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 orbital first to complete a structure, after which it pairs to complete the orbital.
- 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 orbitals with unpaired electrons, after which they attach to orbitals with paired electrons, if necessary, to complete their own orbitals.

While this paper is concerned with only electron orbitals, 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.

REFERENCES.

Aldersey-Williams, H. (1995) The Most Beautiful Molecule, p. 75, Aurum Press Ltd., London.

Foo, P.D., Innes, K.K. (1974) Journal of Chemical Physics pp. 60-11.

Fuller, R.B. (1975) Synergetics, p. 164, Macmillan Publishing Co., Inc., New York.

Lewis, G. N. (1916) Journal of the American Chemical Society, Vol. 38, pp. 762-786.

Zumdahl, S. S. (1989a) Chemistry, pp.292, D.C. Heath and Company, Toronto.

Zumdahl, S. S. (1989b) Chemistry, pp.358, D.C. Heath and Company, Toronto.

Zumdahl, S. S. (1989c) Chemistry, pp.359, D.C. Heath and Company, Toronto.