

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

Edward SUZUKI HOERDT

1-15-23 Seta, Setagaya-ku, Tokyo 158-0095, Japan

E-mail address: esa@edward.net

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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. 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). 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 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.

1. Introduction

The author knows well that the electron behavior is described based on quantum mechanics and the electron orbits are obtained by solving the Schrodinger 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

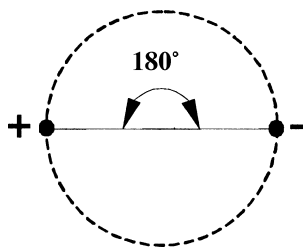


Fig. 1. Paired electrons in an orbit (orbital) as a "line" relationship.

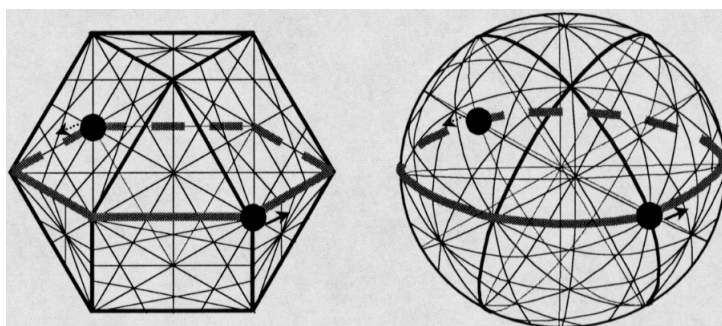


Fig. 2. Hydrogen as a point and Helium as a line.

"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 (see Fig. 2) 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,

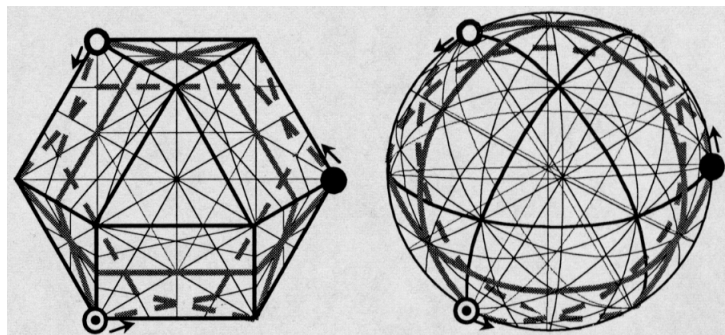


Fig. 3. Trigonal planar for Boron atom.

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 (see Fig. 1).

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, 1989a) throughout the different sublevels.

2. Electron Configurations and Orbits

2.1. Level 1: 1 orbit with 1–2 electrons

The Hydrogen has 1 orbit with 1 electron ($1s^1$). The Helium has 1 orbit with 2 electrons ($1s^2$). 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.

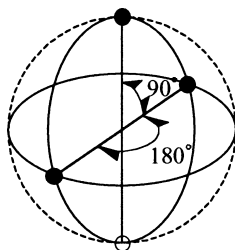


Fig. 4. Two electron separation angles of 180 degrees and 90 degrees.

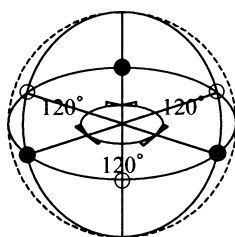


Fig. 5. Common separation angles of 120 degrees.

2.2. Level 2: 3 orbits with 3 electrons and 4 orbits with 4–8 electrons

The Boron has 3 orbits with 3 electrons ($2s^1 2p^2$ instead of $2s^2 2p^1$). It is generally accepted that Boron and other atoms with three valence electrons are in the $s^2 p^1$ form. It is postulated here that instead the form is of $s^1 p^2$ 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 (see Fig. 4).

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 (see Fig. 5).

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 ($2s^1 2p^3$ instead of $2s^2 2p^2$).

This tetrahedral configuration included in Fig. 6 is the simplest and the most stable three-dimensional relationship that can exist among four electrons (Fig. 7). 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)

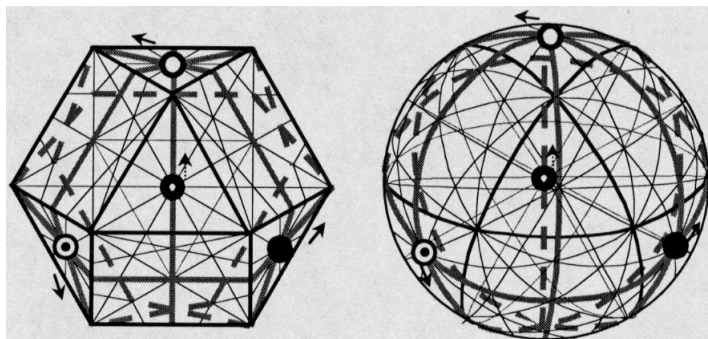


Fig. 6. Tetrahedral for Carbon.

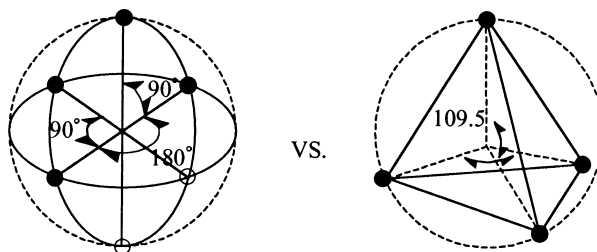


Fig. 7. 3 orbits vs. 4 orbits.

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.

When all the electrons in Fig. 8 make half a revolution (*in terms of the great circle and not necessarily in actuality*) around their respective orbits, the resulting configuration is thus: (see Fig. 9)

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

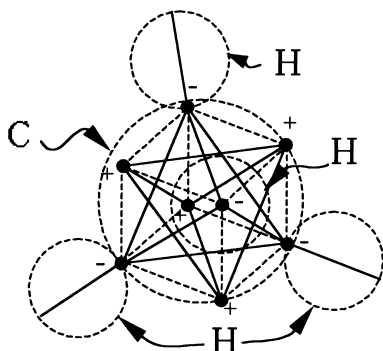


Fig. 8. Molecular structure of methane. (With Carbon electrons paired. Atoms not to scale.)

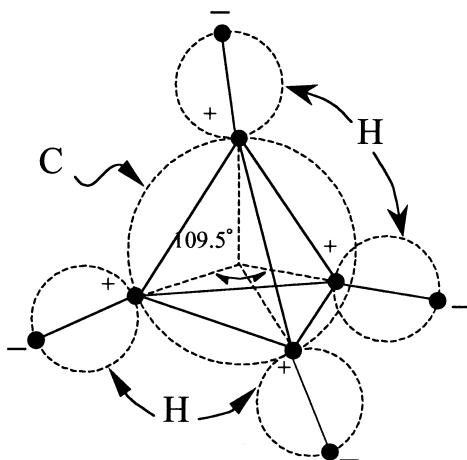


Fig. 9. Molecular structure of methane. (With Hydrogen electrons paired, as seen from a different angle. Atoms not to scale.)

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. 10).

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.

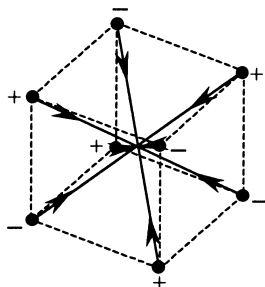


Fig. 10. Four diagonal “bracings” through the center of Carbon in methane. “Plus” and “minus” signs indicate pairing of electrons of opposite spins. Arrows indicate tensile, attractive forces.

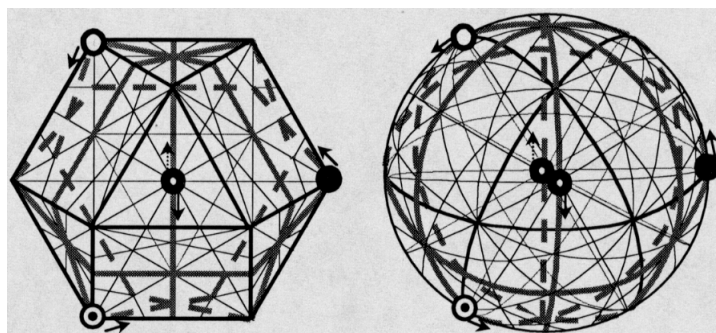


Fig. 11. Trigonal bipyramidal for Nitrogen.

The Nitrogen has 4 orbitals with 5 electrons ($2s^2 2p^3$). The four orbitals are the same as those of the previous 4-electron arrangement (Fig. 11). The opposite ends of one orbital is now filled, and the 3 electrons of the 3 other orbitals 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 (Fig. 12).

The Hydrogen atoms attach to the empty, opposite ends of the three non-paired electrons. In doing so, the three 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

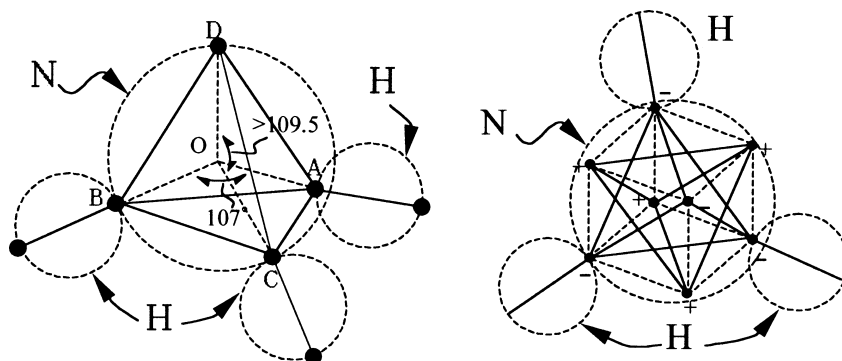


Fig. 12. Bonding angles and pairing of ammonia. (Atoms not to scale. The 1 electron that pairs with D to form a lone pair is not drawn in the left diagram.)

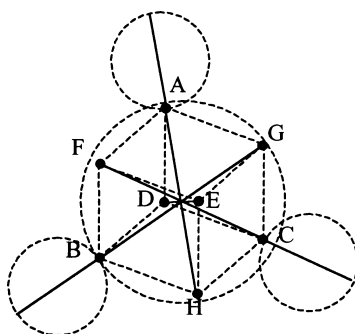


Fig. 13. "Lone pair" and "bonding pairs" of ammonia (atoms not to scale).

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 equilibrals 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 (Fig. 12). The paired electrons (DE) in Fig. 13 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 (Fig. 13).

The Oxygen has 4 orbitals with 6 electrons ($2s^2 2p^4$). To the previous Nitrogen configuration an electron is added to fill one of the unfilled orbitals. 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

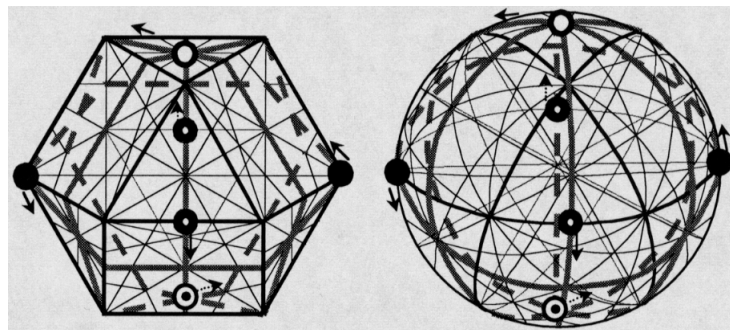
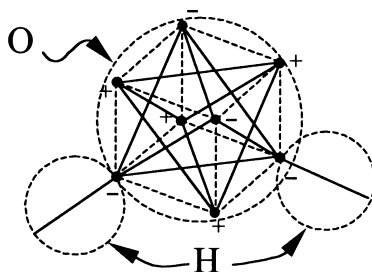


Fig. 14. Octahedral for Oxygen.

Fig. 15. Two interlocking tetrahedra in the Oxygen of H_2O . (With Oxygen electrons paired. Atoms not to scale.)

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 (Fig. 14).

One may wonder why there are 4 orbits instead of 3, as 3 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 triangular faces to form 2 interlocking tetrahedra, or cube. The molecular structure is thus modeled as shown in Fig. 15.

When all the electrons rotate 180 degrees, the molecular structure is thus, as in Fig. 16.

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

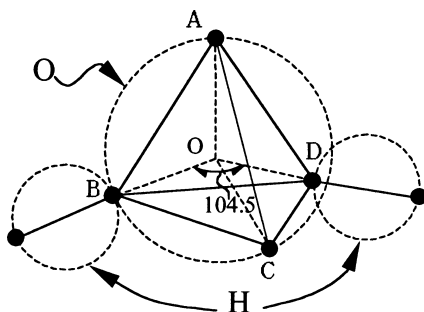


Fig. 16. Molecular structure of H_2O . (With Hydrogen electrons paired. Atoms not to scale. The 2 electrons that pair with A and C to form lone pairs are not drawn.)

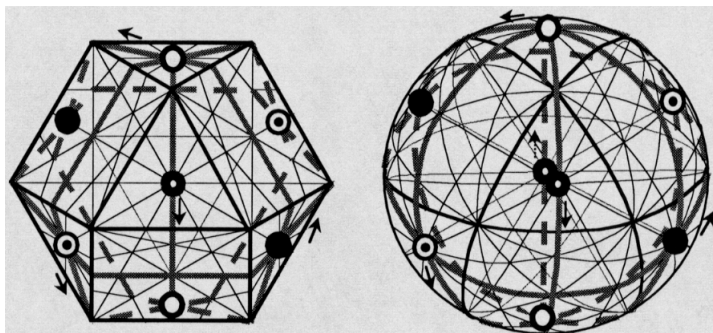


Fig. 17. Two interlocking tetrahedra (cube) for Neon.

the center of mass of the resulting molecule from the center of Oxygen to cause a shift in the regular vector equilbral 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.

Fluorine has 4 orbits with 7 electrons ($2s^2 2p^5$). The Neon has 4 orbits with 8 electrons ($2s^2 2p^6$) as in Fig. 17. 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.

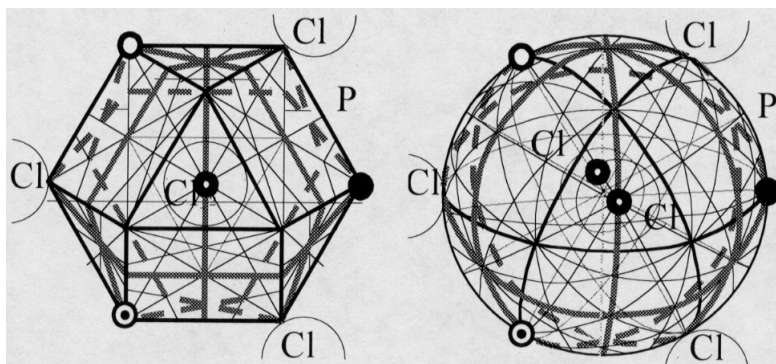


Fig. 18. Molecular structure of PCl_5 (atoms not to scale).

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 (PCl_5)

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 PCl_5 is considered to be as shown in Fig. 18.

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, 1989b). 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

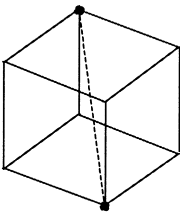
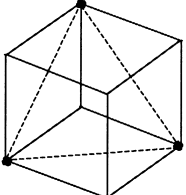
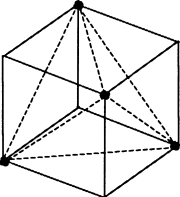
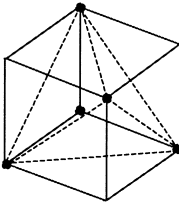
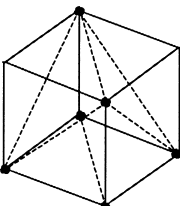
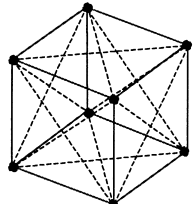
	Number of Orbits	Number of Electrons	Electron Arrangements	Remarks
	1	2	Linear	1 Pair of Electrons
	3	3	Trigonal Planar	Triangle small and lop-sided
	4	4	Tetrahedral	Regular
	4	5	Trigonal Bipyramidal	Triangles small and large: lop-sided. 1 Pair of Electrons
	4	6	Octahedral	Triangles small and large: lop-sided. 2 Pairs of Electrons
	4	8	Double Tetrahedral	Regular. 4 Pairs of Electrons

Fig. 19. Regular arrangements of electrons in "cubes."

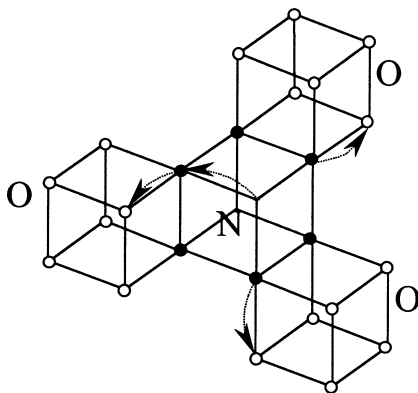


Fig. 20. Molecular structure of NO_3^- with 3 double bonds. Phase 1: All electrons paired.

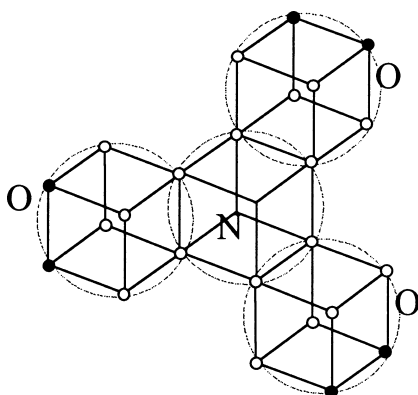


Fig. 21. Molecular structure of NO_3^- . Phase 2: All electrons paired, with Nitrogen electrons in Oxygen orbits (ionic bonding). Spheres around the cubes show how the atoms interpenetrate each other.

as well as molecular arrangements of atoms, each atom shall henceforth be presented not as part of double tetrahedra but simply of cube, as follows: (see Fig. 19)

For sake of brevity, only the cube arrangements without the vector equilibrals 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. NO_3^- ion

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.

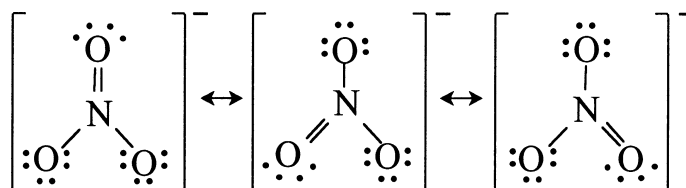
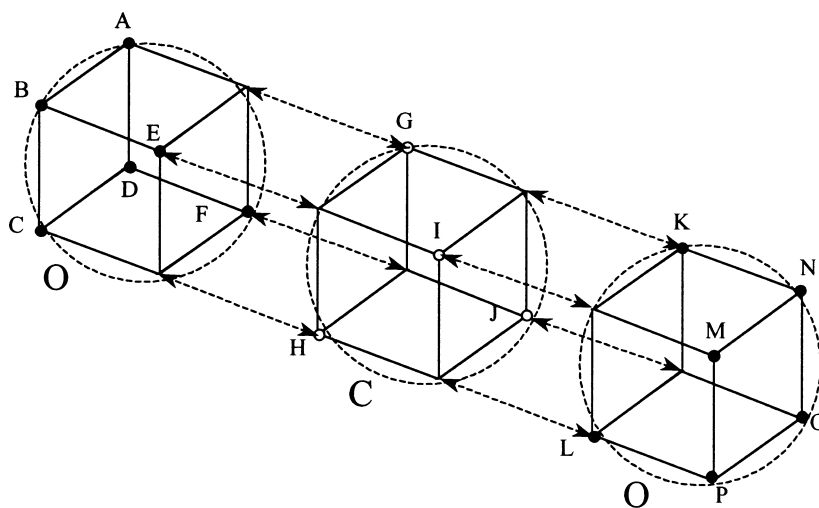
Fig. 22. Lewis structure for NO_3^- .

Fig. 23. Carbon and Oxygen atoms before bonding.

Nitrogen has 4 orbitals with 5 electrons ($2s^2 2p^3$) and Oxygen has 4 orbitals with 6 electrons ($2s^2 2p^4$). With an electron added, all the atoms have 6 valence electrons each.

As is evident from the diagrams, the bond angles are 120 degrees. Again, it should be noted that Nitrogen and Oxygen have 4 orbitals 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 Fig. 20).

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: (see Fig. 22)

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, 1989c). 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.

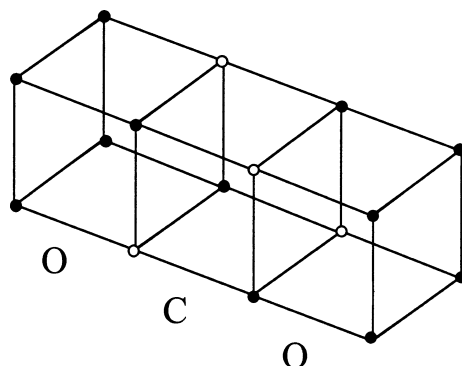


Fig. 24. CO_2 molecule. Phase 1: All electrons in their respective atomic orbits (covalent bonding).

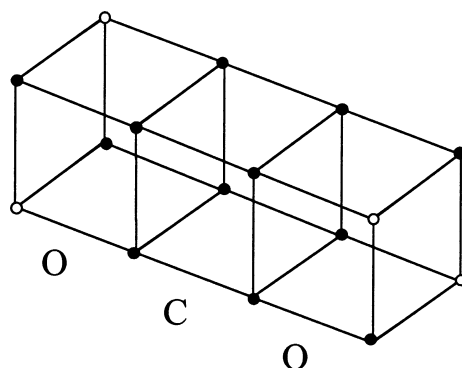


Fig. 25. CO_2 molecule. Phase 2: All Carbon electrons in their respective Oxygen orbits (ionic bonding).

3.3. Carbon dioxide (CO_2)

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

As is evident in the 2-phase diagrams of the CO_2 molecule (Figs. 24 and 25), 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 (Fig. 23) 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.

In the same way as was done for PCl_5 , NO_3^- , and CO_2 , structures of PCl_6^- anion, ethylene, acetylene, carbon monoxide, fullerene (C_{60}), carbon nanotube, and methanol can be given. However, they shall be presented on another occasion.

4. 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 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 structure 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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