Exploration

Cubic Lattice Bonding of Graphene, Benzene & Ozone

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Abstract

We demonstrate that a cubic lattice nucleus model provides a rational and physically viable representation of carbon allotropes, polycyclic and other molecules. The demonstration focuses on the carbon allotrope graphene, the benzene ring, and the oxygen/ozone molecule. We describe a trifid bond structure based on the cubic lattice model to illustrate the nature of molecular bonds. We suggest that the trifid and derivative bond structures supersede the orbital electron-sharing and covalent bond models and the Lewis bond diagrams.

Keywords: Lewis structure, van der Waals force, chemical bond modes, graphene, deuteron module.

1. Introduction

Graphene is an allotrope of carbon. It is represented as a two-dimensional, atomic-scale, hexagonal array in which a carbon atom occupies each vertex. Graphene is the basic structural element of other allotropes, including graphite, charcoal, carbon nanotubes and fullerenes. It consists of an indefinitely extended single atomic layer molecule, the ultimate case of the family of flat polycyclic aromatic hydrocarbons. Graphene was isolated in 2004 by researchers Andre Geim and Kostya Novoselov at The University of Manchester who won the Nobel Prize in physics for their pioneering work. We argue that the representation of the graphene molecule and similar cyclic structures - such as benzene - may be correctly visualized with the cubic lattice model. In the cubic lattice characterization of graphene, carbon atoms are not vertices but sides of the hexagonal Lewis substructure for graphene.

2. Cubic Lattice Nucleon

In Figure 1, a carbon-12 atom is depicted as a cubic lattice configuration where the nucleus consists of six deuteron modules, surrounded by an electron orbital envelope [1]. Each electron orbits a specific deuteron module. The disc-like or toroid-like representation of the electron orbitals represents a Parson magneton [2]. Alternate orbital electrons are assumed to 'spin' in opposite directions in accordance with deuteron orientations. The schematic of the carbon atom in Figure 1, shows abstractions of the essential components.

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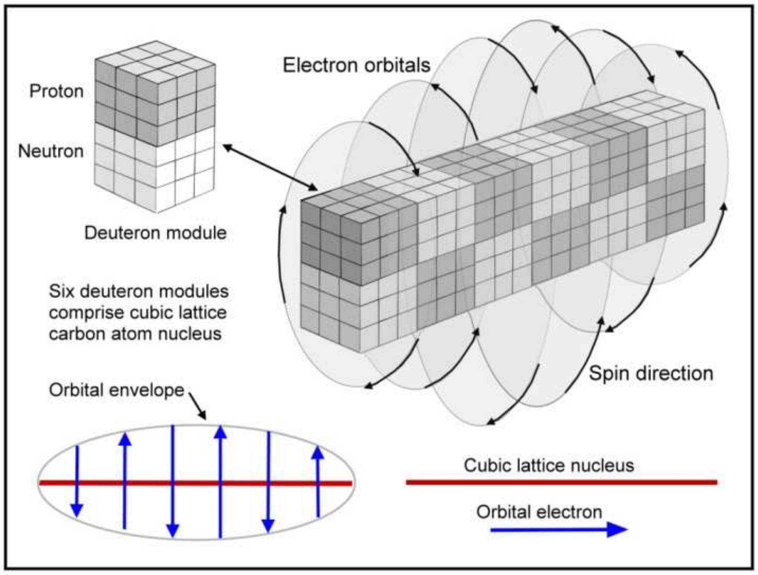

Figure 1 - Cubic lattice and schematic representations of carbon atom.

The concept of atomic orbitals is itself an abstraction which attempts to describe the probabilistic locations of electrons orbiting a spheroidal nucleus, as conceived in the Standard Theory of Particle Physics. The orbital conception describes wave-like (or cloud-like) electrons spinning around an assumed spheroidal nucleus. Quantum theory visualizes orbitals in terms of concentric shells and subshells which each hold a specific number of electrons determined by quantum mechanics. The cubic lattice nucleus model does not assume specific numbers of electrons in particular orbital shells but assigns a specific orbiting electron to each deuteron in the nucleus modular architecture. Accompanying wave mechanics, periodicity, and orbit energy parameters should apply to each Parson magneton as in the standard concentric orbital shell visualization.

3. Carbon Bond Trifid

The carbon bond trifid as depicted in Figure 2 appears to be fundamental to the formation, structure, and strength of the graphene allotrope of carbon. We can find and demonstrate its repeated appearance in other cyclic molecules such as the benzene ring and in other instances where it explains the geometric arrangement of molecular atoms. In Figure 2 we assume that the three carbon nuclei are the same plane, but allow that each defines its own plane as would be the case for graphene nanotubes or other buckminsterfullerenes.

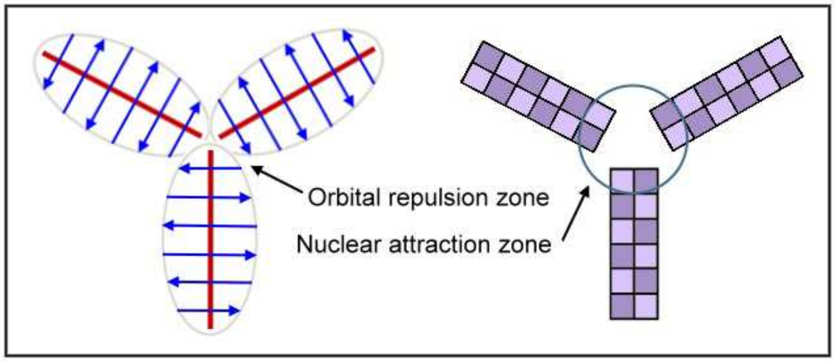

Figure 2 - Schematic of trifid bonding of three carbon atoms and nuclei.

Figure 2 suggests that the trifid bonding of three carbon atoms involves a balance between the repulsion of their negatively-charged orbital envelopes and the attraction between close deuteron pairs of their nuclei. Our argument assumes the existence of a zone of attraction between deuterons which extends beyond the orbital envelope within which the nucleus resides. Appendices A, B, C, D, and E provide supplemental data.

4. Graphene Array based on Cubic Lattice Model

Figure 3 compares the currently-accepted standard visualization of graphene with our visualization based on the cubic lattice nucleon/nucleus model. The standard visualization assumes an atomic-scale, hexagonal substructure in which one atom occupies each vertex, where each atom is represented as a small sphere. The bonding between atoms is represented by small rod-like connectors. The bond lengths represented by the rods are of the order of one angstrom or slightly greater. These typically represent lengths of single bonds (~1.5 angstroms) or double bonds (~1.3 angstroms) depending upon the orbital shells surrounding the assumed spheroidal nucleus of the carbon atom. This standard Lewis structure representation is also assigned to carbon atom hexagons that comprise the benzene ring, discussed later.

We argue that in the correct representation of the graphene array the spheres and rods are reversed and that the bonding of the carbon atoms occurs where they meet (in trifid bonding) while the atoms occupy a similar space (≈ or ≥angstrom) in between - instead of the rods, as depicted in Figure 3.

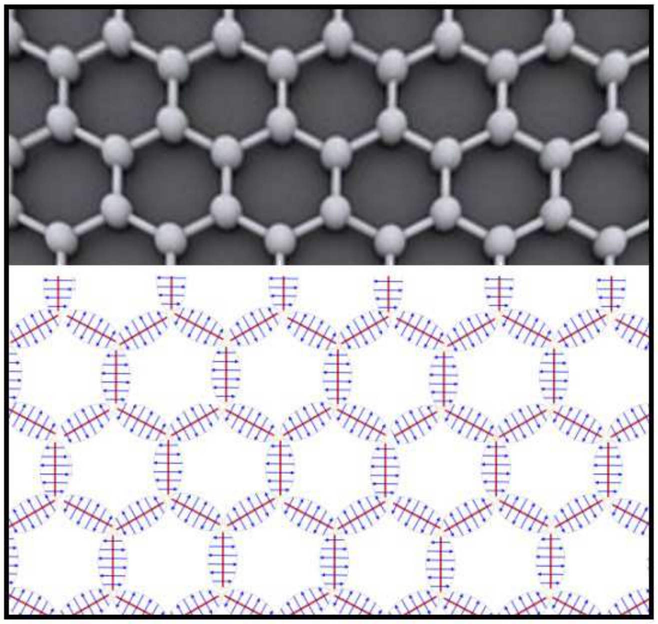

Figure 3 - Standard and cubic lattice-based graphene matrix.

Figure 4 compares an atomic scale quantitative annular dark-field scanning transmission electron microscopy (ADF STEM) image with the cubic lattice-based array of graphene. STEM intensities simply image the energy variations of the hexagonal array in the interior of a graphene grain [3].

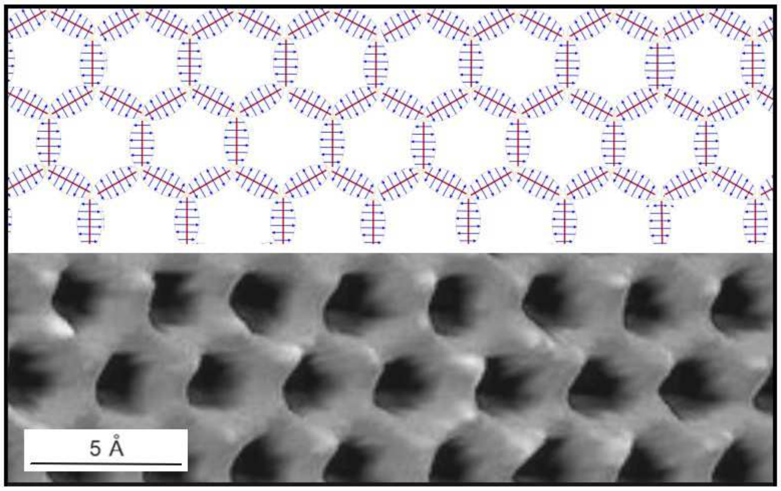

Figure 4 - Comparison of cubic lattice matrix and STEM image of graphene.

Figure 4 compares an atomic scale quantitative annular dark-field scanning transmission electron microscopy (ADF STEM) image with the cubic lattice-based array of graphene. STEM intensities simply image the energy variations of the hexagonal array in the interior of a graphene grain [3].

The ‘high’ points in the STEM image correspond to loci of trifid bonding and therefore of regions with more intense energy content. We argue that these loci are not coincident with carbon atoms but that the atoms constitute the sides of the hexagons, as depicted by the cubic lattice model in Figure 4.

5. The Benzene Ring and Ozone

Benzene, C_6H_6, is conventionally depicted with the Lewis structure as a ring of six carbon atoms, with alternating double bonds and single bonds, as in Figure 5. The bond lengths in the benzene rings are measured as 1.397 angstroms. The notions of double or single bond lines are unnecessary in the alternative cubic lattice trifid bonding scheme depicted in Figure 5 where carbon atoms rather than imaginary bond lines form the sides of the benzene hexagon.

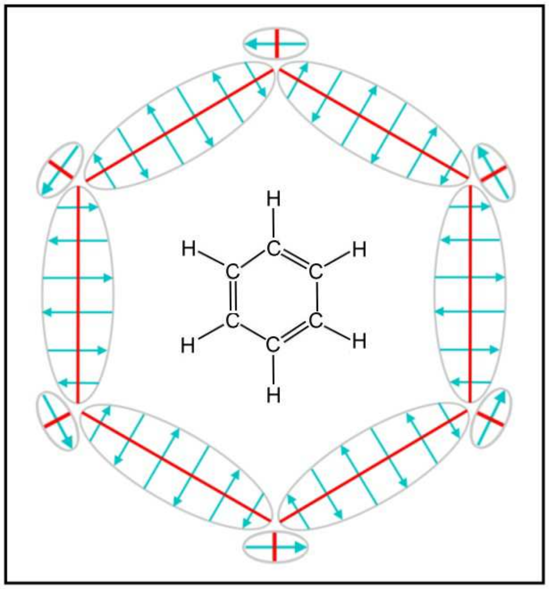

Figure 5 - Alternative representations of the benzene ring.

Figure 6 depicts the cubic lattice bond scheme for the oxygen molecule and the most likely of three allotropes of ozone. The cubic lattice ozone molecule is rendered as being in one plane with an angular spacing of 120°. The inter-atomic angle may be less if the atom lobes occupy different planes, like the petals of a flower. According to experimental evidence from microwave spectroscopy, ozone is a bent molecule, with an angle of 116.8° between its atoms [4]. In Figure 6 the Lewis structure ozone molecule is represented as a resonating polarized hybrid with two alternate structures, each with a single bond on one side and double bond on the other. In the standard depiction the O – O bond distances are 1.278 Å. We suggest that the notions of electron-sharing and covalent bonding assumed in the Lewis structure, although serviceable, are obsolescent and that the trifid and derivative bond structures presented here are preferable.

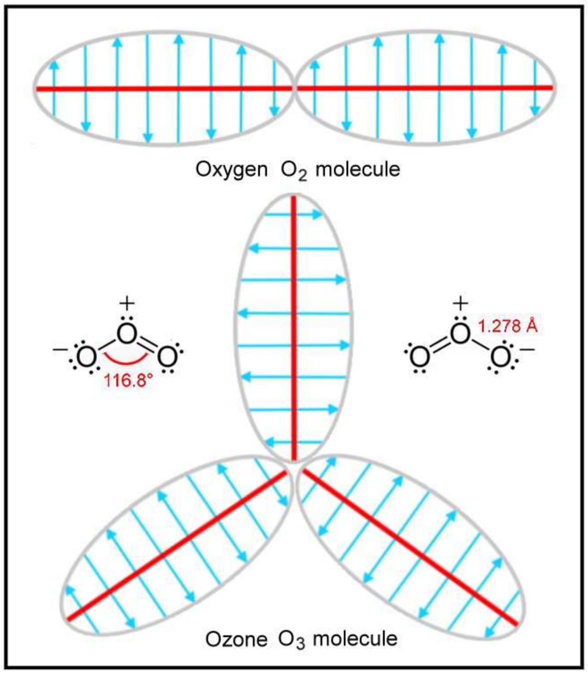

Figure 6 - Alternative ozone bonding schemes.

6. Alternative to the Lewis Structure

Lewis structure diagrams are devised to show the bonding between atoms in terms of shareable electrons [5]. Lewis diagrams show each atom and its position in the structure of the molecule using its chemical symbol. Lines or pairs of lines are drawn between atoms that are bonded to one another. So-called ‘excess’ electrons that form lone pairs are represented as pairs of dots, and are placed next to the atom symbols, as in Figure 6. Main group elements of the second period and beyond are assumed to bond by gaining, losing, or sharing electrons until they have achieved a valence shell electron configuration with a full octet of electrons, other periodic table elements obey different rules.

The Lewis structure is based on the shell model for atoms and upon the assumption that atoms *seek or share additional electrons in order to complete or complement a prescribed shell configuration*. The cubic lattice nucleus model of the atom makes no such assumption. We contend that the bonding of atoms that form molecules is based on the mutual attraction or affinity between pairs of deuterons, as depicted in Figure 7 for the oxygen molecule O_2. The rationale is that the zone of attraction extends beyond the electron orbital envelopes of the oxygen atoms and balances the mutual repulsive force of their negatively-charged envelopes.

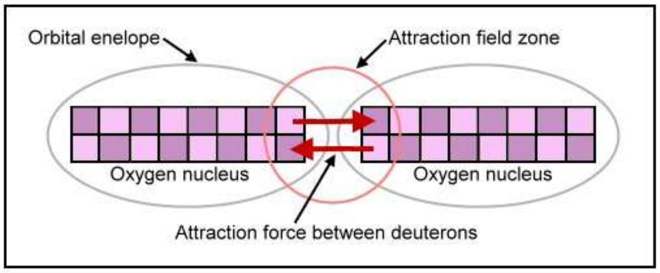

Figure 7 - Bond zone between atoms in O_2 molecule.

The cubic deuteron is an essential module common to every element nucleus from deuterium, helium and beyond. The exception is protium [6]. The conceptual cubic architecture of the oxygen nucleus may be taken as the fusion of eight deuterons or four alpha particles. The latter demonstrates the affinity of deuterons which fuse to produce alpha particles. Energy (≈ 24 MeV) between deuteron pairs is released when they fuse**.** Supplemental data are discussed in Appendix A and B.

7. Nature of the Chemical Bond - Myth and Fact

It is still common to speak of shells and subshells of electrons around the atomic nucleus despite the advances in understanding of the quantum-mechanical nature of electrons. Quantum mechanics cannot predict the exact location of an electron, only the probability of finding it at different locations. The form of the periodic table is closely related to the assumed electron configuration of the atoms involved. In general, the periodicity of the periodic table is presumed due to the number of electrons needed to fill shells and subshells.

An electron shell is one set of allowed states that electrons may occupy while sharing the same principal quantum number, n. According to the shell model, an atom's nth electron shell can accommodate $2n^2$ electrons, e.g. the first shell can accommodate 2 electrons, the second shell 8 electrons, and the third shell 18 electrons. The factor of two arises because the allowed states are doubled due to electron spin - each atomic orbital admits up to two otherwise identical electrons with opposite spin, one with a spin +½ and one with a spin −½. A subshell is the set of states defined by a common azimuthal quantum number, ℓ, within a shell. The values ℓ = 0, 1, 2, 3 correspond to the s, p, d, and f labels, respectively. For example, the 3d subshell has n = 3 and ℓ = 2. The maximum number of electrons that can be placed in a subshell is given by 2(2ℓ+1). This gives two electrons in an s subshell, six electrons in a p subshell, ten electrons in a d subshell and fourteen electrons in an f subshell. According to this elaborate scheme, the 3d subshell has n = 3 and ℓ = 2.

The numbers of electrons that may occupy each shell and subshell arise from the equations of quantum mechanics and the Pauli exclusion principle which states that no two electrons in the same atom can have the same values of the four quantum numbers. *Quantum numbers provide a rationale for why electrons which normally repel each other may commingle in various orbital configurations.* By contrast, each electron in the cubic lattice nucleus model has a distinct quantized energy state and a distinct and separate orbit, as depicted in Figure 1.

In atoms or molecules with more than one electron, the motion of electrons are correlated and the orbital or shell picture fails. A very large number of electronic configurations are needed to describe any multi-electron system, and no energy can be associated with one single configuration. Electron wave functions may describe a small number of configurations, therefore the notion of electronic orbital configurations remains satisfactory for many multi-electron systems. The cubic lattice model avoids these configurational problems.

In both the standard and cubic lattice model, a fundamental application of electron configurations is in the interpretation of the facts of atomic spectra. It is necessary to assume electrons with one or more different energy levels in an atom. Energy levels can be calculated for the ground-state configuration of atoms, although not all the energy levels are observed in practice. It is through the analysis of atomic spectra that the ground-state electron configurations of the elements were experimentally determined.

The most practical application of quantum mechanical electron configurations is in the rationalization of chemical properties, in both inorganic and organic chemistry. In effect, some simplified forms of molecular orbital theory, have become the modern equivalent of the valence concept, describing the number and type of chemical bonds that atoms can be expected to form. Valence bond theory is one of two basic theories, along with molecular orbital theory, developed to use the methods of quantum mechanics to explain chemical bonding. The focus is on how electron orbitals of separate atoms combine to give individual chemical bonds when a molecule is formed. In contrast, molecular orbital theory has orbitals that cover the whole molecule.

A covalent bond involves the sharing of electron pairs between atoms. These electron bonding pairs allow, a stable balance of attractive and repulsive forces between atoms. For many molecules sharing of electrons allows each atom to attain the equivalent of a full outer shell, a stable electronic configuration. The means that the atoms share ‘valence’ as is discussed in valence bond theory. Theoretically, in the molecule H_2, the hydrogen atoms ‘share’ two electrons via covalent bonding. Covalent bonding that entails sharing of electrons over more than two atoms is said to be delocalized. Supplemental data are discussed in Appendix C, D, E.

8. Conclusion

The cubic lattice nucleon model avoids the valence concept altogether and accepts the fact that like charges repel - that free electrons mutually repel and that atoms lacking ‘complete shells’ do not ‘invite’ itinerant electrons in. As explained previously in this paper, and as illustrated in Figure 7, it is the attraction between deuterons which overcomes the mutual repulsion of electron orbital envelopes to form molecular bonds.

The Lewis structure ‘bond length’ conventionally depicted for various hydrocarbons and other molecular structures clearly correspond to the size of their atomic orbital envelops as conceived with the cubic lattice model. The cubic lattice representation of molecular structures makes Lewis structures and conventional chemical bond concepts obsolete. The bond linkages of carbon allotropes, the benzene ring, and other molecular structures are better represented by deuteron attraction fields shared by adjacent atom nuclei.

Appendix A

The hydrocarbon compound ethane has the chemical formula C_2H_6. Methane with the chemical formula CH_4 is the simplest alkane. In the Lewis structure depiction, Figure 1A, methane is assumed to be a tetrahedral molecule with four equivalent C–H bonds. Its electronic structure is described by four bonding molecular orbitals resulting from the overlap of the valence orbitals on C and H. Ethylene (ethene) is has the formula C_2H_4 or $H_2C{=}CH_2$. Acetylene (ethyne) the simplest alkyne has the chemical formula C_2H_2.

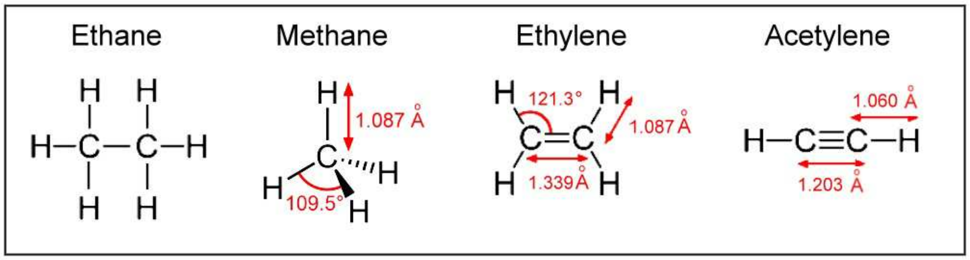

Figure 1A - Lewis structure representations and measurements of four hydrocarbon molecules.

Figure 2A depicts the conjectured cubic lattice nucleon-based structures of ethane, methane, ethylene, and acetylene molecules. In accordance with our argument, the bonding of carbon and hydrogen atoms is related to the affinity and attraction of terminal deuterons of adjacent cubic lattice nuclei. The deuteron-deuteron fields, as conceived here, adapt to a quadrifid as readily as a trifid configuration, as in the ethane molecule.

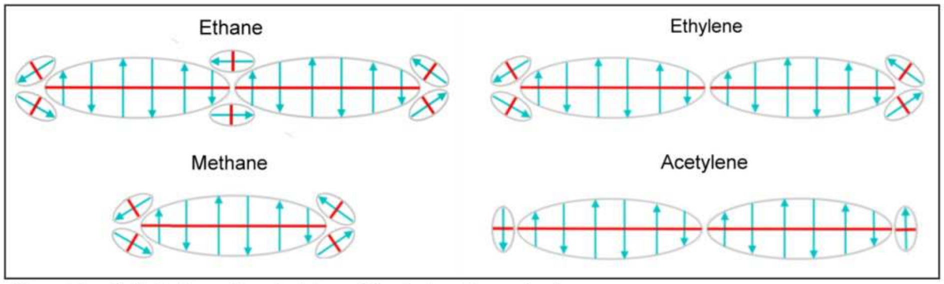

Figure 2A - Cubic lattice nucleon depictions of four hydrocarbon molecules.

Appendix B

We propose that the physical-chemical bond field depicted in Figures 2 and 7, and implied elsewhere in this paper, is a manifestation of the van der Waals force which is a distance-dependent interaction between atoms or molecules. Van der Waals forces play a fundamental role in fields as diverse as supramolecular chemistry, structural biology, polymer science, nanotechnology, surface science, and condensed matter physics. Van der Waals forces define many properties of organic compounds and molecular solids.

Unlike the ionic or covalent bond, the van der Waals attraction is not a chemical-electronic bond but a comparatively weak and susceptible to being perturbed. The van der Waals force quickly vanishes at long distances between interacting molecules. In Figure 1B we illustrate a concept of the hydrogen-carbon nuclear van der Waals bonds (proton to neutron affinity) in terms of the cubic lattice nucleon model.

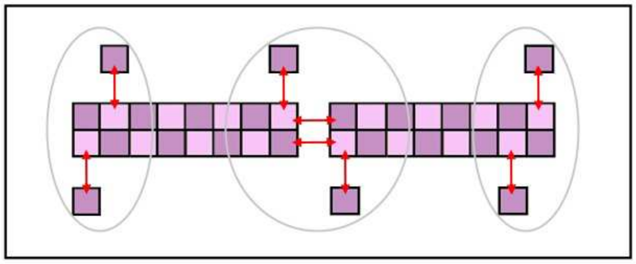

Figure 1B - Van der Waals attraction zones for ethane.

Appendix C

The spherical shell model is a visualization of the electron configuration surrounding the atomic nucleus. The spherical nuclear shell model is a model of the atomic nucleus which uses the Pauli exclusion principle to describe the structure of the nucleus in terms of energy levels. The nuclear shell model is analogous to the shell model which describes the arrangement of electron orbitals.

Protons and neutrons in the nuclear shell model are independent of each other and unlike the cubic lattice nucleus model protons and neutrons are not paired as deuterons. Indeed, neutrons in the spherical nucleus move about independently while in the cubic lattice model neutrons are fixed structural components [1]. Because neutron-proton pairs form deuteron substructure modules of atomic nuclei, as in Figure 1, it is possible to assign a separate orbit to each electron associated with each deuteron with no orbital commingling.

The spherical shell model must provide a way to overcome mutual repulsive forces of electrons commingling in orbitals surrounding the atomic nucleus. The model invokes the Pauli exclusion principle which states that two or more identical fermions (electrons in orbit around the atom nucleus) cannot occupy the same quantum state within a quantum system simultaneously. Quantum mechanics theory resolves the electron charge repulsion problem with rules associated with four quantum numbers. It is impossible for two commingled electron orbitals to have the same values of the four quantum numbers: n, the principal quantum number, ℓ, the angular momentum quantum number, m_ℓ, the magnetic quantum number, and m_s, the spin quantum number. If two electrons reside in the same orbital, and if their n, ℓ, and m_ℓ values are the same, then their m_s must be different, and the electrons must have opposite half-integer spins of +½ and −½. No two electrons can share the same allowed combinations of the four quantum numbers. These elaborate rules are unnecessary with the cubic lattice nucleus model but comparable rules may apply to each orbital electron energy level.

Appendix D

The cubic lattice nucleon model readily explains why some elements are inert and form no compounds while other elements are highly interactive and compound-forming. This makes it unnecessary to invoke the notion of electron-sharing to complete orbital shells. We illustrate with fluorine and neon:

Fluorine with atomic number 9 is the most electronegative element, it is extremely reactive. Almost all other elements, including some noble gases, form compounds with fluorine. Neon with atomic number 10 is a noble gas. Neon is chemically inert and forms no uncharged chemical compounds. Some compounds of neon may include ionic molecules, molecules held together by van der Waals forces and clathrates (substances in which a molecule of one compound fills a cavity within the crystal lattice of another compound).

Assuming the shell model: The fluorine atom has 2 and 7 electrons per shell while the neon atom has 2 and 8 electrons per shell. The complete octet of eight electrons in the outer atomic shell makes neon stable and resistant to bonding with other elements while fluorine with only seven electron in the outer atomic shell makes fluorine prone to compound-forming by 'borrowing' the electron needed for completing the outer shell, and is therefore highly reactive.

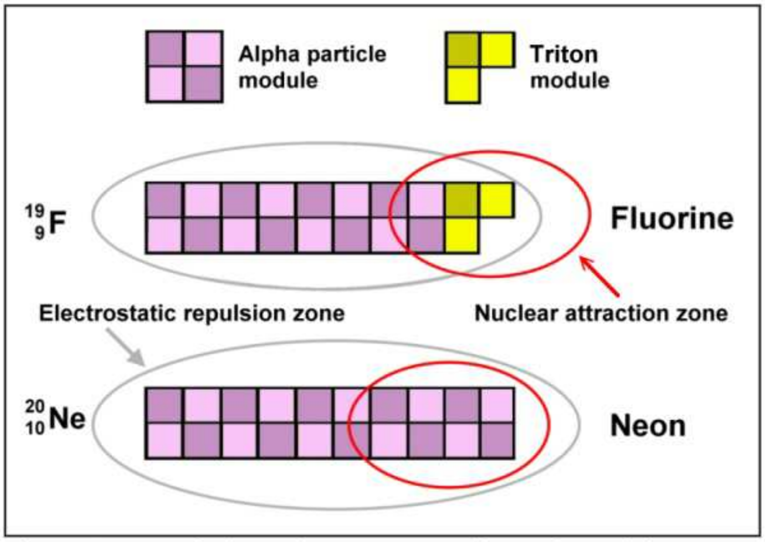

Figure 1D - Imbalance between attraction and repulsion zones.

Figure 1D shows a conceptual imbalance between attraction and repulsion which according to the cubic lattice nucleon model explains the chemical activity of fluorine and the inertness of neon. The underlying rationale is that the triton module and associated electron orbitals allow the nuclear attraction zone to extend beyond the electrostatic repulsion zone. Apparently, the 10 alpha modular structure of the neon nucleus is such that the nuclear attraction zone is drawn within the repulsion zone.

A similar rationale may be applied to chlorine and argon: Chlorine with atomic number 17 is an extremely reactive element and a strong oxidizing agent. Among the elements, chlorine has the highest electron affinity and the third-highest electronegativity, behind only oxygen and fluorine. Argon with atomic number 18 is a noble gas and undergoes almost no chemical reactions. The chlorine atom has 2, 8, 7 electrons per shell while the argon atom has 2, 8, 8 electrons per shell. The complete octet of eight electrons in the outer atomic shell makes argon stable and resistant to bonding while chlorine with only seven electron in the outer atomic shell makes chlorine prone to completing the outer shell and therefore highly reactive. As in the case of fluorine-19, the cubic lattice model chlorine-35 has a triton module which distorts the repulsion-attraction balance while argon-36 with a complete set of 18 alpha modules draws the nuclear attraction zone within the repulsion zone.

Appendix E

The Aristotelian and Ptolemaic geocentric model of the cosmos - in which the Sun, the Moon, stars, and planets all revolve around the Earth - prevailed until replaced by the Copernican heliocentric model. Until Kepler demonstrated that the Earth and planets follow elliptical orbits around the Sun, theorists imagined cycles and epicycles to explain the erratic periodic retrograde motions of the planets based on the geocentric model. It has been determined that the Copernican, Ptolemaic and even the Tychonic models provided identical results to identical inputs. They are *computationally* equivalent, though Kepler showed that physical observations reveal heliocentricity and that the Sun is one of the foci of elliptical planetary orbits.

We are confronted with a comparable quandary with the currently accepted model of the atom in which the nucleus, nucleons, and electron shells are assumed to be essentially spheroidal as opposed the cubic lattice model depiction. The clever application of theoretical mathematics and quantum mechanics stratagems provide a *computationally* consistent base for accepting the spheroidal model of the nucleus and surrounding electron shells. The model persists in modified forms wherein electron orbitals are depicted as teardrop-shaped, doughnut-shaped, or as electron clouds.

Modifications of the spheroidal shell model arose because ongoing studies show that electrons behave in ways that defy classical physics. In the electron cloud model, electrons are no longer depicted as particles moving around a central nucleus in fixed orbits. Instead, their instant locations are described as being loci in clouds around the nucleus where the electrons are likely to be found.

In *Fashion, Faith, and Fantasy in the New Physics of the Universe*, Roger Penrose contemplates models adopted by theoreticians in their pursuit of truths about the nature of atoms and other physical entities [7]. Penrose acknowledges the remarkable effectiveness of mathematics in describing and predicting their nature and properties. However, Penrose cautions that discovering mathematical truths is not the same as discovering physical truths: ". . . we need a change in the physics, not just some clever mathematics, brought in to cover the ontological cracks!" Indeed, we need to reexamine the models that represent atoms.

The cubic lattice nucleus model is offered as a rational approach for depicting the atom nucleus and for depicting the nature electron orbitals in a way which avoids the esoterica of electron clouds. We are in effect obliged to imagine a structure for the nucleus and to discover the nature and arrangement of orbital electrons associated with that structure. Figure 1E compares the conventional and the cubic lattice structures for the oxygen nucleus. In the conventional depiction, protons which would mutually repel are held tightly together by the strong force between quarks. This assumes that gluons mediate strong interactions among quarks. Gluons are posited as a gauge bosons that act as the strong force between quarks. The cubic lattice nucleus model adopts the chromodynamics of quark 'asymptotic freedom' wherein attraction grows stronger as deuterons are separated. This accounts for attractive forces that extend beyond the orbital envelope.

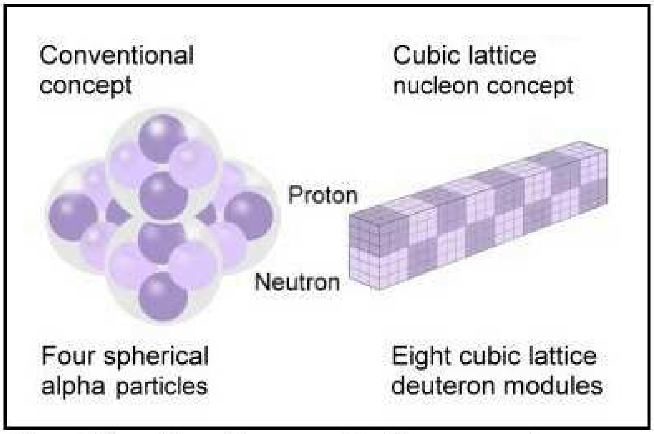

Figure 1E - Alternative concepts of oxygen nucleus.

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