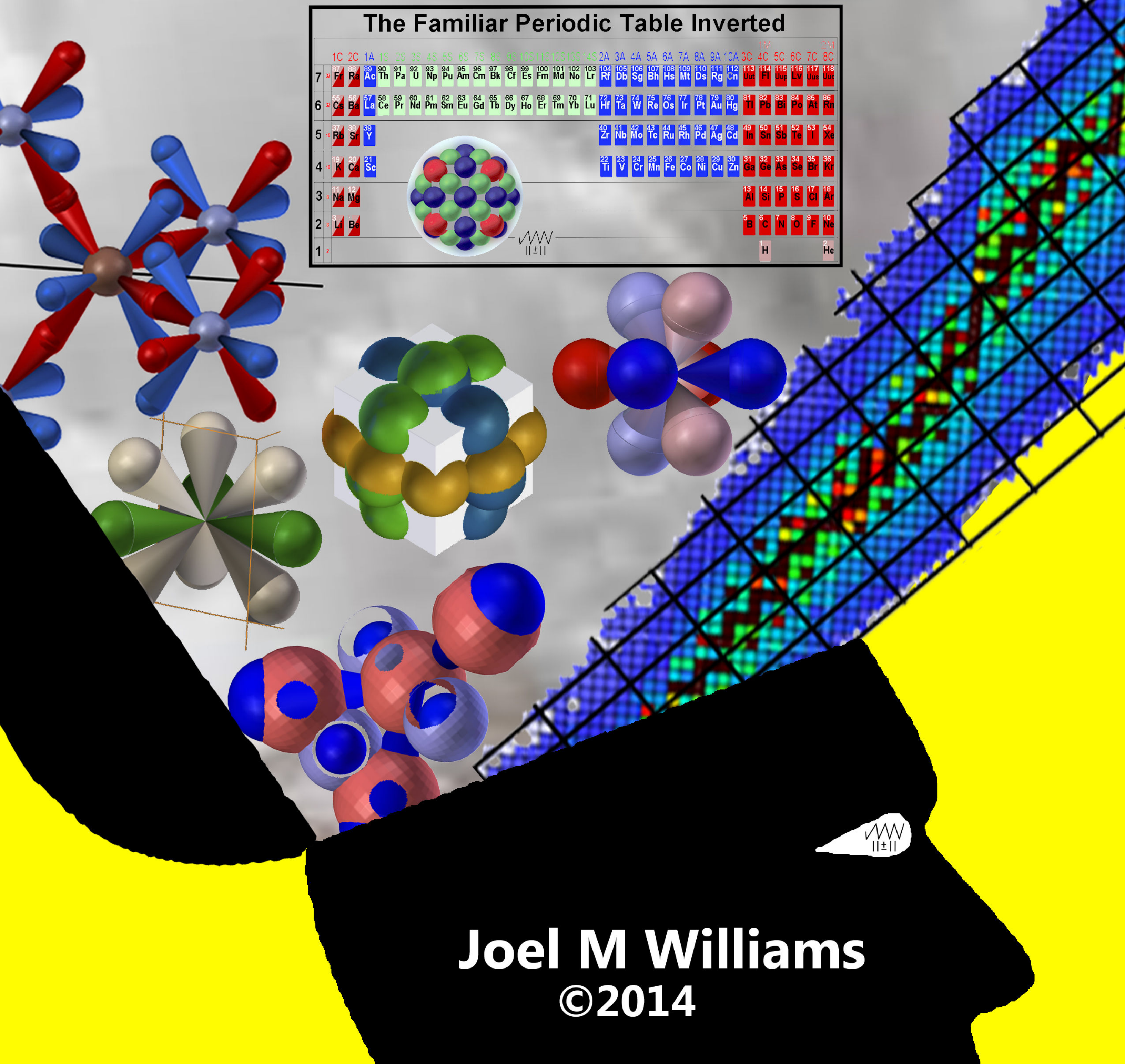
Rethinking the Atom

A Compilation of Papers by the Author



The Familiar Periodic Table Inverted

																													1M				2M
		1C	2C	1A	1S	2S	3S	4S	5S	6S	7S	8S	9S	10S	11S	12S	13S	14S	2A	3A	4A	5A	6A	7A	8A	9A	10A	3C	4C	5C	6C	7C	8C
7	32	87 Fr	88 Ra	89 Ac	90 Th	91 Pa	92 U	93 Np	94 Pu	95 Am	96 Cm	97 Bk	98 Cf	99 Es	100 Fm	101 Md	102 No	103 Lr	104 Rf	105 Db	106 Sg	107 Bh	108 Hs	109 Mt	110 Ds	111 Rg	112 Cn	113 Uut	114 Fl	115 Uup	116 Lv	117 Uus	118 Uuo
6	32	55 Cs	56 Ba	57 La	58 Ce	59 Pr	60 Nd	61 Pm	62 Sm	63 Eu	64 Gd	65 Tb	66 Dy	67 Ho	68 Er	69 Tm	70 Yb	71 Lu	72 Hf	73 Ta	74 W	75 Re	76 Os	77 Ir	78 Pt	79 Au	80 Hg	81 Tl	82 Pb	83 Bi	84 Po	85 At	86 Rn
5	18	37 Rb	38 Sr	39 Y															40 Zr	41 Nb	42 Mo	43 Tc	44 Ru	45 Rh	46 Pd	47 Ag	48 Cd	49 In	50 Sn	51 Sb	52 Te	53 I	54 Xe
4	18	19 K	20 Ca	21 Sc															22 Ti	23 V	24 Cr	25 Mn	26 Fe	27 Co	28 Ni	29 Cu	30 Zn	31 Ga	32 Ge	33 As	34 Se	35 Br	36 Kr
3	8	11 Na	12 Mg																									13 Al	14 Si	15 P	16 S	17 Cl	18 Ar
2	8	3 Li	Be																									5 B	6 C	7 N	8 O	9 F	10 Ne
1	2																												1 H				2 He

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A Compilation of Papers

by

Joel M Williams

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Preface

I received a formal education through the post-doctoral level in Chemistry, taught it, worked on a wide variety of projects and have written many papers (see vitae). For the first 35 years, I labored without questioning formal texts for a viable career. Interestingly, the literature flap about classical vs non-classical boron bonding was heavy during the early portion (1960s) of my career. In 1993, while working with supercritical fluids, however, it became obvious to me that the spherical model of the hydrogen atom was too simplistic to explain my observations. At that point, I suggested that the hydrogen atom must be little different than other atoms and that its bonding should likewise be little different. I retired from Los Alamos National Lab at that point and began, unbounded by peer-pressure, to look more deeply into the structure of atoms and their bonding to each other. Unable to get articles printed in mainstream publications (chemistry or physics), I posted articles in "arxiv" until "permission" to do so was required. I then self-published a book entitled "Challenging Science" in 2005 where I summarized my efforts to that date. The present book is a compilation of my mental efforts since then and is generated to preserve them for posterity. Doctors-of-Philosophy should think and not just pronounce and apply accepted doctrine.

It became increasingly clear to me that the early mathematical definitions of the electronic structure of atoms were not as clean and neat as literature text and teachings would have all to believe. Beyond the s- and p-orbitals, the collective groupings are a jumbled mess. The first and foremost is the assertion that orbitals are orthogonal, yet that orthogonality is readily violated with orbitals of even the same shell occupying common physical space. The declaration that two solutions for the d-orbitals were equivalent in order to reduce the mathematical treatment to the observed data was a slick ruse to "validate" the spdf orbital approach. Single sets for each of the spdf orbitals are still taught to the masses. As two f-orbital sets are now being voiced, it is clear that the classical spdf approach has stifled consideration of models that do not require that "things become different just as one approaches the atomic realm", that "solutions can be merged if the model does not quite fit", that "electrons can be paired without repelling one another", etc, etc.

The papers included herein cover a number of aspects of atoms: nuclei of the isotopes, electron orbitals, placements in the periodic table, chemical behavior, and bonding to others atoms. Since atoms are "countable", the mole and Avogadro's number are discussed. And, since atoms have mass, an alternate explanation of "gravity" is included. The papers are presented in reverse chronological order so that the reader is exposed to the most current thoughts first with earlier efforts available for further delving and background.

"We are like dwarfs sitting on the shoulders of giants. We see more, and things that are more distant, than they did, not because our sight is superior or because we are taller than they, but because they raise us up, and by their great stature add to ours."

- John of Salisbury in a treatise on logic called Metalogicon, written in Latin in 1159.*

"If I have seen a little further it is by standing on the shoulders of Giants."

- Isaac Newton to Robert Hooke in 1676.*

I, too, have had the good fortune to "stand on the shoulders of giants"!
With a broader vista, however, some things appear to be quite different than have been posited.

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* http://www.phrases.org.uk/meanings/268025.html

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CONTENTS

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Chapter XX

Nucleotopes and the Nuclei of the Elemental Isotopes
Nucleotopes — The Nuclei of the Isotopes

Abstract

Elements are characterized by the charge on the nuclear without regard for its arrangement. Isotopes of an element merely indicate that the nuclei have different masses, but the same outward charge. Isotopes are a chemical description based on that outward charge. The nuclear component interactions are largely independent of the exo-nuclear electrons that control the chemical interactions.

The current concept of the nuclei of isotopes is that they all have the same number of protons and only differ by the number of included neutrons. This paper proposes an alternate model for the nucleus: the nucleotope. This model of nuclei has the number of protons and neutrons not differing from one another by more than a single unit. The outward nuclear charge is determined by the number of included β^- *particles. The model is applied to the elements of the periodic table, particularly addressing tritium and why elements above lead are unstable α-particle emitters. All images were generated by the author.*

Introduction

"The nucleus of an atom consists of protons and neutrons (two types of baryons) bound by the nuclear force (also known as the residual strong force). These baryons are further composed of subatomic fundamental particles known as quarks[1] bound by the strong interaction. Which chemical element an atom represents is determined by the number of protons in the nucleus. Each proton carries a single positive charge, and the total electrical charge of the nucleus is spread fairly uniformly throughout its body."[2] This view is little different than it was a century ago, except for the quarks.

"While protons define the entire charge of a nucleus and, hence, its chemical identity, neutrons are electrically neutral, but contribute to the mass of a nucleus to the same extent. Neutrons explain the phenomenon of isotopes – varieties of a chemical element which differ in atomic mass."[2] The nucleus has minor influence on an element's chemistry beyond its charge and the orbitals of the electrons. Isotopes relate to chemistry; the character of the nuclei is a separate issue. In other words, the nuclei of an element's isotopes may have little in common with one another! Figure 1 provides a typical display of the elements (nuclear

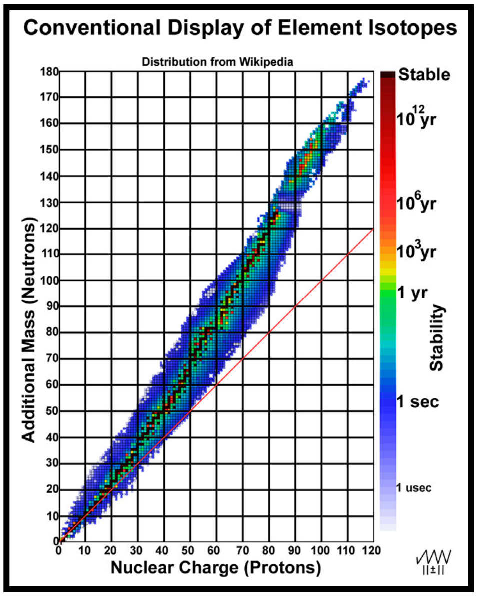

Figure 1. Conventional Display of Elemental Isotopes

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[1] Standard Model: (a) M. Gell-Mann, Phys. Let. **8,** 214 (1964); (b) G. Zweig, *An SU3 Model for Strong Interaction Symmetry and Its Breaking*, CERN Report No. TH 412 (Geneva, 1964); Quarks: Michael Riordan, *The Discovery of Quarks*, SLAC-PUB-5724, April 1992 (http://www.slac.stanford.edu/cgi-wrap/getdoc/slac-pub-5724.pdf)

[2] *Atomic nucleus*, http://en.wikipedia.org/wiki/Atomic_nucleus

charge/proton number/atomic number) with varying additional mass (neutrons) with each isotope color-coded[3] to indicate its individual stability.

Plotting the distribution of the elemental isotopes as a function of their masses gives a decidedly different perspective of how the nuclei of the isotopes relate to one another. In Figure 2, the data in Figure 1 is tipped 45-degrees so that nuclear mass is evenly spaced along the x-axis. The y-axis grid is set 2 units/line with the 20-unit line passing through mercury (at #80, mass = 200) for reasons that will be clear later.

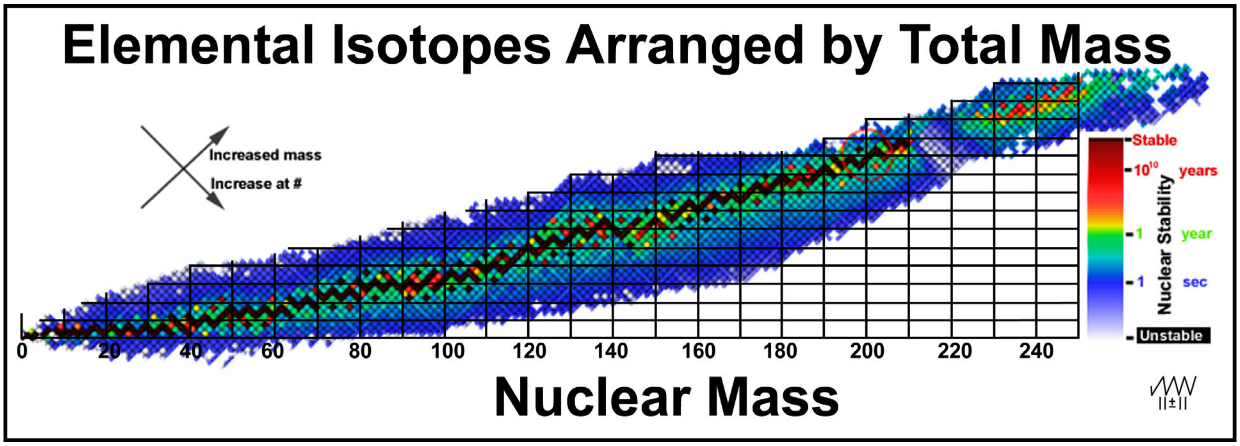

Figure 2. Elemental Isotopes Arranged by Total Mass

A number of general trends can be seen.

- The elements do not have a sharply defined, "valley of stability"[4]; instead there is a general "stability zone" indicated by the majority of black diamonds.
- A prevailing black zigzag pattern of threes: up2 [2 higher mass units at the same nuclear charge (atomic number)] and down2 [2 higher mass units in the form of 2 higher nuclear charges] for stable nuclei should be obvious.
- There are occasional up4s, 1 up7 (Sn; at#50, mass 114-120), with very few >down2 (which occur in upheaval regions).
- Persistent 2x2 stable outliers occur on either side of the prevailing up2/down2 pattern. These outliers are separated from the main pattern by unstable nuclei.

Before preceding to an explanation about the relationship of the nuclei of the different elements that have the same total mass, it is useful to explore the elements in the lowest mass region. The nuclei of the first eleven elements are illustrated in Figure 3. Beta-particle decays give vertical changes in elements without changing the nuclear mass: β^- downward (increased atomic number) and β^+ upward (decreased atomic number). Vertical changes should involve minor changes in the nucleus other than the beta-particle changes.

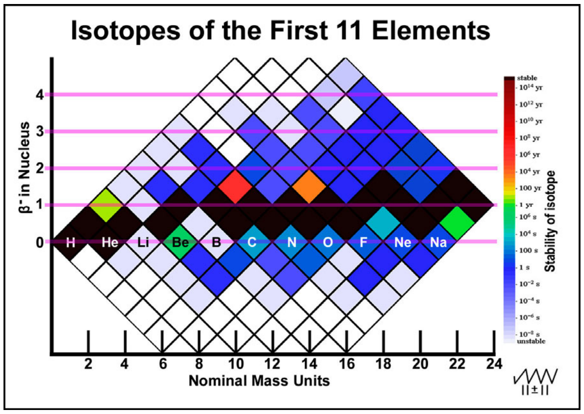

Figure 3. Isotopes of the First 11 Elements

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[3] Background image is from *Isotope half-lives*, http://en.wikipedia.org/wiki/Isotope

[4] Dave Jacque, *Gammasphere leads explorers along the rim of the valley of nuclear stability*, http://www.phy.anl.gov/gammasphere/pub/logos_98.html

The first few elements do not have many ways for their nuclei to be assembled and therefore have few stable nuclei. Below are a few observations. Decay data is from Wikipedia.[5]

- No stable elements occur for masses 5 and 8; both break the zigzag.
- Be-8 is unique as it neatly splits in half to an α-particle (nee He-4) and He-4.

- β^- decay occurs above the black stability zone
    - T-3 (green), Be-10 (red), C-14 (orange) and C-17 each β^- decay to the next higher atomic numbered element (straight down in the figure) with hardly a change in mass.

- Non-β decay
    - Li-4 and Li-5 release a proton to yield the corresponding He; this is a lower energy mechanism for these nuclei than the release of a β^+ particle through the dissociation of a bit of neutral material.
    - Be-7 exhibits EC (electron capture) and moves to Li-7 as it is deficient a β^- particle based on its nuclear charge (+4); here EC is a lower energy mechanism than β^+ particle or proton release. ^{18}Ar-37, ^{20}Ca-41, ^{22}Ti-44, ^{23}V-49, ^{24}Cr-51, ^{25}Mn-53, ^{26}Fe-55, ^{27}Co-57, ^{28}Ni-56, ^{31}Ga-67, ^{32}Ge-68, and ^{34}Se-72 also decay by EC; all are just below the stability zone.

- β^+ decay occurs below the stability zone. It is called β^+ decay, but is more appropriately called "β^- build with β^+ release". Either a β^+ is in the nucleus or more likely a neutral component of the nucleus separates into two oppositely charged beta-particles with the β^- particle being retained and the β^+ particle released with energy. This occurs vertically in the figure with hardly any change in mass and is often a lower energy mechanism than EC or proton release.
    - C-11 emits a β^+ to B-11; N-13 to C-13; O-15 to N-15; F-18 to O-18; and Na-22 to Ne-22.

The Nucleotope Model of the Nucleus

Without belaboring the issue, suffice it to say that the conversion of a neutron to a proton (down-quark converted to an up-quark) with the release of a β^- particle and a neutrino defies logic[6] when up and down quarks are considered basic, non-compounded, nuclear components. Similarly, the conversion of a proton to a neutron (up-quark converted to a down-quark) in the nucleus with the release of a β^+ particle also defies logic for the same reason. While Feynman diagrams[7] may describe such conversions, these quark conversions are, nonetheless, still illogical. A more logical model would have the β^- and β^+ particles derived from entities separate from the quarks which should remain unaltered.

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[5] *List of nuclides*, http://en.wikipedia.org/wiki/List_of_nuclides

[6] Joel M Williams, *ON QUARKS, NUCLEI and BORON-10 NEUTRON CAPTURE*, http://pages.swcp.com/~jmw-mcw/On Quarks, Nuclei and Boron-10 Neutron Capture.htm; also at http://vixra.org/abs/1308.0005 and http://gsjournal.net/Science-Journals/Essays/View/4998

[7] (a) *Feynman diagram: β− decay of a neutron into a proton*, http://www.physi.uni-heidelberg.de/Forschung/ANP/Perkeo/theorie.php
(b) *Feynman diagram: β+ decay of a proton into a neutron*, http://hyperphysics.phy-astr.gsu.edu/hbase/forces/funfor.html

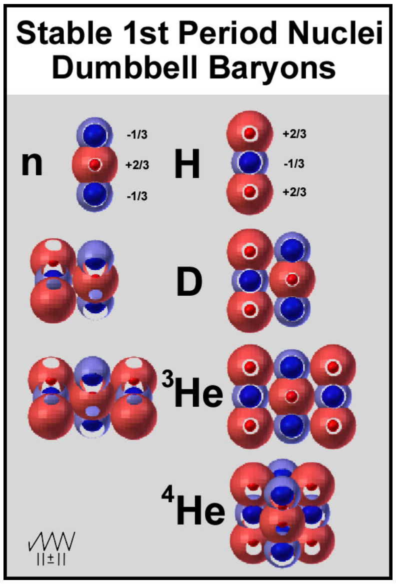

Figure 4. Stable First Period Nuclei

Dumbbell models of the baryons (proton and neutron) provide the essence of the two observed quarks. While some would decry these dumbbells as too simplistic, they do indicate strong, multiple, electrostatic interactions between the two types of baryons. These features are presented in Figure 4. That the nucleus of each element in Figure 4 is stable attests to the stability of the baryons. Equal or near equal numbers of the two baryon types provide maximum electrostatic interactions. It is logical that as the total number of baryons increases that the baryons do so in pairs to maintain their template interactions. This was the rationale for putting a "20" line in Figure 2 through the 200 mass isotope of Hg-80. The Hg-80/200 nucleus would be composed of equal numbers of protons and neutrons (100 each) and 20 β^- that set the outward charge of the nucleus to positive 80.

The y-axis of Figure 2 is now expanded in Figure 5 to show the effect of the included β^- particles on the isotope stabilities more clearly. A periodic table[8] is included for easy referencing to the elements.

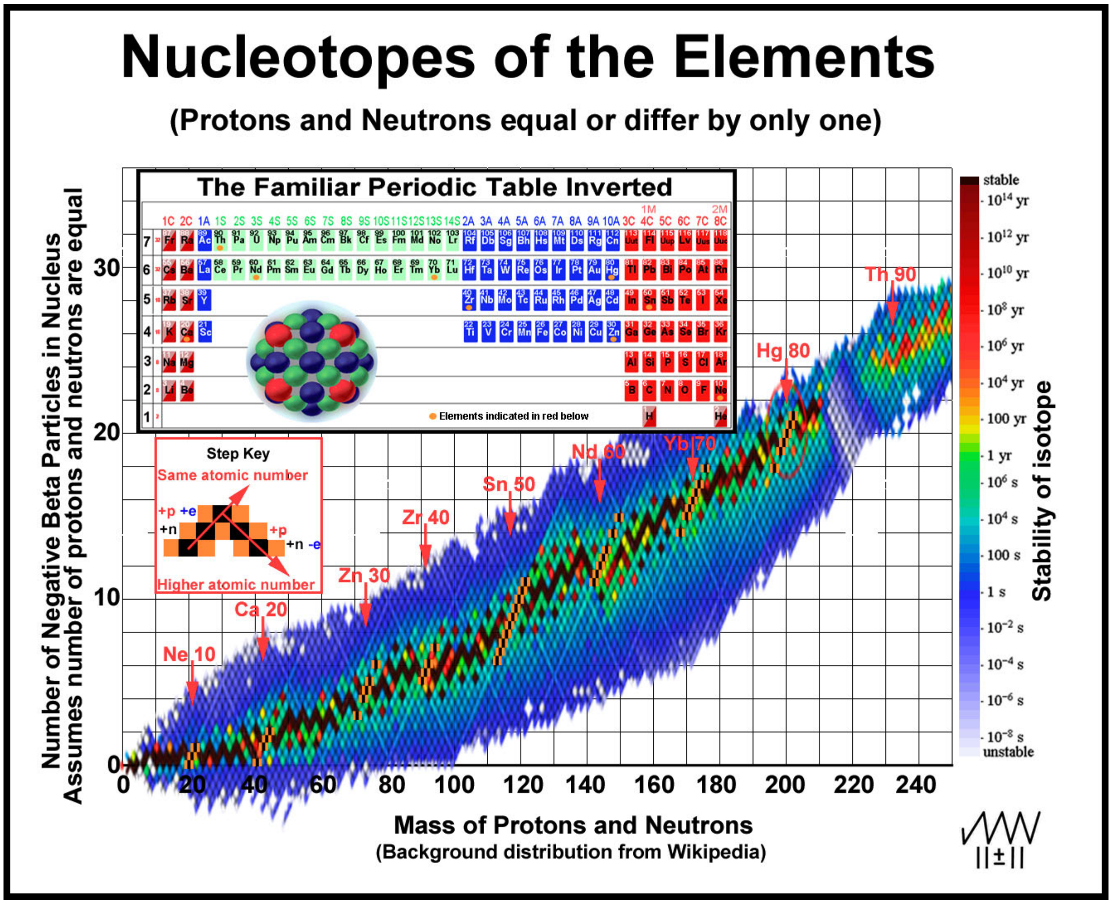

Figure 5. Nucleotopes of the Elements

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[8] Joel M Williams, Creating the Familiar Periodic Table via MCAS Electron Orbital Filling, http://pages.swcp.com/~jmw-mcw/The Familiar Periodic Table of Elements and Electron Orbital Filling.htm

Isotopes of an element "step" with alternating "neutral baryonic pairs": (a neutron) and (a proton with a separate β^- particle). Element to element changes of single mass units also "step", but do so with alternating "positive baryonic pairs": (a neutron minus a separate β^- particle) and (a proton). Vertical changes from one element to another occur without a mass change, but with a β^- particle release or addition. Horizontal changes from one element to another occur with a proton-neutron pair. Nuclear stability is related to the arrangement of the proton and neutron baryons with the added complication of accommodating the included β^- particles. Some elements, e.g., Sn-50, have many possible stable nucleotopes and thus many stable isotopes. Promethium-61, on the other hand, has NO stable nucleotope arrangements and, thus, no stable isotopes. Why is there a relatively narrow "stability zone" or "Valleys of Stability"? Because the protons and neutrons need to be equal or not more than one or two in either direction! The zone's location shifts from the straight-and-narrow to accommodate the included β^- particles. It is the β^- particles that keep the nuclei on an even keel as the mass increases through the "Valleys of Stability" (Figure 6). As the cargo (mass) increases, more crew (β^- particles) is needed. Sometimes the nuclear boat must navigate through some rocky stretches where the crew can find no stable arrangements.

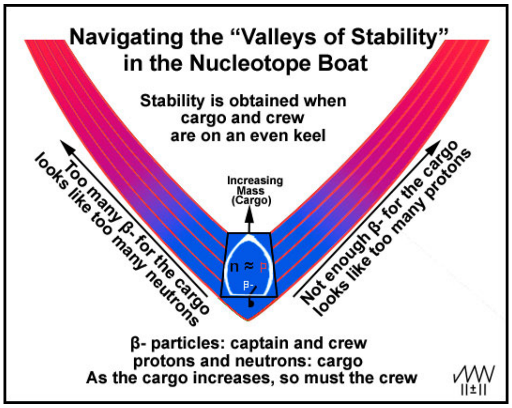

Figure 6. Navigating the "Valleys of Stability"

The hydrogen-helium isotopes provide a simple contrast between the nucleotope model and the current model with its over/under-loading of the nuclei with neutrons to produce the elemental isotopes. Dumbbell models of the stable nuclei of the +1 and +2 nuclei have been placed in the diamonds of Figure 7. The question is what model to put in the tritium diamond.

According to the step key of Figure 5, the tritium image should be the deuterium nucleus plus a proton plus a β^- particle which is just the He-3 nucleus plus a β^- particle! This, of course, is not the current model. The current and nucleotope models are shown at the bottom of Figure 7 for comparison. Both must liberate a β^- particle as this is what tritium does to yield helium-3. The current model requires that a down quark be converted to an up quark with the β^- particle being released in the process and that the baryons then reorder to produce maximum electrostatic interactions. Since most of the stable isotopes of the periodic table have many more neutrons than protons according to the current model, it is not clear why this model of tritium would have a propensity to decay at all.

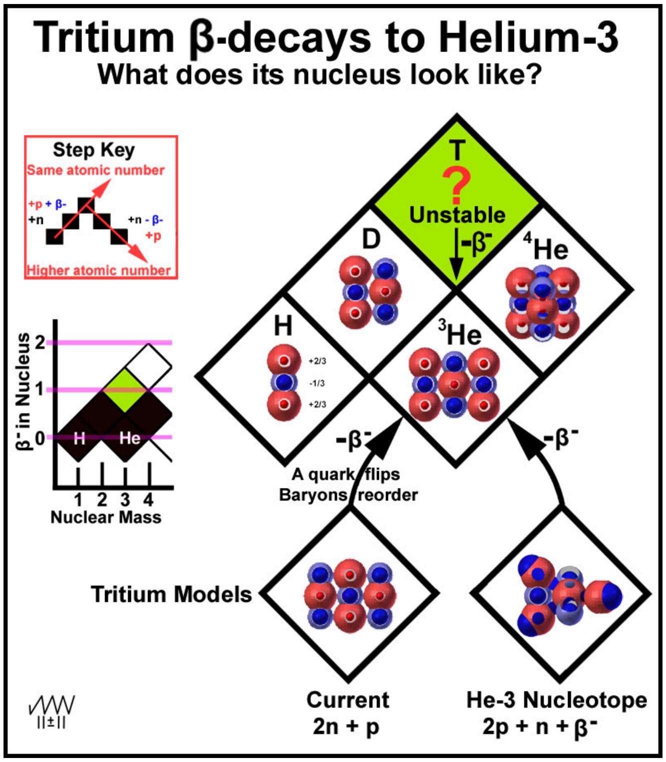

Figure 7. The +1/+2 Nuclei

In contrast, the He-3 nucleotope tritium nucleus simply releases an included β^- particle to yield the helium-3 nucleus. How is this β- particle incorporated in the tritium He-3 nucleus? It simply orbits, as indicated by the four blue orbital extremes in Figure 8, around the 5 +2/3 quarks in a manner similar to the tetrahedral movement of an external, nucleus-orbiting electron, ala the MCAS electron model.[9] What is the driving force for the decay of this nucleotope? The answer is the center neutron. This baryon has no single low energy position to provide ultimate stability. While the β^- particle moves in its orbital path, the neutron oscillates in its plane. At some point, the down quarks of the neutron (light blue spheres) will be positioned just right to force the β^- particle, as it move towards it outer limits, beyond its normal extreme and out of the nucleus. T-3 now decays to He-3 with nothing more than the β^- particle and subsequent binding energy being released.

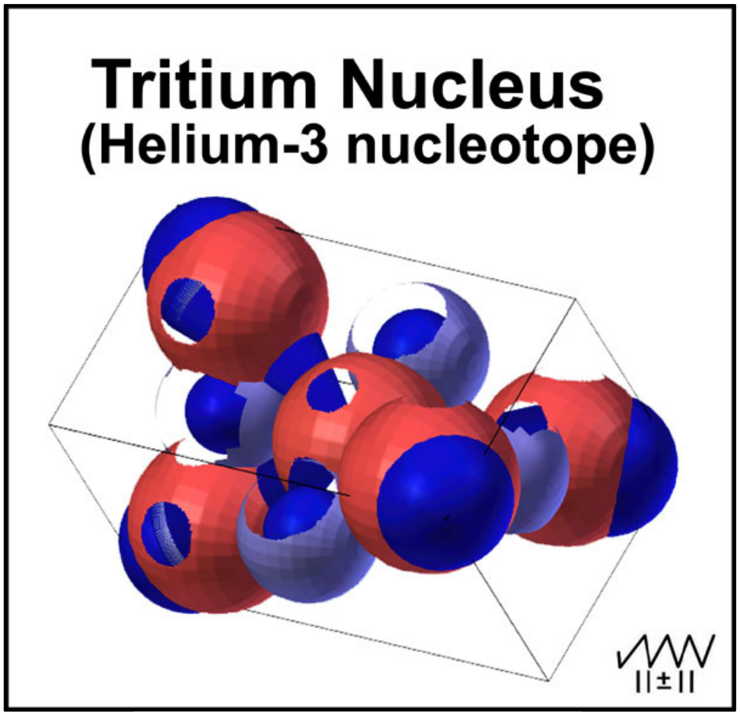

Figure 8. Tritium Nucleus (He-3 Nucleotope)

Analyzing the Binding Energy of Nuclei

What is binding energy, but mass that is no longer there and has become energy somewhere else? Binding energy is calculated by the following equation where the mass of the nucleus is independent of its constituents:

Binding Energy = ∑(mass of the unbound nuclear components) - the mass of the nucleus
E_{binding} = mass lost when the baryons shed some neutral matter to cozy up for more optimal electrostatic (pos-neg attractions and pos-pos & neg-neg repulsions) interactions

Binding energy per nuclear component using published data[10] has been calculated for a number of elements and plotted[11] in Figure 9.

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[9] Joel M Williams, *The MCAS Electronic Structure of Atoms*, http://gsjournal.net/Science-Journals/Essays/View/4019; discussed in *The spdf Electron Orbital Model Parsed*, http://gsjournal.net/Science-Journals/Essays/View/5032

[10] *Exact Masses and Isotopic Abundances*; http://www.sisweb.com/referenc/source/exactmaa.htm

[11] Similar plots for the conventional approach:
(a) *Nuclear binding energy*, http://en.wikipedia.org/wiki/Nuclear_binding_energy;
(b) Hendrik Schatz, *The Mass of a Nucleus*, http://www.nscl.msu.edu/~schatz/PHY983_13/Lectures/mass.pdf

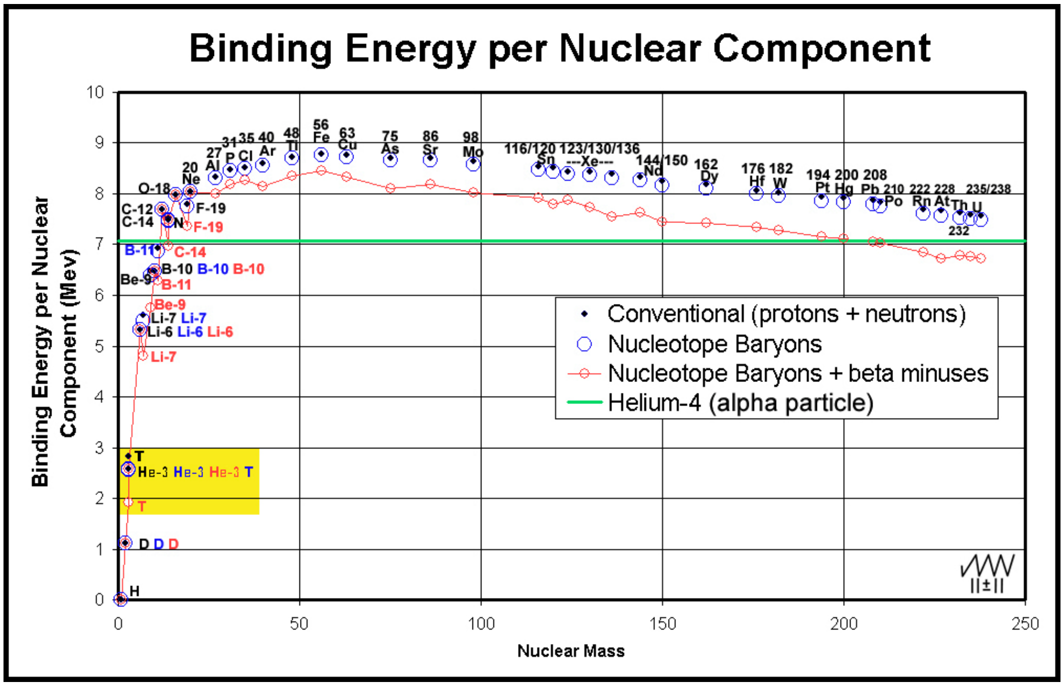

Figure 9. Nuclear Binding Energy per Nuclear Component

Attention is drawn to the trio of T and He-3 entries in the yellow rectangle in the lower left of Figure 9. The conventional determination of the binding energy (black dots) for tritium (T) and helium-3 (He-3) gives the binding energy per baryon of T greater than that of He-3. This is strange considering that T → He-3 + β^- + energy. The enigma, of course, lies in the choice of starting nucleons.

In the conventional model, the nucleus has only baryons: protons (charge/atomic number) and neutrons (additional mass).

T (1p+2n)$_{\text{conventional}}$ = 3.0246 amu; He-3 (2p+1n) = 3.0232 amu. Ending measured element masses less the valence electrons: T = 3.0155 amu; He-3 = 3.0149 amu; Δ = 0.0006 amu (the mass of a β^- + some energy).

- Binding energy/baryon: (T$_{\text{conventional}}$ = ~2.9mev) > (He-3 = ~2.6mev).

In the nucleotope model, a β^- particle is included and the number of each baryon is reversed with the result that the binding energy of T and He-3 are approximately the same per baryon — blue points in Figure 9.

T (2p+1n+1e)$_{\text{nucleotope}}$ = 3.0238 amu; He-3 (2p+1n) = 3.0232 amu. Ending measured element masses less the valence electrons: T = 3.0155 amu; He-3 = 3.0149 amu.

- Binding energy/baryon: (T$_{\text{nucleotope}}$ = ~2.6mev) ≈ (He-3 = ~2.6mev).

If, with the nucleotope model, however, binding energy is expressed per nucleon (2p +1n +1β^-), the value for T is less than that for He-3, as expected for T → He-3 + β^- + energy — red points in Figure 9.

- Binding energy/nucleon: (T$_{\text{nucleotope}}$ = ~1.9mev) < (He-3 = ~2.6mev).

Further examination of Figure 9 shows that, while the binding energy per nucleotope nucleon is less than that per baryon, significant "corrective" measures like that for tritium only occur for masses below 19 amu where a few β^- particles in a nucleus of baryons makes a large difference in the nucleon number. Maximal bonding occurs at Fe regardless of the methodology.

Why do Elements above Lead release α-Particles?

Unstable elements that occur above the "stability zone" and have atomic numbers less than 82 (lead, Pb) decay mainly by β^- release. Elements with atomic numbers greater than 82 decay by α-particle (He-4 nucleus) release. While the binding energy of nuclei decreases after a maximum at Fe, there seems to be little rationale for this behavior in the conventional, proton/neutron model. Inspection of Figure 9 indicates that the binding energy of these nuclei is well above that of the helium-4 nucleus (see the black dots versus the green α-particle line). When binding energy is determined per nucleon and the nucleotope model, however, the reason for α-particle release becomes clear. Lead (Pb-82) is the highest atomic number/mass element that is stable. It is also the last element whose nuclear binding energy/nucleon is greater than that of helium-4. Beyond Pb, the binding energy per nucleon dips below that of Helium-4 (the α-particle). Elements with atomic numbers greater than that of Pb are α-emitters as this more stable chunk of baryons breaks away from the more poorly bound nuclei. The process continues until the binding energy/nucleon of the nucleus is greater than that of the α-particle. This often occurs when the sum of the emitted α-particle chunks reduces the mass to Pb-82. That α-particle release by these elements occurs is not at all surprising with the nucleotope model.

Chapter XIX

Parsing spdf Orbital Hybridization and Simple Bonding

Abstract

The current spdf-QM electron orbital model is a forced one based on the precepts of a spherical starting point that requires that macro-physical laws no longer apply. For atoms to actually bond to one another, atomic orbitals have to be "hybridized". π-bonds formed by overlapped, unhybridized, p-orbitals may make sense mathematically, assuming spin-reversal electron pairing actually occurs, but the nebulous clouds hardly make sense from a 3D, real world, perspective with mobile, interacting electrons. This paper looks at the sp-QM orbital hybridization from a 3D perspective, carries that hybridization a step further, and offers an alternative.

Introduction

The current spdf-QM electron orbital model of atoms is a forced one based on the precept of a spherical starting point. Not only does the QM model require established macro-physical laws to cease near the nucleus area, but the basic set of orbitals that are generated in the model have no resemblance to those needed to model the materials of our substantive world. For atoms to actually bond to one another, the spdf-QM orbitals have had to be "hybridized". Initially, the hybridizing involved only the s and p-orbitals, but eventually essentially all of the orbitals had to be "hybridized" as metal complexes were modeled. This paper looks at the "hybridizing" of the s and p-orbitals. It should be noted that, despite the extensive "hybridizing" of all the other atomic orbitals, the spherical 1s-orbitals of hydrogen and helium have been off limits.[*13,14,15,16,17]

Before addressing the mechanics of "atomic orbital hybridization and atom bonding", it is appropriate to note that experimental data[18] demonstrates that electrons are observed as

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[*] A non-spherical starting point addresses hydrogen's position in the period table[13]; hydrogen's bonding with itself[14] and its bonding between two oxygen atoms[15] and between two boron atoms[16]; and helium's ortho/para phenomenon[17].

[13] Joel M Williams, *Creating the Familiar Periodic Table via MCAS Electron Orbital Filling,* http://pages.swcp.com/~jmw-mcw/The%20Familiar%20Periodic%20Table%20of%20Elements%20and%20Electron%20Orbital%20Filling.htm; *The Century-old spdf/nlms Quantum Model is Incorrect,* http://www.fqxi.org/data/essay-contest-files/Williams_spdf_is_the_Wrong.pdf

[14] Joel M Williams, *Comparing Several Orbital Approaches to the Hydrogen Molecule,* http://pages.swcp.com/~jmw-mcw/Orbital%20Models%20and%20the%20Hydrogen%20Molecule

[15] Joel M Williams, *Hydrogen Bonding and Orbital Models,* http://pages.swcp.com/~jmw-mcw/Hydrogen%20Bonding%20and%20Orbital%20Models.htm

[16] Joel M Williams, *Nixing the 3-Center Orbital Bond Concept of Diborane,* http://pages.swcp.com/~jmw-mcw/Nixing_the_3-center_Orbital_Bond_Concept_of_Diborane

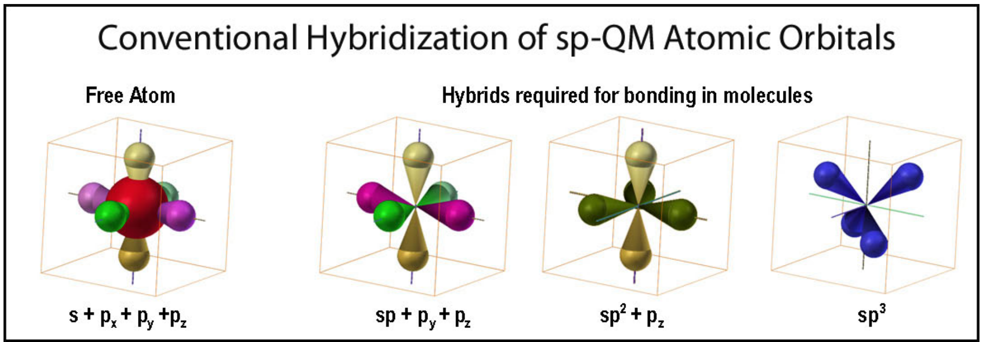
[17] Joel M Williams, *Electron Orbitals for Ortho and Para Helium,* http://pages.swcp.com/~jmw-mcw/electron%20orbitals%20for%20ortho%20and%20para%20helium.htm

[18] A. S. Stodolna1, A. Rouzée, F. Lépine, S. Cohen, F. Robicheaux, A. Gijsbertsen, J. H. Jungmann, C. Bordas, and M. J. J. Vrakking, *Hydrogen Atoms under Magnification: Direct Observation of the Nodal Structure of Stark States*, Phys. Rev. Lett. 110, 213001 (2013)

particles and do not exist everywhere at once[19]. Orbitals should be considered as defining where electrons occur around a nucleus and where atom-atom interactions can occur. A 'hard' orbital gives a sense of behavioral constancy and 3-dimensional direction of electron movement or static presence. It is this 3-D modeling that practitioners find useful in assembling atoms like tinker-toys into molecules.

While physicists were content with the "file-cabinet stacking" of spdf orbitals for their spectral data, chemists were unable to explain the geometry of real molecules with them. As G.N Lewis was pointing out in the early 1900s, simple real molecules followed a "rule-of-eight". Thus, methane (CH_4) had its 4 hydrogen atoms in a tetrahedral arrangement around a carbon center. The orthogonal projection of the p-orbitals and the spherical s-orbital did not yield the correct structure even for this simplest of molecules. The octet rule imagery, on the other hand, gave good indications of molecular form. Elementary level, "tinker toy", ball-and-stick models still provide the best simple, "hands-on", understanding of atomic interactions, in my estimation, with a caveat about just what those stick single and spring "double and triple" bonds actually are. The equivalent 2-D paper representations are also quite useful to the chemist who is interested, for example, in replacing "the multiple bond" between two atoms with bonds to each of them by two other atoms.

In the early efforts of molecular modeling, it was accepted that the spdf-QM model was correct for individual atoms. If molecules needed different ones, then so be it. The logical approach was to determine what orbitals "were needed" for real molecules and to "hybridize" (mix, whirl, blend, whatever) the atomic ones to give these "needed" ones. The simplest cases to be addressed by "atomic orbital hybridization" were linear, trigonal, and tetrahedral arrangements of atoms. To this end, the s and p orbitals were combined in three ways: s+1p (sp), s+2p's (sp^2), and s+3p's (sp^3). In the current spdf-hybridization, the s-orbital combines with the p-orbitals to produce a major plus (+) lobe and a tiny negative (-) lobe. Presumably as an orbital, the s-orbital is synchronous +/-! [As noted above, an s-orbital is not "hybridized" to complimentary tetrahedral orbitals (t^+ and t^-).] Thus, a s-orbital combining with a p-orbital should have 4 equal lobes (2+ and 2-). Eight (8) lobes are maintained in the various hybrids. In the sp^1-hybrid, the "negative lobes" coincide with the positive lobes in linear fashion and are ignored. For the sp^2 and sp^3 hybrids, the complementary lobes are also simply ignored or shown as tiny insignificant appendages. The sp, sp^2, and sp^3 hybrid sets are shown in the figure on the right.



The cubic outlines are all the same size to emphasize what is occurring during "hybridization". A bit of color mixing is used to further the imagery. All of the images are based on the spdf-QM assumption that a single electron or spin-mated pair of electrons will occupy an orbital. The transformation of the s and p orbitals to these hybrids is quite straightforward with the assumption that the original atomic model is correct.

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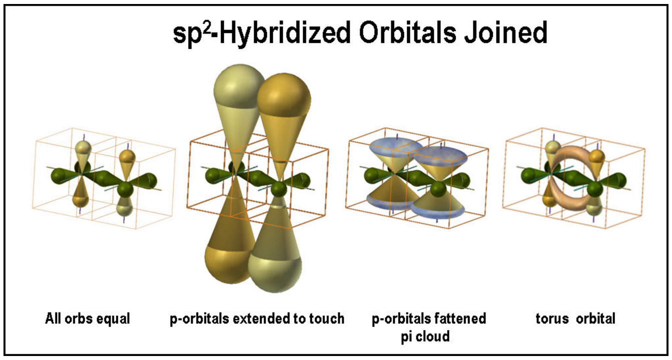
[19] Joel M Williams, *Nixing the 'Balloons-of-Electron-Dots' Atomic Orbital Models*, http://pages.swcp.com/~jmw-mcw/Nixing%20the%20'Balloons-of-Electron-Dots'%20Atomic%20Orbital%20Models.htm

Parsing the sp-QM Hybridization and Bonding Concept

In current methodology, “molecular orbitals” are formed from overlapped hybrid atomic orbitals that have the same electron occupancy assumptions as the hybrid atomic orbitals do. An in-axis molecular orbital is straightforward for each of the atomic hybrids assuming that the vernacular of the QM mated-pair of electrons is correct. It is a bit of a problem accepting that a pair of electrons just mill around in the confined space between the nuclei, however. One of the attributes of mathematical treatments of bonding (and the focus of the MO approach, for that matter) is that one does not actually need to know how things work, only that they do.[20]

Maximum bonding should occur when the orbitals of two atoms from a linear molecular orbital (bond) between the two atoms. While it is traditional to present sp^3–sp^3 bonding first, sp^2-sp^2 bonding is discussed here first. The figure at the right allows in-axis (on a line from nucleus to nucleus) and off-axis interactions to be seen.



The in-axis orbital overlap [called a sigma (σ) bond] indicated in the first image is easily grasped. It is the orbital occupancy of spin-paired electrons that is more difficult.

Overlap of the p-orbitals is more difficult to comprehend as they are parallel to one another. Convention teaches that these adjacent, parallel, “unhybridized”, p-orbitals form a strong π-bond. Taught and accepted; believable and correct? The second image in the figure shows greatly extended p-orbitals to effect “touching” and the extreme bending angle of the bond. The third image shows flattened p-orbitals with the touching portions forming “π-clouds”. Just how these “clouds” of electrons hold the nuclei together is a bit dicey.

According to the spdf-QM model *an electron has an equal probability of being in each lobe of an orbital* (hybridized or not); how they do that is another matter. In other words, particulate electrons “flow” through the lobes of an orbital “freely” to populate them equally. With this in mind, the atoms are shown linked as a torus in the fourth image of the joined “sp^2 hybridized orbitals”. (The p-orbitals are left to indicate what needs to happen.) Obviously there needs to be much bending of the p-orbitals to accomplish this. What this indicates is that the bond is NOT between two parallel “8”-shaped orbitals, but rather between two “<”-shaped orbitals, or, more likely, one side of an X-shaped orbital. What is a bent p-orbital, but a “self-hybrid” orbital? More later.

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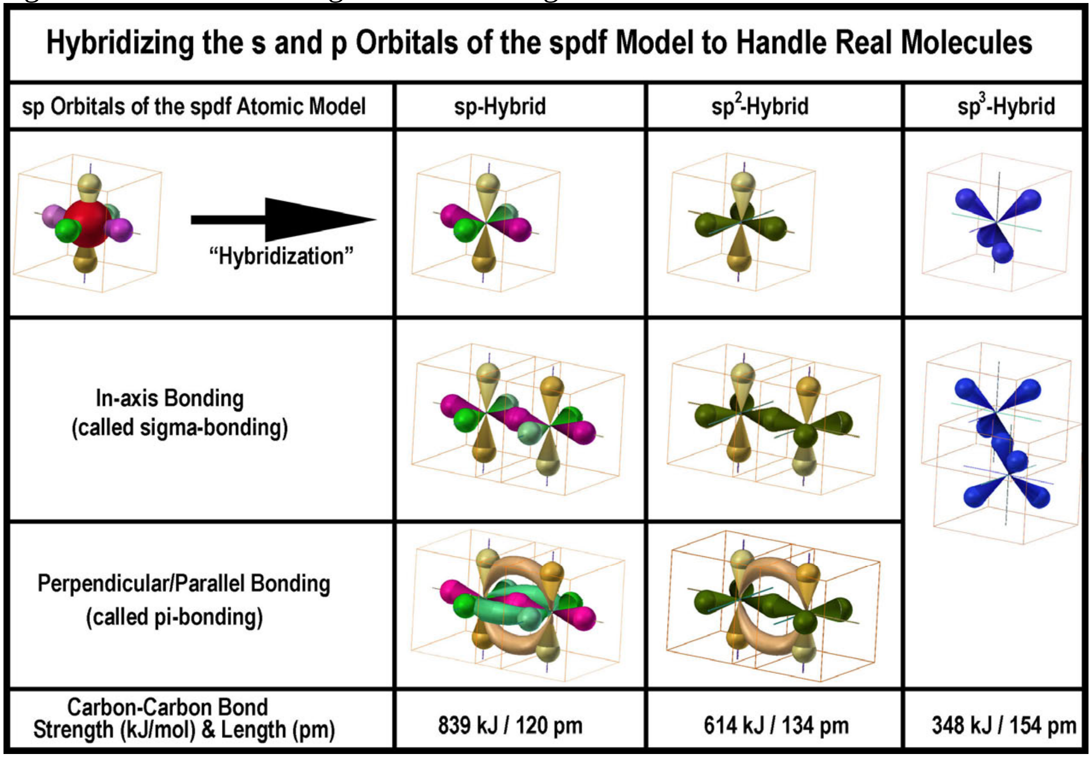
[20] Bertrand Russell, “*Physics is mathematical not because we know so much about the physical world, but because we know so little”; in* Eugene Wigner, *The Unreasonable Effectiveness of Mathematics in the Natural Sciences*, Communications on Pure and Applied Mathematics 13: 1–14 (1960); http://en.wikipedia.org/wiki/The_Unreasonable_Effectiveness_of_Mathematics_in_the_Natural_Sciences#cite_note-1

The interaction of two atoms with three different degrees of sp^x-hybridization is shown in the next figure without considering electron loading or other atoms attached.

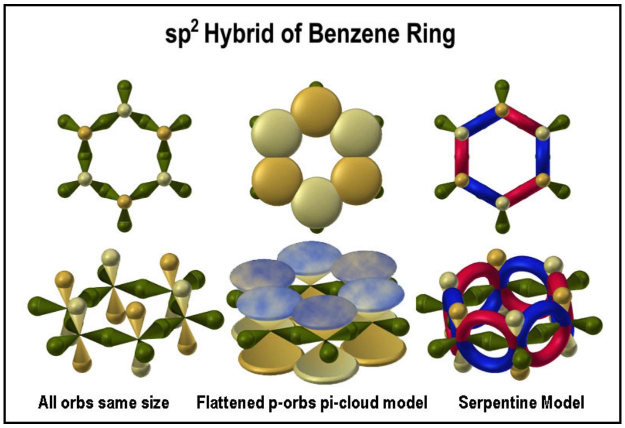


Hybridizing the s and p Orbitals of the spdf Model to Handle Real Molecules

sp Orbitals of the spdf Atomic Model	sp-Hybrid	sp^2-Hybrid	sp^3-Hybrid
"Hybridization"			
In-axis Bonding (called sigma-bonding)			
Perpendicular/Parallel Bonding (called pi-bonding)			
Carbon-Carbon Bond Strength (kJ/mol) & Length (pm)	839 kJ / 120 pm	614 kJ / 134 pm	348 kJ / 154 pm

Bent bonds are energetically higher in energy and thus less stable. That highly "bent bonds" can provide the large incremental bonding strengths[21] indicated in the bottom of the above figure seems improbable.

The "π-cloud" alluded to for p-p orbital bonding is a key feature in describing benzene and other aromatic compounds. The σ-bond network is shown in the left images of the figure on the right. The flattened p-orbitals and π-cloud are shown in the next images. While the p-orbital overlap issue was pointed out for a simple double bond, the interlaced π-cloud presents a number of other issues: how do particulate electrons flows round an atom, between atoms and through the "cloud"? The traffic flow issue is easily handled by mirrored serpentine orbitals as seen in the last image in the figure. This provides electron density above and below the 6-carbon plane. The above and below plane atomic orbitals of the serpentine molecular orbitals are clearly not vertical "8"-shaped ones, but rather crossed orbitals; in other words, they form an X. While 3D orbital models provide pleasant imagery, many chemists find simple Kekulé-type images[22] provide an easier understanding of how and why olefins and aromatic compounds behave the way they do chemically[23].



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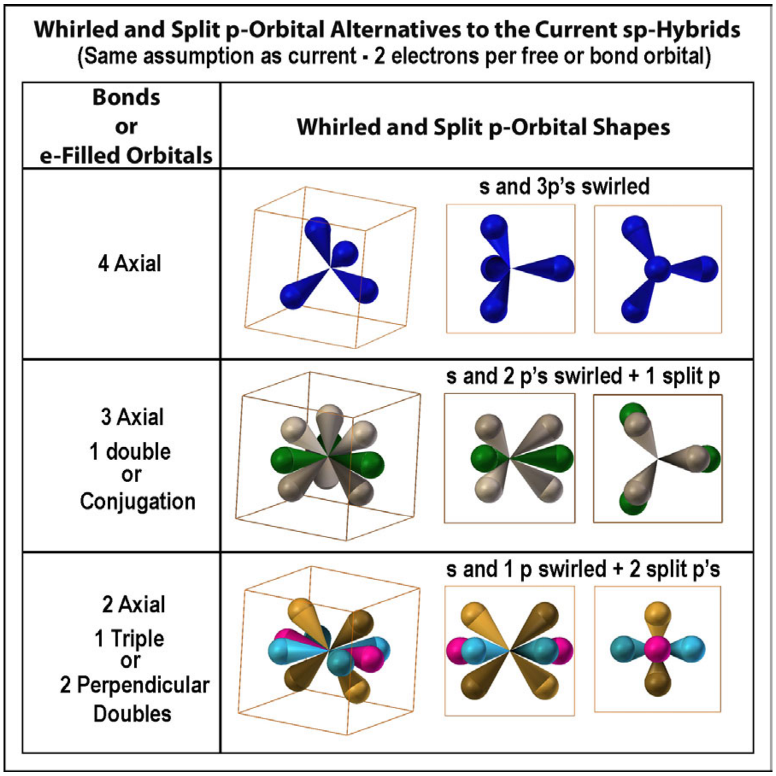
[21] C Chieh, *Bond Lengths and Energies*, http://www.science.uwaterloo.ca/~cchieh/cact/c120/bondel.html

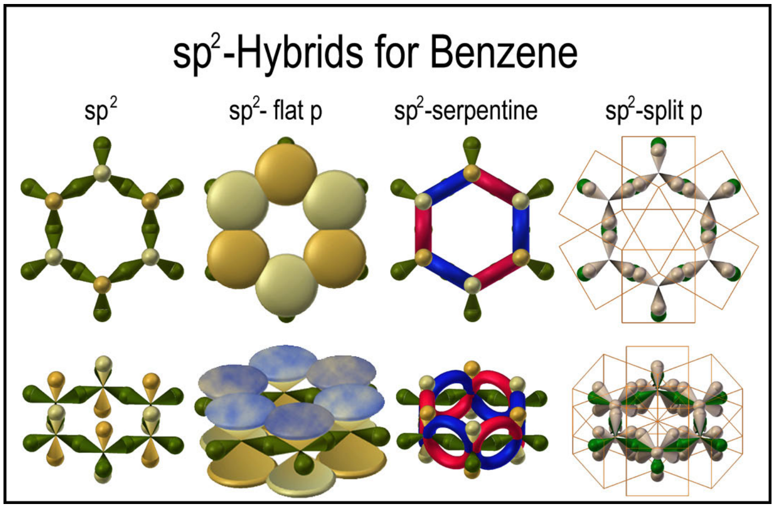
[22] *Kekulé structure for benzene*, http://www.chemguide.co.uk/basicorg/bonding/benzene1.html; *Organic Chemistry/Aromatics*, http://en.wikibooks.org/wiki/Organic_Chemistry/Aromatics

[23] For example, *Alkene*, http://en.wikipedia.org/wiki/Alkene

Carrying Orbital Hybridization a Step Further



Pre-computer mathematical modeling was mostly xyz-coordinate driven. The first emphasis was on linear, then planar, and finally 3-D. With the need for directionally oriented orbitals, the simplest hybridizing of the orbitals evolved. The tetrahedral sp^3 could handle many connection issues and even some non-tetrahedral ones like ethylene, allene, carbon dioxide. Planar, non-linear connections, like those needed for carbonate ions and aromatic molecules were the problem. So, p's were whirled with the s. Why stop with whirled p's? Why not "split p's"? If entirely different atomic orbital sets can be chosen (and, yes, there are several!)[24] and orbitals can be merged and split into differing sets, then it hardly seems a problem to just split an orbital without merging it. The figure at the right shows "whirled and split p-orbital" alternatives to the current sp, sp^2, and sp^3 hybrids. These alternatives provide significant orbital overlap where perpendicular p's do not.



The benzene carbon network modeled with the sp^2-split-p orbital hybrid is now added to the other models in the figure on the right. The π-bonds are not fully overlapped here in order not to conceal the σ-bonds below. The sigma bond is now surrounded by two orbital lobes with time averaged <1 electron. Compare this with a sp^3 sigma bond where its end of the bond would have three orbitals with an electron each. The p-NMR response of attached hydrogen atoms would be different because of the difference in shielding and, indeed, such is observed.

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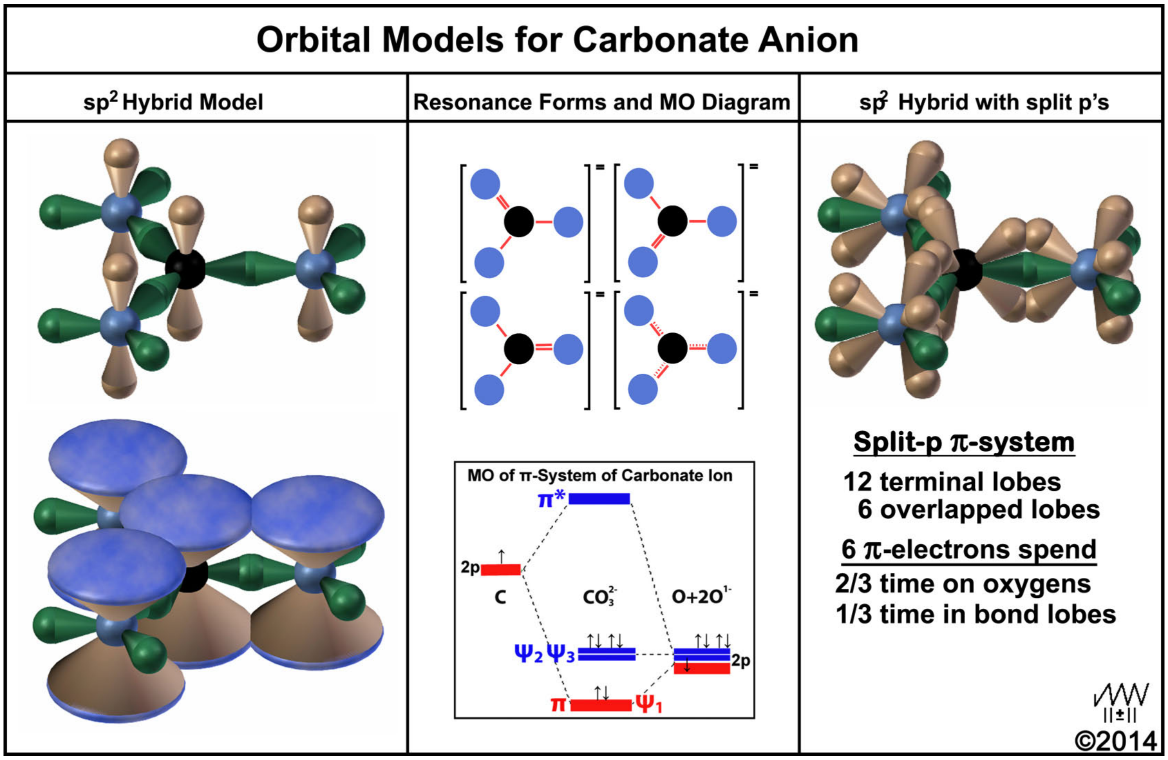
[24] Joel M Williams, *Parsing the spdf Electron Orbital Model*, http://pages.swcp.com/~jmw-mcw/Parsing%20the%20spdf%20electron%20orbital%20model.htm

Consider now the carbonate anion. sp^2 hybrid models, resonance forms, a MO diagram of the π-system, and a sp^2-split-p model are shown in the figure below.



The upper left image is the typical sp^2-p model without p-p bridging. The lower left shows the π-in-the-sky cloud representation. How the 6-electrons of the p-orbitals move around in this cloud is very vague. The upper middle images show the venerable resonance forms that indicate that these 6-electrons move back-and-forth from carbon to oxygen. Actually, there should be a fourth form shown in which there is no π-bond (net positive carbon and three negative oxygen atoms). The dotted line form is intended to summarize the three other forms. The MO image[25] in the lower middle conveys what one of the three "double-bond resonance forms" indicates. This is used to indicate that the C-O bonds are 1/3rd order with respect of the π-bonds. Of course, one would expect all 6-electrons to be equal. So three of these MO forms would be needed, too.

The image on the right of the figure illustrates the situation when the p-orbitals are split-p's. Electrons are assumed to flow from atom to atom through the connected orbital lobes. Click here for a shockwave file by the author of a particle moving in an elliptical orbit. As indicated in the figure, each electron will spend 1/3rd of its time in the overlapped orbital lobes (bonds) and 2/3rd of its time in the terminal lobes of the oxygen atoms. Since there are 6-electrons, 2 will, on average, be in overlapped orbitals at any given time. Since the electrons are "paired" they must be so by reciprocal motion; a tenet of the MCAS model.

Of course, the question is whether an atom "hybridizes". The answer is that the spdf-QM model leaves no other choice. By requiring electrons to be spin-paired, the model restricted the number of orbitals to half the number of total possible orbitals. This, in turn, greatly restricted the number of bonding options.

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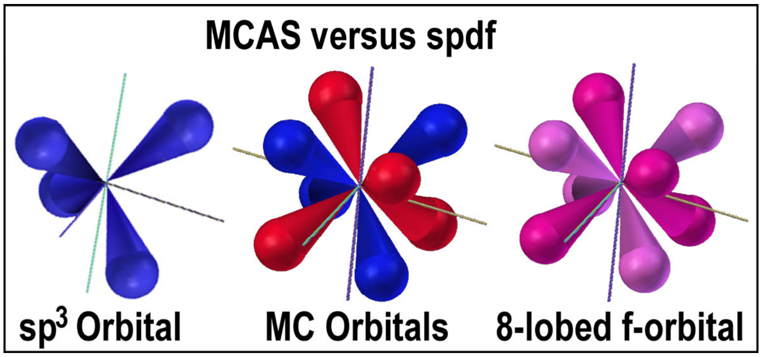
[25] Lower Moreland Township School District text, www.lmtsd.org/cms/lib/PA01000427/Centricity/Domain/219/Ch2-MO-Theory.pdf

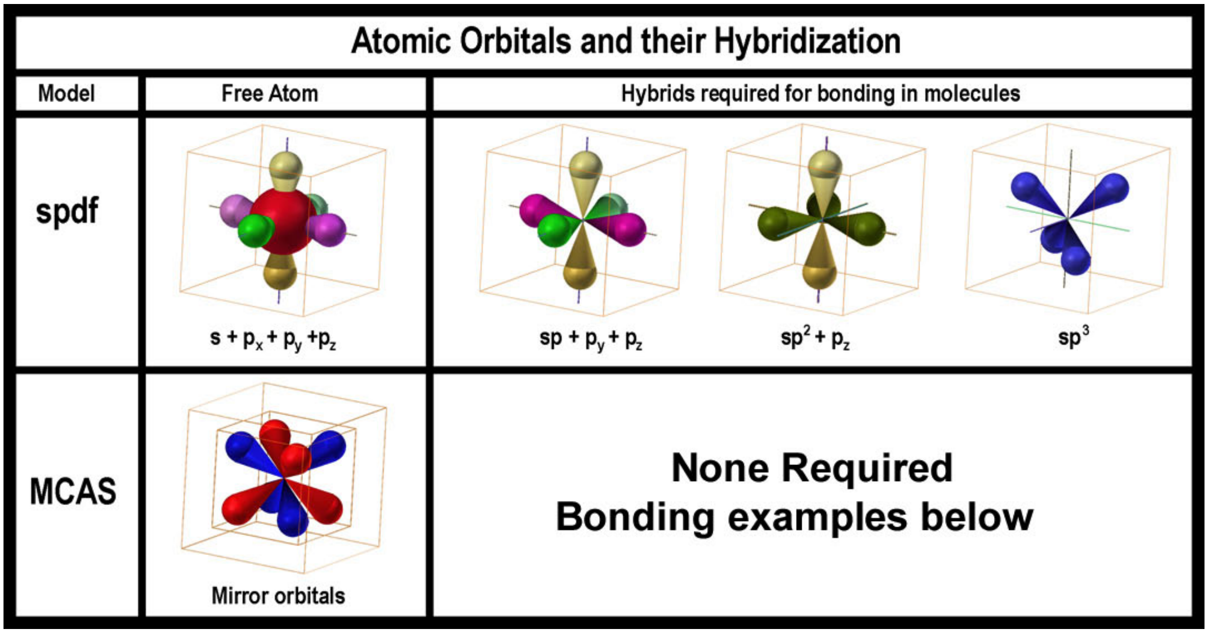
Consider a Different Approach



Consider the MCAS atomic model which does not require ‘hybridization” as it is already in the needed form. The MCAS model also has the needed “mirrored” orbitals that negate the need for spin-reversed pairing of electrons in the same orbital and provides the mechanism for electron flow in aromatic compounds. It also provides twice the number of orbitals that can be used for bonding; thus, it provides options not possible with the sp^x-hybrids.

Note the similarity of the sp^3-QM orbital and a MC orbital of the MCAS model. spdf-QM has provided the precedence for the MC orbitals in its 8-lobed f-orbital. The difference is that the two 4-lobed, tetrahedral MC orbitals are separate with an electron able to move within a tetrahedral group. Up to 4 electrons can be accommodated as the tetrahedral unit has 4-lobes. The f-orbital has a +/- tetrahedral pair also, but only one or two electrons are deemed able to occupy ALL of the lobes equally. How they do so is not clear. Unlike the MC orbitals, the 8-lobed f-orbital is not allowed to contain more than 2 electrons and those two are said to be spin-paired.

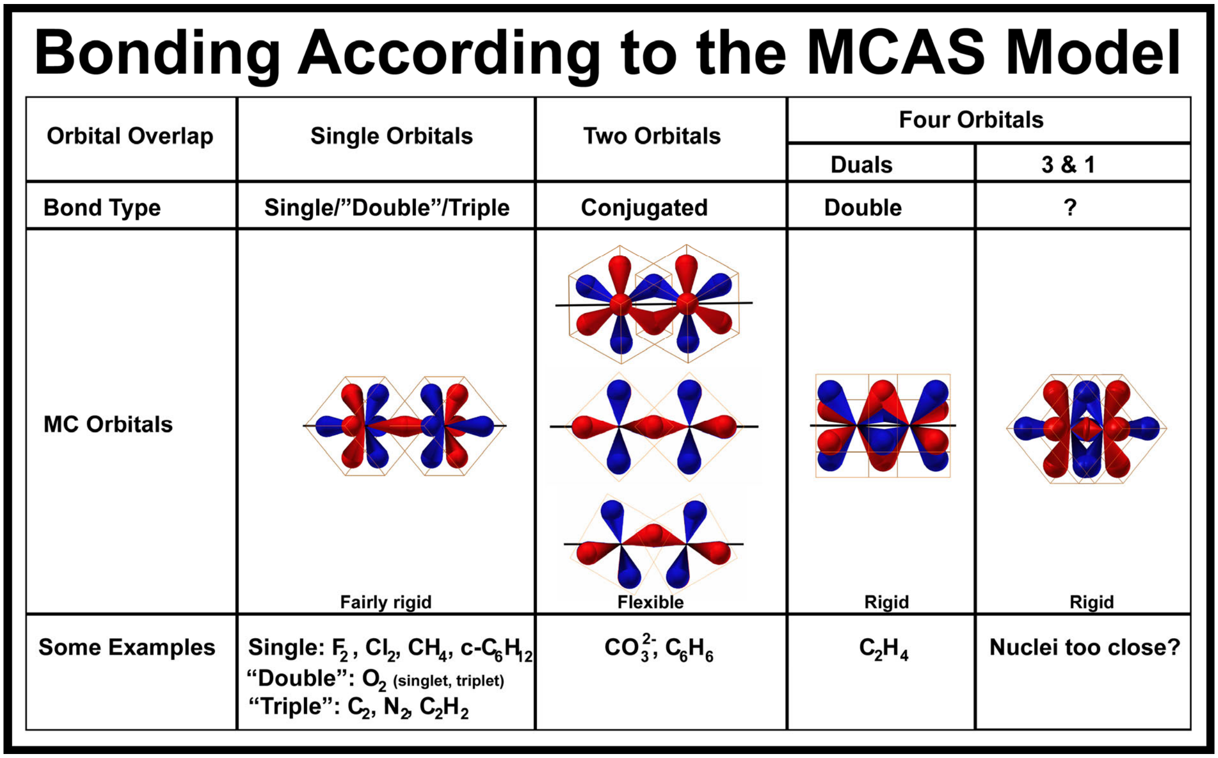
The MC orbitals provide a simpler set of orbitals compared to those of the hybridized sp-QM orbitals. There is no need to have two electrons occupy the same orbital via spin-reversal of an electron. There is also no need for hybridization of the MC orbitals and certainly not for simple molecules! Two summary figures are presented below.



Atomic Orbitals and their Hybridization

Model	Free Atom	Hybrids required for bonding in molecules		
spdf	$s + p_x + p_y + p_z$	$sp + p_y + p_z$	$sp^2 + p_z$	sp^3
MCAS	Mirror orbitals	None Required Bonding examples below		

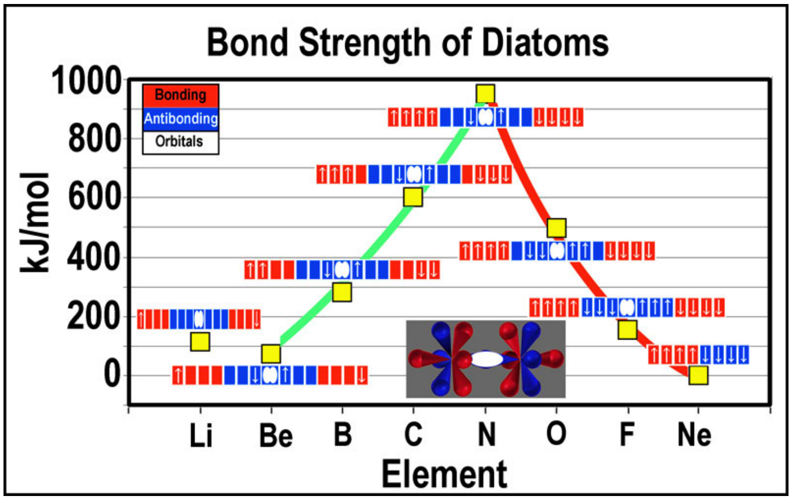
The ways in which the mirrored tetrahedral pairs can overlap between two atoms is easily comprehended. It is their electron-filling and connection to other atoms that requires more attention. The internuclear distance of the overlap modes decreases from left to right in the figure below. Briefly, the "single", "two", and "four" overlapped orbitals relate to the single, conjugated, and isolate double bonds that are typically taught.



Bonding According to the MCAS Model

Orbital Overlap	Single Orbitals	Two Orbitals	Four Orbitals	
			Duals	3 & 1
Bond Type	**Single/"Double"/Triple**	**Conjugated**	**Double**	**?**
MC Orbitals	Fairly rigid	Flexible	Rigid	Rigid
Some Examples	Single: F_2, Cl_2, CH_4, c-C_6H_{12} "Double": O_2 (singlet, triplet) "Triple": C_2, N_2, C_2H_2	CO_3^{2-}; C_6H_6	C_2H_4	Nuclei too close?

As indicated in "Some Examples", the single orbital overlap can cover more than common single bonds. Indeed, the diatomic molecules of the second row of the periodic table are properly described by the single orbital overlap model — the strengths of the bonds (single, double, triple) are just related to the amount of anti-bonding electrons (those in blue orbitals in the figure on the right; those orbitals, incidentally, are part of the tetrahedral orbital unit that forms the overlap bond!). The singlet/triplet oxygen duality is caused by different distributions of the electrons in the bonding and antibonding orbitals. A discussion of these phenomena can be found in *Understanding the Bonding of Second Period Diatomic Molecules*[26]. The image is hyperlinked to the article.



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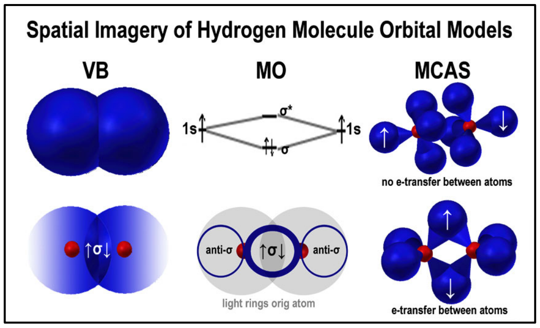
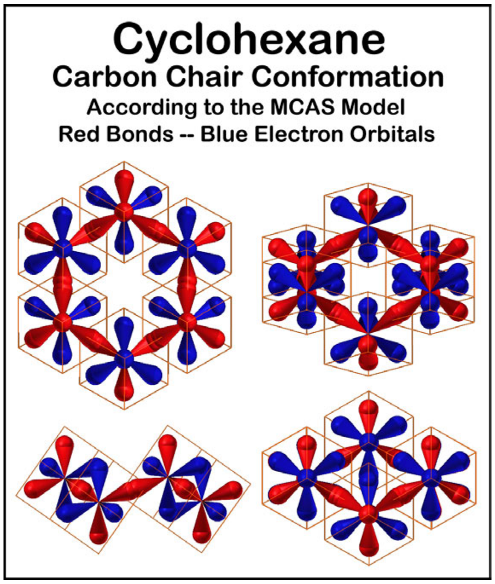
[26] Joel M Williams, *Understanding the Bonding of Second Period Diatomic Molecules*, http://pages.swcp.com/~jmw-mcw/understanding%20the%20bonding%20of%20second%20period%20diatoms.htm

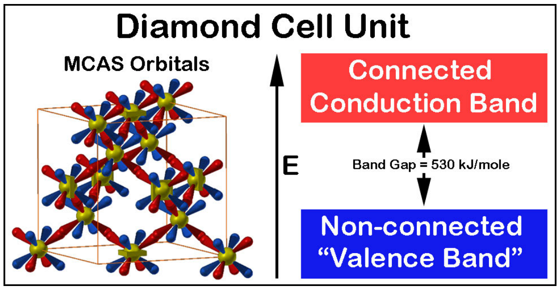
Application of the MCAS model to the hydrogen molecule can be found in *Comparing Several Orbital Approaches to the Hydrogen Molecule.*[14] The image on the right is hyperlinked to the article. Only one of the tetrahedral orbital units of each hydrogen atom is shown in the figure.



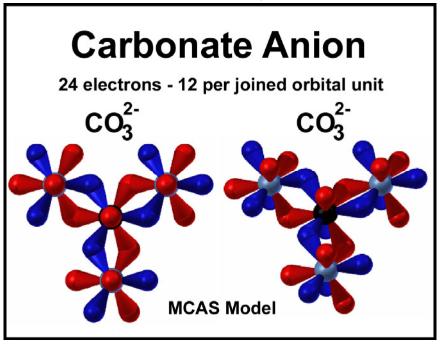
Several more examples are now presented for the MCAS approach.

- The carbon structure of cyclohexane in its chair conformation is shown on the right. The four electrons of each carbon are unshared and in the blue orbitals. Bonding between carbon atoms and to other atoms, such as hydrogen, is through the red orbitals. Electrons in the three blue orbitals surrounding each bond provide the electrostatic attraction with the nucleus on the other end of the bond that gives the bond its strength. 60° staggering and eclipsing energies are related to the electrostatic interactions of the 6 blue orbitals around a bond as rotation around the bond occurs. Rotation about a C—C bond is limited to flexing in cyclohexane, but occurs "freely" in molecules like ethane and butane.





The reader might find it interesting that crystalline carbon is simply repetitive C_6 carbon chair units in 3D.[27] The crystal bond network (red in the figure on the right that is hyperlinked to the article) of pure carbon has no electrons in it. This is the conduction band! The band gap is the energy required to move an electron from an atom's "non-sharing", tetrahedral orbital unit to its overlapped orbital, sharing network. Extremely tiny amounts (<1 per 10,000 cell units!) of interstice-doping with electron or hole providing atoms allows it and silicon to be semiconductors.



- The MCAS orbital structure for the carbonate anion is shown on the right. Note the reciprocal configuration of the red and blue orbital units. There are 26 orbitals (6 bonds and 20 terminals). Start with 6 electrons in each of the oxygen terminal orbitals and 6 in the

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[27] Joel M Williams, *Crystalline Carbon and Silicon - Covalent or Ionic?*, http://pages.swcp.com/~jmw-mcw/Crystalline_carbon_and_silicon-Covalent_or_Ionic.htm

overlapped orbitals; this is the fourth resonance form described above where there is a net -1 around each of the oxygen atoms and a net +1 around the central carbon atom (assigning half a bond electron to each of the atoms that forms the bond. Electrons flow through each joined orbital unit (red and blue) reciprocally to give the average of all the other resonance forms and to provide "pairing".

As noted in the beginning, the MCAS model starts with a different base orbital: a tetrahedral one instead of a spherical one. In doing so, it handles many of the current ambiguous orbital issues, such as hydrogen's position in the period table[13], hydrogen's bonding with itself[14], and its bonding between two oxygen atoms[15] and between two boron atoms[16], and helium's ortho/para phenomenon[17], without the need to "hybridize"!

Chapter XVIII

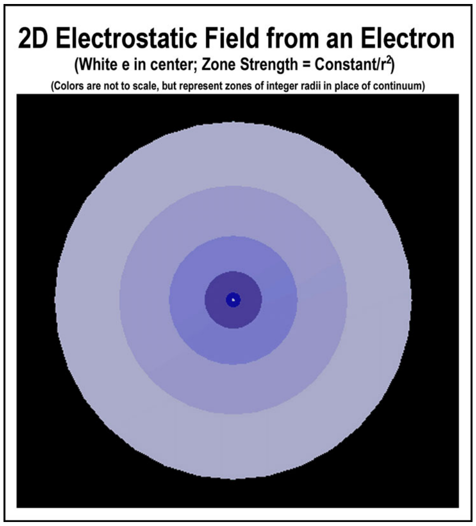
Are Electron Orbitals Fleshy, Hollow Pods

Abstract

It is one thing to draw lobes for electrons with the understanding that one does not know what is going on inside those lobes. It is something entirely different to indicate that those lobes are filled with clouds or bits of electron presence! The wave approach to indicate an electron's path is quite appropriate, however. Electron movement is well defined per the precise spectral data generated. Movement of electrons to and fro within and between atoms will be on well-defined pathways with their electrostatic fields moving with them. The movement of an electrostatic field is illustrated as its associated particle moves along an elliptical path.

If a ray of sunlight hits the retina of your eye, can the sun itself exist in your eye? In other words, what is the probability that the sun is actually in your eye? Is this probability really finite? In the vernacular of quantum probability, the answer would be yes! Where is the flaw in this logic?

Consider the same situation with an electron. If a tiny bit of negative field is detected, does it mean that an electron has a finite probability of being there or ever has been there in the context of the matter studied? If an electron were held in-place (physics thought experiment), it would have a surrounding field whose strength would be inversely related to the distance from the electron squared (r^2); see the figure at the right. Would anyone deem that the electron is anywhere in these zones and even beyond as depicted in a dot representation like that just to the right? The sharpness and constancy of observed spectral lines when electrons move from one energy level to another would be most unlikely from such randomness to other such randomness. But, this is the reasoning of QM atomic probability modeling. Fortunately, experimental evidence[28] is demonstrating that electrons are particulate at the nucleus level and have orderly behavior in orbitals.



2D Electrostatic Field from an Electron

(White e in center; Zone Strength = Constant/r^2)

(Colors are not to scale, but represent zones of integer radii in place of continuum)

Consequently, random dot representations of electrons in atomic and molecular orbitals need to be put aside.[29]

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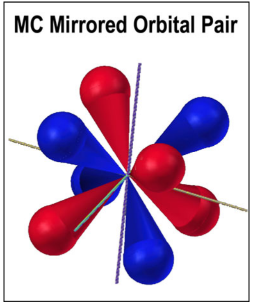
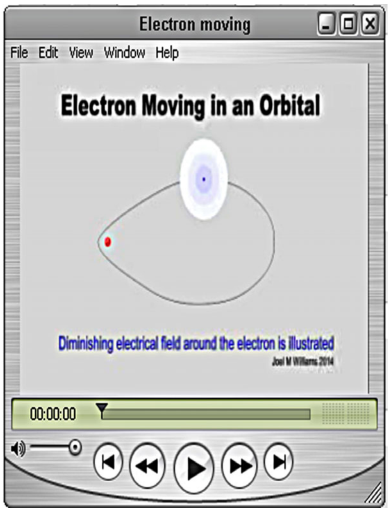
[28] A. S. Stodolna1, A. Rouzée, F. Lépine, S. Cohen, F. Robicheaux, A. Gijsbertsen, J. H. Jungmann, C. Bordas, and M. J. J. Vrakking, *Hydrogen Atoms under Magnification: Direct Observation of the Nodal Structure of Stark States*, Phys. Rev. Lett. 110, 213001 (2013)

[29] Joel M Williams, *Nixing the 'Balloons-of-Electron-Dots' Atomic Orbital Models*, http://pages.swcp.com/~jmw-mcw/Nixing%20the%20'Balloons-of-Electron-Dots'%20Atomic%20Orbital%20Models.htm

Orbitals are deemed to contain the motion of electrons about a nucleus. In this way, they contain a collection of electron orbits. *If* electrons move around a nucleus, their motion is likely to be contiuous, closed-loop, and eliptical. The MCAS model possesses these characteristics. The MC mirrored orbital pair of this model is illustrated at the right. Electrons move from orbital to orbital within a tetrahedral set in the style of a hypotrochoid.[30] From this figure, the reader should get the impression that electron behavior around a nucleus is precise and not a nebulous cloud.



The reader can get a feel for the movement of an electron on a closed loop in the video on the right. Clicking the figure opens the attached file list. Open the mp4 file to run the video. The electron with a diminishing field (3D actually, but shown in the video as a plane) is moving in a tear shaped path. A full cycle lasts <1 sec in the video, but it will loop continuously if the video player is set to "loop". The electron in the video is on a single lobe path. In the MC model, it will pass through each of the 3 other lobes of a tetrahedral unit before returning to this one to complete the circuit. An orbital should be about the expanse of negativity as well as actually containing an electron; i.e., it should contain most of the electrostatic field of an electron as it repeatedly moves in its appointed path around the nucleus. In some video players, the moving field begins to streak.

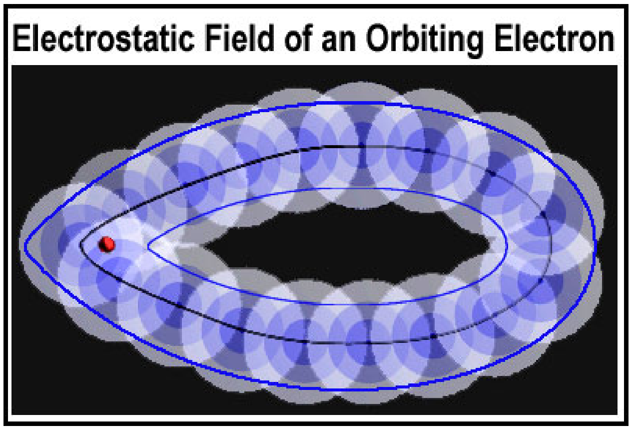


Electron Moving in an Orbital

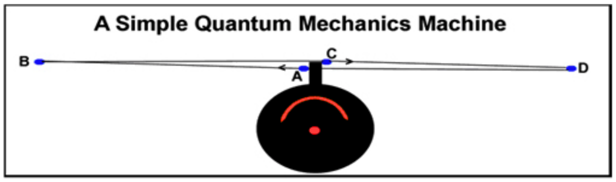
Diminishing electrical field around the electron is illustrated

Joel M Williams 2014

Since electrons move at nearly the speed of light, the electron will create a nearly continuous presence of its electrostatic field. A feel for that continuum is presented in the figure at the right where 17 locations are shown. The electron is following the black middle path. Some posit that an orbital contains the electron 90-95% of the time. A counter position is that the orbital contains the electron all of the time and that it is only the lessened magnitude of the electrostatic field that is outside of the orbital and not the electron itself. The outer bound of the orbital would thus be the outer blue line. The presence of a small amount of negative charge is not the same as an electron possibly being at that point (vide supra).



The energy levels of the orbitals of a hydrogen atom are scale as the square of integers from 1 upwards. This is predictable from classical physics! A simple "quantum" machine (shown in the figure on the right) is



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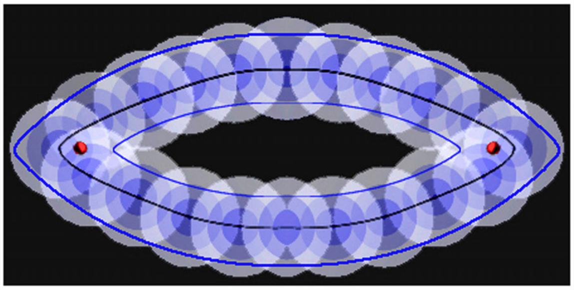
[30] Joel M Williams, *Modeling the MCAS WAY*, http://pages.swcp.com/~jmw-mcw/science; original at http://arxiv.org/html/physics/9902046v2

sufficient to explain why this happens. The explanation has been presented elsewhere[31]; the article can be accesssed easily by clicking here. The relationship of this "quantum machine" to the orbital movement in the video should be obvious. For a tetrahedral MC unit, the four orbital extremes will be BDBD.

Have you ever considered that atomic orbitals could be hollow? That is how the experimental results could be interpreted.[31] In an analogy to the outer limit of the orbital, a thin blue inner line is drawn in the figure above. While the electrostatic field of a electron decreases "forever" (the connecting fabric of the universe?), its magnitude could be very small in the middle of the orbital. It seems quite reasonable to think of an electron orbital as a "fleshy, hollow pod". Since an electron follows a precise path dictated by its electrostatic interactions with the nucleus and other electrons, the orbital path will be flattened and pad-like; similar to a spineless, prickly pear cactus stem shrunken in the middle. Another analogy would be a "pulled" torus. Without knowing where the path is, a cone with a single scoop of icecream provides the reasonably good orbital exterior that I used in the MC mirrored orbital pair figure.

Electrostatic Field of an Electron Moving between Two Nuclei



The figure on the right is a combination of two atomic orbitals to create a molecular orbital. In the current spdf-QM hybrid approach, this would be a sigma orbital. Two electrons would be in the same orbital; here paired by movement in opposite directions instead of the spin-reversal premise of the spdf-QM model. In the MCAS model, the electrons continue on to the connected orbitals of the quartet before returning to this molecular orbital. Again, electrons are paired by reciprocal motion relative to a molecular center and not by electron spin-reversal. Note that there is NO actual electron presence on the axis between the nuclei. Two electrons would not go directly AT a nucleus; to do so, they would collide! Coordinated movement of electrons is more "Virginia Reel" than Brownian.

G.N Lewis pointed out in the early 1900s that simple, real, molecules followed a "rule-of-eight" and that the orthogonal projections of the p-orbitals and the spherical s-orbital of the spdf-QM model did not yield the observed molecular structures. The octet rule imagery, however, did give good indications of molecular form. This is the concept that the MCAS model of the electron orbitals is based on. At the elementary level, "tinker toy" stick models still provide the best, simple, "hands-on", understanding of atomic interactions, in my estimation, with a caveat about just what those stick single and spring "double and triple" bonds actually are. I would add that the balls need 8 holes instead of the current 4 (just drill the current four holes straight through the sphere) with the tetrahedral quartets ringed with two different colors... The equivalent 2-D paper representations of "single", "double' and "triple" bonds are also quite useful to the chemist who is interested, for example, in replacing "the multiple bond" (electron-deficiency) between two atoms with a bond to each of them from other atoms.

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[31] Joel M Williams, *The Bohr Model, Electron Transfer and Newtonian-derived Quantum Numbers*, http://pages.swcp.com/~jmw-mcw/MCAS/MCAS_Jai-Alai_and_the_Ballmer_Series.pdf

SUMMARY

It is one thing to draw lobes for electrons with the understanding that one does not know what is going on inside those lobes. It is something entirely different to indicate that these lobes are filled with clouds or dots of electron presence and that, incidentally, some electrons will even be randomly present outside these lobes! With electrons being detected as particles around nuclei, wave/particle duality and probability models that indicate electrons can be anywhere and everywhere become less believable. The wave approach as an indication of an electron's path is quite appropriate, however. The mathematical probability approach steers the scientific mind away from how electrons move and reside. An electron's movement is well defined per the precise spectral data it generates. Movement to and fro between atoms will be on well-defined pathways with an electron's electrostatic field moving with it.

We live in a society exquisitely dependent on science and technology, in which hardly anyone knows anything about science and technology. -- Carl Sagan

Chapter XVII

Nixing the 3-Center Orbital Bond Concept of Diborane

Abstract

The bonding of the hydrogen atom in the B—H—B sequence of diborane is just a standard overlapping of atomic orbitals. With the MCAS model, hydrogen naturally has the capacity to form linear and non-linear bonds between two atoms when necessary. There is no need for the nebulous 3-center, two-electron, bond that has been used to honor the unassailable 1s-orbital of the spdf-QM model.

INTRODUCTION

A century or so ago, the electronic structure of atoms began to take shape. Spectral physics and mathematics led the charge. Making some assumptions, like electrons not behaving near the nucleus like they do between anodes and cathodes of a battery, but instead “buddy up”, the spdf-quantum mechanical (spdf-QM) model arose. The physicists were satisfied, got lots of Nobel prizes, and ventured off to dig into the nucleus and its particles.

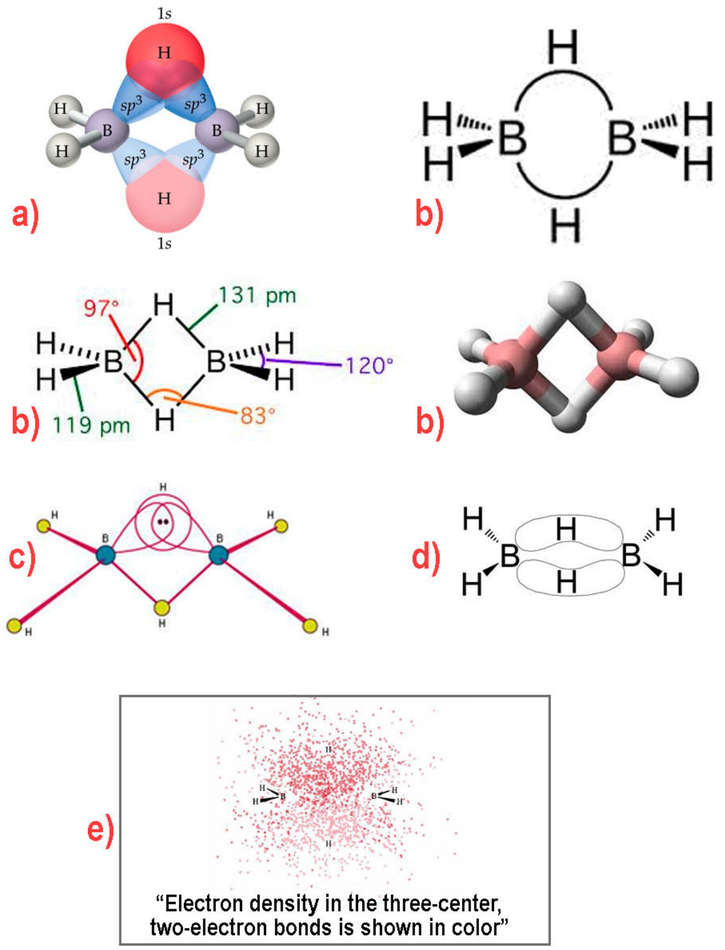
Chemists were left with an “unassailable” model of how electrons could be arranged around various atoms and thus be connected to one another to form the polyatomic matter of the world. That the spdf-QM model could not even model a simple molecule, like methane, was the chemists’ problem. Brew up some “hybrids” of the orbitals, if you need to, but do not mess with the hydrogen 1s-orbital. The spdf-QM model is based on the “holiest of holies” – the electron spin-paired sphere. The hydrogen orbital can be nothing else.

While organic chemists generated polymers, dyes, metal complexes, assorted drugs, etc., physical chemists and chemical physicists brewed in their caldrons complex hybrid orbitals that sometimes looked like misty particle clouds. Treatises were received and published as long as the “holiest-of-holies” was treated with respect.

Hydrogen atoms bonded to something singularly glided along smoothly. Hydrogen bonding in things like water was glossed over as not a real molecular bond, but an electrostatic addition to its real covalent bond. That a proton might have two “real” molecular bonds when placed between some oxygen atoms hardly caused a ripple, although it should have.

When chemists began studying boron chemistry, multiple molecular bonding of hydrogen to boron atoms became a more onerous problem. Did the scientific world “hybridize” hydrogen as it had carbon to convert s+3p’s to 4sp^3’s? Nope. The “holiest-of-holies” was unassailable. Thus was born the 3-center, two-electron, bond.

Web Images of Diborane Bonding



"Electron density in the three-center, two-electron bonds is shown in color"

(See REFERENCE SECTION for specific web references)

The figure at the right contains a sampling of some of the images that appear on the web to portray the B—H—B, 3-center, two-electron, bond. The red letters correspond to those in the reference at the end of this paper.[32] The upper left image[32a] indicates that a spherical hydrogen bonds with two sp^3 hybrid orbitals. Just how is unclear; it just does. The upper right image[32b] indicates that there are B-to-B bonds, just what those bonds are is not clear, and that somehow hydrogen gets involved. The left middle image[32b] gives physical data and indicates two bonds for the middle hydrogen atoms, but orbital types are indicated; a 122-degree bond angle instead of the 120-degree angle is listed elsewhere.[33] The middle right image[32b] makes the hydrogen atoms appear a bit like an oxygen atom of a water molecule with the electrons omitted. The next lower left image[32c] presumably indicated what a 3-center, two-electron, bond is; well, it shows 3 orbitals at a juncture. How those orbitals interact is not clear. This is especially problematic now that electrons are being detected as particles flowing in orbits.[34] The next lower right image[32d] looks like there is a pi-cloud between the boron atoms and somehow the hydrogen atoms are afloat in it. Experimental evidence shows that electrons really are particulate at the nuclear level, however.[34] The very bottom image[32e] takes the cake in my estimation and shows what

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[32] Web reference for the images of diborane in the text:

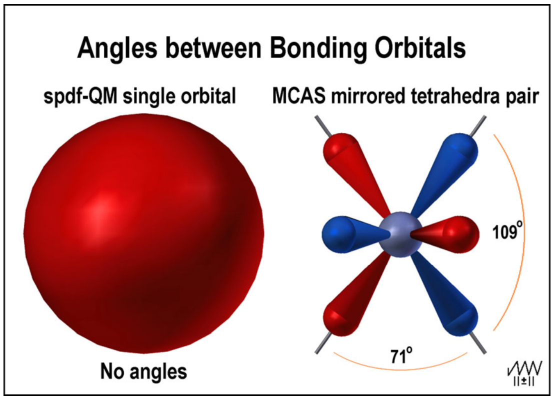
- a) http://wps.prenhall.com/wps/media/objects/948/971150/ch19_04.htm
- b) http://en.wikipedia.org/wiki/Diborane
- c) http://www.britannica.com/EBchecked/media/956/The-structure-of-the-three-centre-two-electron-bond-in
- d) http://de.wikipedia.org/wiki/Diboran
- e) http://chempaths.chemeddl.org/services/chempaths/?q=book/General Chemistry Textbook/2568/chemistry-representative-elements&title=CoreChem:Group_IIIA

[33] http://www.chemteam.info/VSEPR/diborane.html

[34] Joel M Williams, *Nixing the 'Balloons-of-Electron-Dots' Atomic Orbital Models*, *http://pages.swcp.com/~jmw-mcw/Nixing the 'Balloons-of-Electron-Dots Atomic Orbital Models.htm*

happens when folks get carried away with those dot matrix representations of orbitals![34] The website[32e] claims that this is “the current picture of bonding in diborane”. You have to wonder what students are learning from this sort of imagery. Little information about the bonding mechanics of the hydrogen atoms is forthcoming from these images, except for the physical location of the hydrogen atoms and that two of the hydrogen atoms ARE each attached to two boron atoms, contrary to the spdf-QM precept that hydrogen forms single, 2-electron, bonds!

While I was studying supercritical fluids,[35] it became clear to me that hydrogen atoms should not have orbitals that differed from those of other atoms and certainly not spherical ones. Indeed, WHY should those of hydrogen be different? So, I sent a submission to the academic press in 1993 indicating that hydrogen should have a tetrahedral orbital rather than a spherical one.[36] This was the birth of the MCAS atomic orbital model.



The figure at the right contrasts the spherical orbital of the spdf-QM model with the mirrored tetrahedral pair of the MCAS model. What differentiates hydrogen and helium from other elements is the tightness (extent) of the first energy level. At the first energy level, each tetrahedral unit (red or blue here) is dimensionally too small to handle more than a single electron. Thus, hydrogen and helium are the only elements of the first period of the periodic table. As orbital extents increase with higher energy levels, the orbitals contain one electron each at first (pairing) and then three more each until there are eight. Thus, a periodicity of eight occurs in the outer energy level as it does in the periodic table. Creating the periodic table via the MCAS model is presented elsewhere.[37] The first level orbitals of hydrogen (and helium) need to be no different than those of any other element![38]

MULTIPLE BONDING OF HYDROGEN ATOMS

Having pointed out that the MCAS atomic orbitals are the same for all atoms, multiple bonds for hydrogen atoms should not be strange at all. The main reason that they are not common results from the fact that a single electron in the non-bonding tetrahedral set is electrostatically sufficient for the singly positive proton. The diametrically opposed tetrahedral sets of the MCAS model signal the logic of linear X—H—X bonds, however. Such linear arrangements are found for protons between two oxygen atoms (O—H—O).[39]

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[35] Joel M Williams and George H. Sprenger, *THE 4TH STATE OF MATTER: THE DELTA STATE*, *http://arxiv.org/html/physics/9904001*

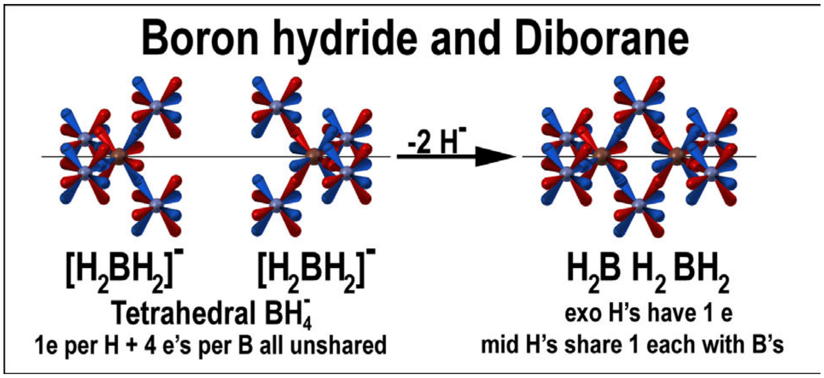
[36] The submission was neither accepted nor peer-reviewed.

[37] Joel M Williams, *Creating the Familiar Periodic Table via MCAS Electron Orbital Filling*, *http://pages.swcp.com/~jmw-mcw/The Familiar Periodic Table of Elements and Electron Orbital Filling.htm*

[38] Joel M Williams, *Comparing Several Orbital Approaches to the Hydrogen Molecule*, http://pages.swcp.com/~jmw-mcw/Orbital Models and the Hydrogen%20Molecule; and *Electron Orbitals for Ortho and Para Helium*, http://pages.swcp.com/~jmw-mcw/electron orbitals for ortho and para helium.htm

[39] Joel M Williams, *Hydrogen Bonding and Orbital Models*, http://pages.swcp.com/~jmw-mcw/Hydrogen Bonding and Orbital Models.htm

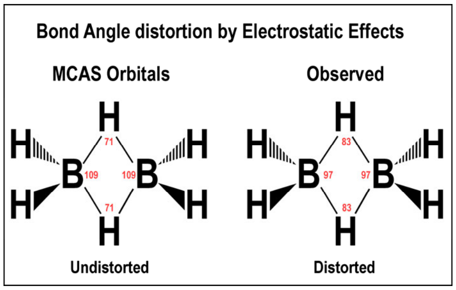
Diborane presents a different problem as the B—H—B bonds are NOT linear!



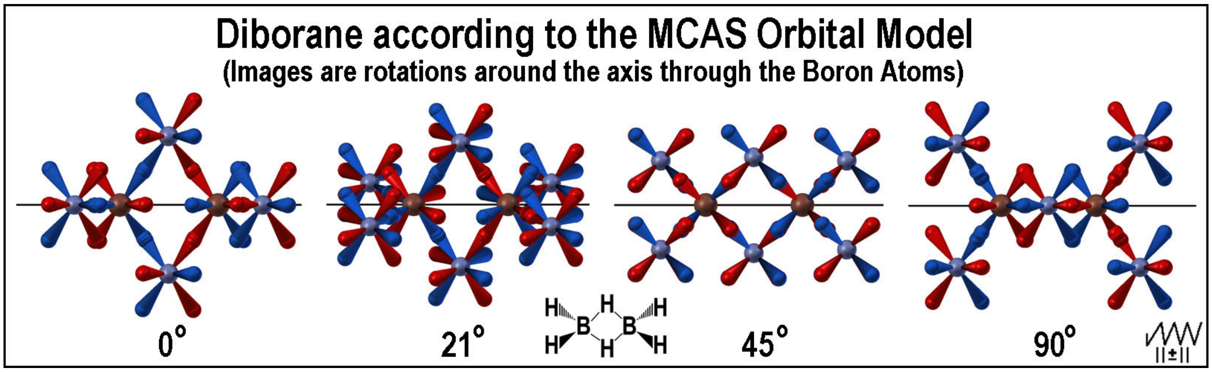
Boron hydride is a "methane analog". Each of the four hydrogen atom is identical and surrounds the boron atom tetrahedrally. A single electron moves around each hydrogen atom in the non-overlapped (bond) orbital set. Since 4 electrons move around the boron atom in its non-bonding set, the negative charge of the boron hydride unit is centered. The images in the left of the figure below show the orbital alignments. The two boron hydride images are reverse color-coded for the purpose of demonstrating their combination to diborane.

Diborane is a molecule wherein two boron hydride anions are merged with the removal of 2 protons and 4 electrons. The figure at the right illustrates this process. The two types of hydrogen atoms differ in their connectivity. Four (4) hydrogen atoms have a normal, single orbital overlapped bond with their electron in the non-overlapped tetrahedral set and thus not shared. Two (2) hydrogen atoms have two bonds formed by the overlap of an orbital of each its tetrahedral sets with that of two different boron atoms. These atoms share electrons with each other and the boron atoms through the bond linkages. There are two different paths: one is indicated "blue" and the other "red".

The undistorted bond angles of the center bridge are 109° for the H—B—H connections and 71° for the B—H—B connections. Repulsion between the boron nuclei forces them apart and narrows the H—B—H angles while lengthen the B—H bonds and widening the B—H—B angle. This is illustrated in the figure at the right.

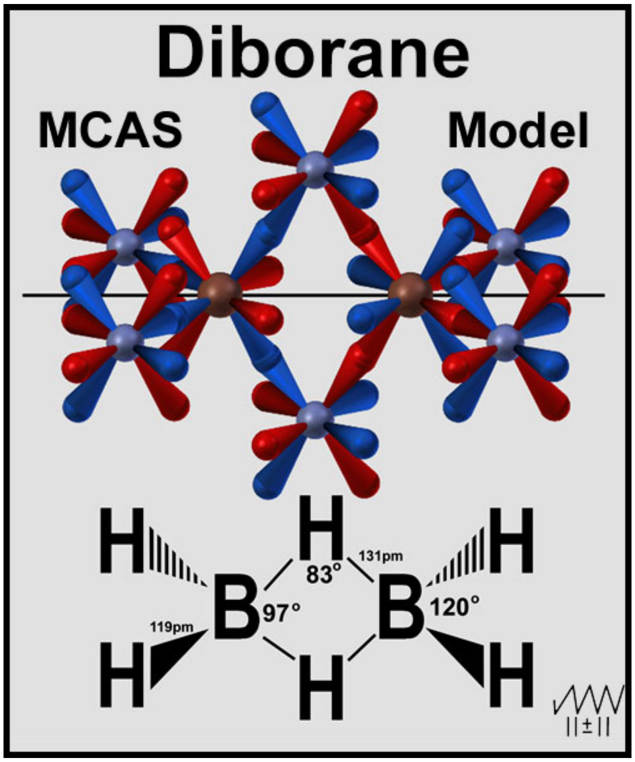


The following figure shows the undistorted orbitals of diborane as the molecule is rotated around the boron-boron nuclear axis.



One wonders, as a reader has pointed out, why linear $(H_2B)_nH_2$ molecules would not occur. The main reason is that boron can form B—B bonds, too. These will promote electron flow through 3D with occasional double-bonded hydrogen atoms.

Below is an enlarged image of diborane by the MCAS model.



CONCLUSIONS

The bonding of the hydrogen atom in the B—H—B sequence of diborane is just a standard overlapping of atomic orbitals. With the MCAS model, hydrogen naturally has the capacity to form linear and non-linear bonds between two atoms when necessary. There is no need for the nebulous 3-center, two-electron, bond that has been used to honor the unassailable 1s-orbital of the spdf-QM model.

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Chapter XVI

Crystalline Carbon and Silicon: Covalent or Ionic?

Abstract

Diamonds and silicon wafers are prized materials that share a common crystal structure. Tetrahedral atom interactions are the basis for their properties: hardness, thermal conductivity, electrical non-conductivity, etc. sp^3-Hybrid orbitals provide the current explanation for the interatomic "bond" connections. These covalent bonds, however, do not provide an adequate mechanism for these materials acting as semiconductors. Ionic bonding between atoms with the crystal lattice fully connected via overlapped, but "unoccupied", orbitals does provide a logical structure to explain how semiconductor doping works, however.

Introduction

A crystal or crystalline solid is a solid material whose constituent atoms, molecules, or ions are arranged in an ordered pattern extending in all three spatial dimensions. Ionic crystals can form upon solidification of salts, either from a molten fluid or upon crystallization from a solution. Ionic crystals with electrostatic attractions are noted for having high melting points and being hard, brittle and good electrical conductors 'in the molten state'. A diamond is a crystal of tetrahedrally aligned carbon atoms in a variation of the face centered cubic structure called 'the diamond cubic crystal structure'. The network lattice is described as covalently bonded, sp^3, atoms that give diamonds the highest hardness of any bulk material.[40] Silicon, as would be expected from its position in the periodic table, also crystallizes in a diamond cubic crystal structure[41], and, unlike diamond, can be fabricated into large spheres.[42]

This brief paper questions the logic of the physical properties for these materials being the result of covalently bonded atoms in the crystals. A few physical facts about diamond carbon and silicon will help set the stage.

Diamond Carbon

Diamond carbon melts at 4440°C. The interatomic distance[43] is 1.54Å with a cubic cell unit[44] of 3.56683Å containing 8 atoms (8 corners*1/8, 6 faces*1/2 and 4 inside*1). It has very high thermal conductivity (2000+ W·m^{-1}·K^{-1}; compare to gold at 318).[45] Most materials that

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[40] http://en.wikipedia.org/wiki/Crystal

[41] http://en.wikipedia.org/wiki/Silicon

[42] Large silicon spheres are being produced in an effort to define the

kilogram (*Scientists look to define kilogram with a super-round silicon sphere, http://ceramics.org/ceramic-tech-today/scientists-look-to-define-kilogram-with-a-super-round-silicon-sphere*)

and

Avogadro's Number (*Avogadro's Number Needs A Simple Expression*, http://pages.swcp.com/~jmw-mcw/binary_mole.htm)

[43] http://en.wikipedia.org/wiki/Bond_length

[44] http://en.wikipedia.org/wiki/Material_properties_of_diamond

[45] http://en.wikipedia.org/wiki/List_of_thermal_conductivities#cite_note-EngineeringToolbox-858-11

conduct heat well have a valence band of free electrons which serve to transfer the heat.[46] On the other hand, diamond carbon is an electrical insulator with a very low electrical conductivity[45] (10^{-13} $\Omega^{-1}m^{-1}$; compare to gold at $4.5x10^{7}$). The first ionization of an electron from carbon[47] is 1087 kJ·mol^{-1} and internal electric charges do not flow freely under the influence of an electric field. However, synthetic diamonds doped with boron are p-type semiconductors, while those doped with phosphorous are n-type. Thin-film diamond n-type semiconductor wafers are now being generated.[48] Silicon wafers are the state-of-the-art in the semiconductor business. However, the much higher melting point of diamond carbon versus that of silicon[41] (1414°C) provides an impetus for replacing silicon.

Silicon Crystal/Wafers

Silicon crystals are strong, but very brittle and prone to chipping. The interatomic distance[49] is 2.22Å with a cubic cell unit[41] of 5.430710Å containing 8 atoms. The thermal conductivity[41] is much lower at 149 W·m^{-1}·K^{-1}than that of diamond carbon. While the electrical conductivity[50] at 1.56×10^{-3} $\Omega^{-1}m^{-1}$ is much higher than that of diamond, but silicon is hardly a conductor. The first ionization of an electron from silicon[47] at 787 kJ·mol^{-1} is 72% that of carbon, but a mere 7% greater than that of magnesium[47] (738 kJ·mol^{-1}). Unlike the difficulty of forming diamond carbon in large sizes, large cylindrical ingots of the high purity (99.9999999%), crystalline silicon, needed for integrated circuit making[41], can be produced by pulling a seed crystal from a 'melt' in the Czochralski process.[51] Silicon wafers are generally not 100% pure silicon, but are doped with tiny amounts of a particular element (<1 atom of additive for >10,000 crystal cell units of silicon!)[52] to make a wafer of the desired semiconductor type and responsiveness. These added atoms greatly increase conductivity and allow the electrical behavior to be set. Like the time-honored cleavage of diamonds along lattice planes to produce brilliant gems, the crystalline silicon ingot is cut into wafers. Scoring the wafer along cleavage planes allows billions of individual circuits to be placed on an average wafer.

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[46] http://en.wikipedia.org/wiki/Helium

> The thermal conductivity of helium II (a liquid) is greater than that of any other known substance several hundred times that of gold. The flow of heat is said to be governed by equations that are similar to the wave equation used to characterize sound propagation in air. (Presumably a shock wave through very closely "connected" atoms; helium atoms would have multiple 'bonding'; how? – jmw)
>
> For orbitals that permit multiple bonding interaction of first period elements, see the references below:
>
> a: *Electron Orbitals for Ortho and Para Helium*,
> http://pages.swcp.com/~jmw-mcw/electron orbitals for ortho and para helium.htm
>
> b: *Hydrogen Bonding and Orbital Models*,
> http://pages.swcp.com/~jmw-mcw/Hydrogen Bonding and Orbital Models.htm

[47] http://en.wikipedia.org/wiki/Molar_ionization_energies_of_the_elements

[48] *Argonne licenses diamond semiconductor discoveries to AKHAN Technologies*, http://www.anl.gov/articles/argonne-licenses-diamond-semiconductor-discoveries-akhan-technologies

[49] http://www.webelements.com/periodicity/

[50] http://en.wikipedia.org/wiki/Electrical_resistivity_and_conductivity

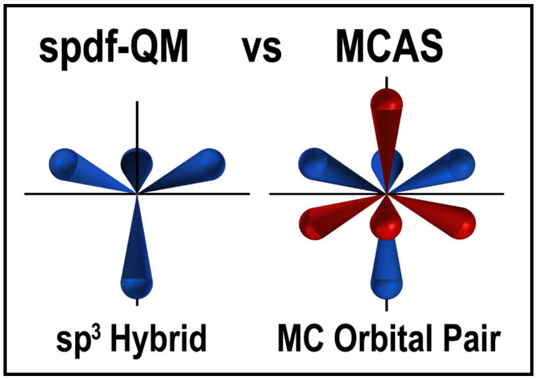
[51] http://en.wikipedia.org/wiki/Wafer_(electronics)

[52] http://en.wikipedia.org/wiki/Doping_(semiconductor)

Factors to be explained by the Atomic Orbital Structure

Dependency	Factor	Carbon	Silicon
Atom Locations	Unit cell structure	Every atom tetrahedrally is surrounded by a nearest neighbor	
	Mechanically strong	Strong, symmetrical, atom interactions are all working together	
	High melting		
	High thermal conductivity	Very rigid crystal matrix gives strong transfer of energy from atom to atom and thus across the crystal; there is no electron flow	3.5x the cell volume of diamond; more room for flexing means less direct energy transfer to adjacent atoms and thus less across the crystal
	Sharp Cleavages	Perfect 111 crystal planes slide easily with a sharp blow	
	Brittle	Diamond hard; tight atomic network	1.44x diamond inter nuclear distance – much weaker crystal planes
Electron Placement And Flows	Unit cell structure	Every atom is tetrahedrally surrounded by a nearest neighbor	
	Electrical insulator	No electron flow from atom to atom; electrons are tightly bound	Silicon is a very weak natural semiconductor; electrons are less tightly bond than in diamond
	Semiconductor behavior	Electron flow through atomic matrix when elements that provide “holes” or “electrons” are present in minuscule amounts; how?	

Electron Orbital Models



The currently accepted electron orbital model of atoms is the spdf-QM model. The figure at the right indicates the sp^3-QM hybrid that is used to address the atomic interactions of diamond carbon and silicon. Included in the figure are the corresponding MC orbitals of the MCAS model. A description of the two is provided elsewhere.[53] Both provide tetrahedral orientation of orbitals with the spdf bonding orbitals having been formed by “hybridizing” the spherical-s and hour-

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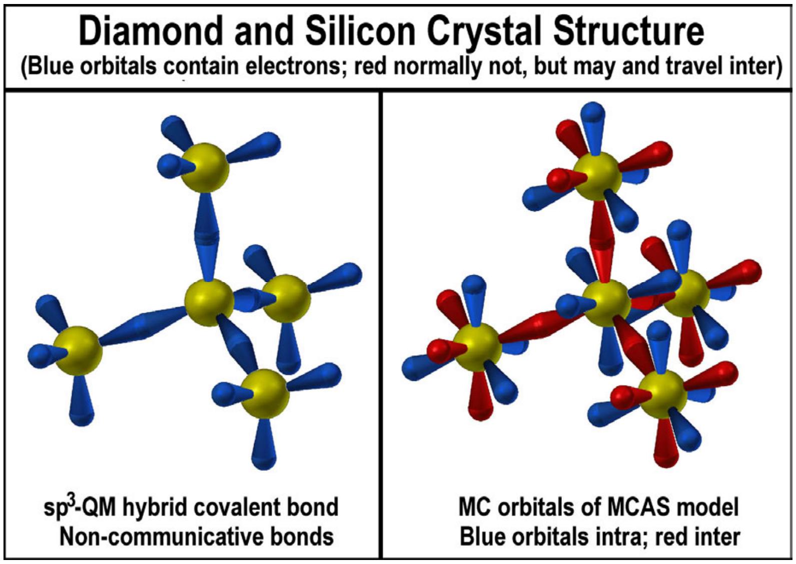
[53] *PARSING THE spdf ELECTRON ORBITAL MODEL*, http://pages.swcp.com/~jmw-mcw/Parsing the spdf electron orbital model.htm

glass-p atomic orbitals. The MC orbitals are not hybrids as they are those of the free atomic element. The primary distinction between the sp^3-QM hybrid and the MC orbitals is what will house the 4 outer ("valence") electrons and what will form bonds. The sp^3-QM hybrid has a singular way to house electrons and form bonds with electron spin-pairing. The mirrored MC orbital pairs allow electrons and bonds to be handled jointly or independently.

Addressing the Tetrahedral Arrangement of Diamond and Silicon Atoms



The figure at the right illustrates how the two models address the tetrahedral interaction of a diamond carbon or silicon atom with its four nearest crystal neighbors. Both show staggered (minimal electrostatic repulsions) configurations for the electron containing orbitals. The sp^3-QM model has the electrons shared as spin-reversed pairs on the axis between two atoms in what is called a "covalent bond". The MCAS model has no electrons shared by atoms as the atoms protect themselves first; thus, there are no electrons on the axis between any two atoms in the perfect crystal. The "bonding" in the MCAS model would be described as "ionic". Electrostatics of such bonds have been present elsewhere.[54]

In the sp^3-QM model, each sp^3 orbital is independent of the others; thus, electrons do not flow from one orbital to another. This is used to describe why diamond carbon is such an excellent electrical insulator. The same can not be said about its explanation of the semiconductor behavior produced by <80 "hole" or "electron" atoms for every million unit cells! It also does not explain why silicon is a natural, but weak, semiconductor.

In the MCAS model, the red, unfilled, but overlapped orbitals provide a continuous "tunnel" network throughout the crystal. With a high, 1st ionization energy, carbon atoms hold their own electrons very tightly. With no readily available electrons, diamond carbon is not a natural semiconductor. With doping, the "tunnel" network allows diamond carbon crystals to become semiconductors. Silicon, on the other hand, has a lower, 1st ionization energy. With the release of just a few electrons into the "tunnel" network, silicon becomes a natural

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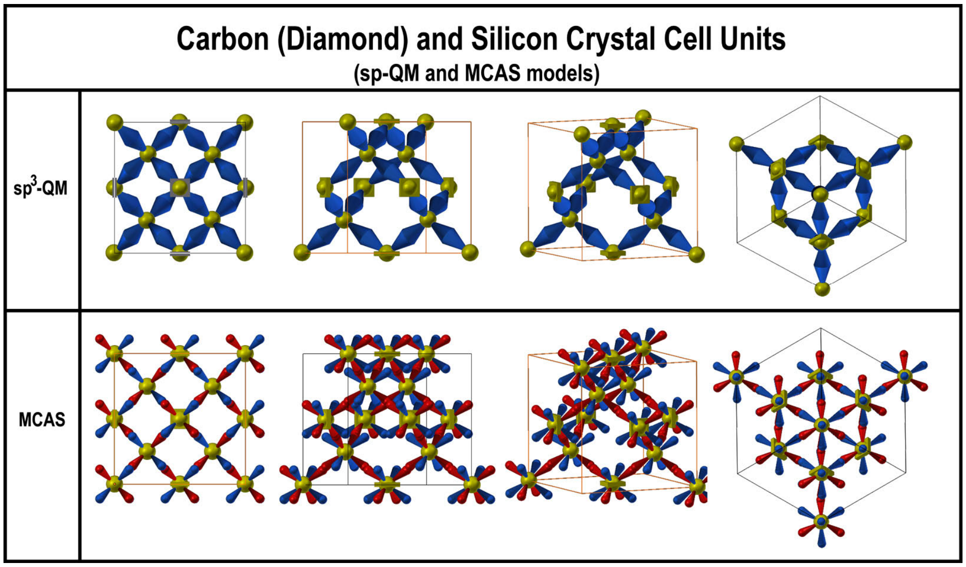
[54] a) Joel M Williams, *Understanding the Bonding of Second Period Diatomic Molecules*,
(Ever wondered how positive charge-forces are transmitted through the electron orbitals of the cations of crystals, like NaCl, to give them their positiveness? The cations are not likely to be solid spheres of simple net positive charge on the exterior, even if it is easier to think of ions as positive and negative balls.)

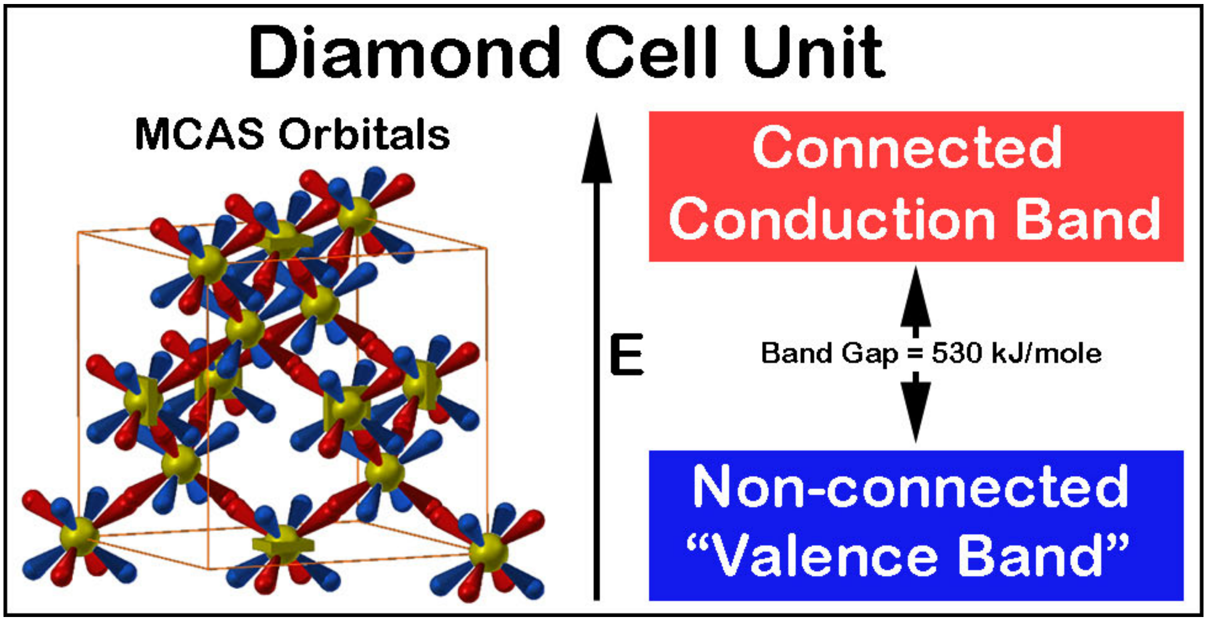
b) Joel M Williams, *Modeling the MCAS Way*,
http://pages.swcp.com/~jmw-mcw/science; http://arxiv.org/html/physics/9902046v2
c) Joel M Williams, *Challenging Science*, AuthorHouse, July 25, 2005,
http://www.amazon.com/Challenging-Science-Joel-M-Williams/dp/1420842382

semiconductor. Doping that places “holes” and “electrons” in the “tunnel” network allows silicon to become the state-of-the-art semiconductor used in integrated circuits.

The figure on the right shows the crystal cell unit according to the two orbital models. Four of the corner atoms are omitted so that the remainder is easier to view.



The reader might find it interesting that crystalline carbon is simply repetitive C6 carbon-chair units in 3D. The crystal bond network (red in the figure below) of pure carbon has no electrons in it. This is the conduction band! The band gap is the energy required to move an electron from an atom's "non-sharing", tetrahedral orbital unit to its overlapped orbital, sharing network. Extremely tiny amounts (<1 per 10,000 cell units!) of interstice-doping with electron or hole providing atoms allows it and silicon to be semiconductors.



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Chapter XV

Hydrogen Bonding and Orbital Models

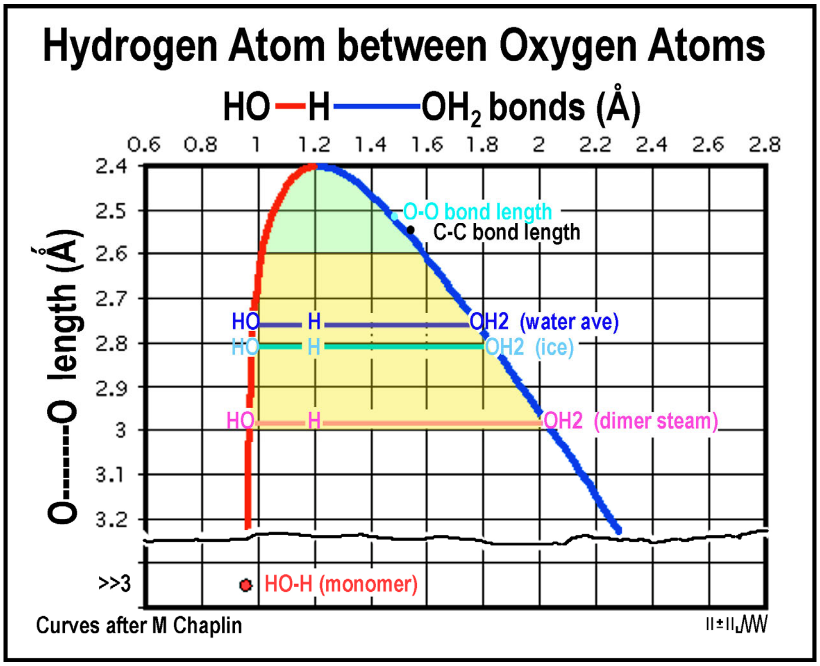
Abstract

There is increasing evidence that the hydrogen atom in X—H—X connections is covalently bound to both X atoms in equal to varying degrees. A spherical s-orbital for hydrogen attached to two 2-electron covalent bonds clearly violates the spdf-QM concept of shared electron bonding. A short discussion of the situation is presented along with a simple alternative orbital model for hydrogen that allows hydrogen to have two, diametrically opposite, covalent bonds.

INTRODUCTION

Molecule interactions form our physical world. While solids indicate strong interactions between atoms and within molecules, e.g. crystals and polymers, water is the epitome of "loose" interactions. As such, water has been one of the most studied substances, both as object and solvent. Martin Chaplin has assembled a website with 2065 references entitled "*Water Structure and Science*"[55].

Since this paper will be about hydrogen bonding in O—H—O systems, the following figure is presented to give the reader a feel for the atomic distances. The figure is adapted from Chaplin[55]. Information presented in the **Data Appendix** at the end of this paper has been added to provide perspective.



The figure clearly indicates the long bond that is associated with the term "hydrogen bonding" that allows H_2O to exist as water. The same bond in ice is just a bit longer. Surprisingly, the bond is much longer in the H_2O dimer that occurs about 1 in 1000 water molecules and about 1 in 20 steam molecules[55]. Chaplin indicates that the hydrogen bonding strength is 15kJ/mole at a length of 2.99Å. The light yellow zone reflects that an extended covalent bond is well within this distance.

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[55] Martin Chaplin, *Water Structure and Science*, http://www1.lsbu.ac.uk/water/hbond.html

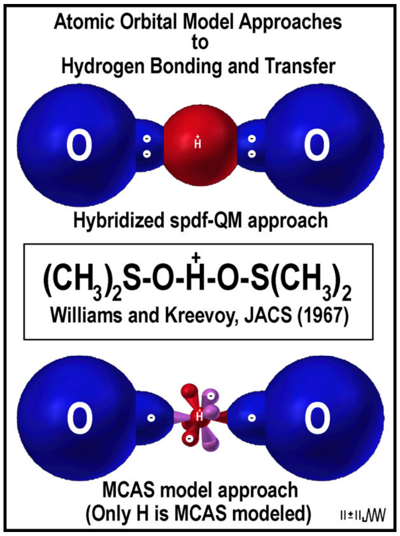
Chaplin covers a number of articles dealing with the covalence of hydrogen bonds. A few of his comments (mainly from footnote 'd'[55]) are presented below to give the reader a feel for the situation. The reader should refer to Chaplin's website for references to each of these comments.

- *The (water)$_{JMW}$ network is essentially complete at ambient temperatures; that is, (almost) all molecules are linked by at least one unbroken hydrogen bonded pathway.*
- *If the water hydrogen bond (the long one)$_{JMW}$ is considered within the context of the complete range of molecular hydrogen bonding then it appears most probable that it is not solely electrostatic.*
- *If the hydrogen bond is substantially bent, it follows that the bond strength is weaker.*
- *The ionization of water, the continuous transformation of ice VII to ice X and the lower ionization potential for liquid water relative to water vapor would all seem to indicate a continuity of electron sharing between water molecules.*
- *In nucleic acids, inter-nucleotide N-H····N coupling (2JNN, using 15N nuclei) confirms some covalent nature in the N-H····N hydrogen bond.*
- *3-bond NMR (3JNC) splitting has been found through peptide N-H····O=C hydrogen bonds in proteins, confirming some covalent nature in the N-H····O hydrogen bonds.*
- *Hydrogen bonds in other molecules, such as DNA, also possess considerable covalent character.*

"Hydrogen bonding" is commonly associated with long, weak, O-----H interactions. When the oxygen atoms are closer, the hydrogen nucleus is more equally distant from each oxygen nucleus (the light green area in the figure above). Such short distances would be expected for proton-transfers from one oxygen atom to another. Proton-transfer might be a fleeting event, but the interaction of the oxygen orbitals with the hydrogen would be instantaneous with the hydrogen atom having two short covalent bonds. How can this occur when, in the current spdf-QM model, hydrogen has only a spherical s-orbital and by definition can only form a single covalent bond having 2 electrons?

A stable molecular arrangement with two oxygen atoms sharing a hydrogen atom equally at short range would definitely require the hydrogen to have two covalent bonds. **Do such molecular arrangements exist? The answer is "Yes".**

DISCUSSION



Dimethysulfoxide solvated proton (DMSO—H—OSDM)$^+$ is a stable molecular arrangement with a symmetrically placed proton between the two oxygen atoms (O—H—O). This molecular species was first reported by Williams and Kreevoy in 1967 when we studied methanesulfonic acid in DMSO.[56] A similar conclusion was drawn by Kirilova, etal.[57] in their 1986 study with ATR. No bands belonging to (DMSO—H—OSDM)$^+$ other than ν(O—H—O) were found. X-ray studies have shown the occurrence of (DMSO—H—OSDM)$^+$ in crystalline salts.[58] In 2002, Denisov, etal.[59], determined the cation to be practically linear with a O—O distance of 2.403Å with the bridging proton located exactly in the center between the two oxygen atoms.

In their 2005 study of crystalline $H_5O_2^+ClO_4^-$, Vener and Sauer[60] found the equilibrium O—O distances to be 2.431Å in the isolated cation and 2.426Å in the crystal.

The covalent orbital reach of an oxygen atom is greater than 0.74Å (½ of O—O) and that of a hydrogen atom is greater than 0.37Å (½ of H—H). The full reach of each atom to the other will be greater than this 1.11Å sum. It is reasonable to expect them to span the 1.2Å distance of O—H bonds easily. In each of the molecular arrangements above, the hydrogen atom is thus clearly involved with two covalent bonds which, in the current spdf-QM bonding model, require it to be coordinated with 4 electrons.

The current spdf-QM electron orbital model is a forced one based on the precept of a sphere as the starting point. The spdf-QM model not only requires that macro-physical laws, such as e-e repulsion, cease in the near-nucleus area, but has a basic set of orbitals with little resemblance to those needed to model the materials of our substantive world. To address how atoms actually bond to one another, the orbitals of spdf-QM model had to be "hybridized". For the simplest orbital connections, sp^3, sp^2 and sp^1 orbital sets were created. Eventually, when inorganic complexes were modeled more "hybridizing" was needed with d-orbitals

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[56] J M Williams and M M Kreevoy, *Structure and infrared spectrum of the solvated proton in dimethyl sulfoxide*, J. Am. Chem. Soc., 1967, **89** (21), pp 5499–5501

[57] A.P. Kirilova, V.D. Mayorov, A.I. Serebryanskaya, N.B. Librovich, E.N. Guriyanova, Izvest. Akad. Nauk USSR, Ser. Khirn. **10** (1986) 2435

[58] References cited in ref 5 below: R.A. Potts, Inorg. Chern. **9** (1970) 1284; B.R. James, R.H. Morris, JACS Chem. Commun. (1980) 31; O.V. Rudnitskaja, T.M. Buslaeva, N.I. Lyalina, Zh. Neorg. Khim. **39** (1994) 922; and V.I. Lobadyuk, V.N. Spevak, N.K. SkVortsov, A.I. Stash, V.K. Belskij, Zh. Obshch. Khim. **66** (1996) 705.

[59] G.S. Denisov, A. Koll, V.I. Lobadyuk, V.M. Schreiber, A.V. Shurukhina, V.N. Spevak, *Hydrogen bonding in coordination compounds containing homoconjugated bis-dimethylsulfoxide cation*, J Molecular Structure **605** (2002) 221-226; http://www.chemie.fu-berlin.de/~limbach/denisov/184.pdf

[60] V. Vener and J Sauer, *Environmental effects on vibrational proton dynamics in H5O2*$^+$*: DFT study on crystalline H5O2*$^+$*ClO4*$^-$, Phys. Chem. Chem. Phys . , 2005, **7** , 258-263; http://edoc.hu-berlin.de/oa/articles/recUjCiEZgtpY/PDF/247whSivydg.pdf

becoming involved. Interestingly, with all of this “hybridizing” of orbitals, the spherical s-orbital of hydrogen was consciously excluded (avoided?). In the bond formation part of the currently accepted spdf-QM hybridized model, bonds contain 2 paired electrons. Consequently, hydrogen is able to form only 1 covalent bond as its unhybridized orbital can only handle 2 electrons. From the real-world cases above, a hydrogen atom does form more than one covalent bond is necessary. Clearly, the spherical s-orbital for hydrogen is incorrect for such bonding. It is even incorrect for a solo hydrogen atom and a helium atom[61].

The upper image in the figure at the right indicates the problem with the current spdf-QM spherical hydrogen orbital. Two identical covalent bonds are needed for the O—H—O connection. Each oxygen atom (only one of their orbital protuberances is shown) supplies 2 electrons, but the hydrogen atom is able to form only one 2-electron bond. Thus, two covalent bonds being attached to the hydrogen atom violates a prime tenet of the spdf-QM orbital approach to molecular bonding.

The MCAS model[62] was created as the result of the need for hydrogen atoms to have two covalent bonds as well as to eliminate the need for spin-reversed electron pairing. “Mirrored tetrahedral orbital twins” (center of the bottom image in the figure at the right) provide precisely the needed orbital configuration for hydrogen. The oxygen atoms are not MCAS-modeled here (shown as spheres with an orbital protuberance), so that the focus is on the MCAS character of the hydrogen orbitals; their orbitals, too, are “mirrored orbital twins”. Electrons are not corralled in the covalent bond, but flow through the orbital sets. The mirrored hydrogen orbital pair establishes an opposing linear orientation of the covalent bonds from the hydrogen atom.

The MCAS model negates the need to “hybridize” an atom’s orbitals for the simplest bonding between atoms! Dogged adherence of the scientific community to Bohr’s orb-turned-sphere for the hydrogen atom has stifled the search for physical model alternatives to the spdf-QM atomic model. Strong pi-bonds from parallel p-orbitals that can hardly touch, and do so at an acute angle, counter experimental evidence that bonds become progressive weaker as they deviate from linearity. Molecular orbital diagrams remove the physical aspects of the orbitals. In essence, MOs simply indicate that bonds are formed without worrying about how electrons in them actually move or reside. How and where electrons move in the atomic and molecular systems is the aim of the MCAS model. A spherical orbital with spin-reversed paired electron twins in highly localized, interatomic, bond space is not part of this model.

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[61] Joel M Williams, *Electron orbitals for ortho and para Helium*, http://pages.swcp.com/~jmw-mcw/electron orbitals for ortho and para helium.htm; a pdf version is available at http://gsjournal.net/Science-Journals/Essays/View/4980; He (11±11) is a gas.

[62] A description of the MCAS atomic model is presented along with the spdf-QM atomic model in this reference: Joel M Williams, *Parsing the spdf electron orbital model*, http://pages.swcp.com/~jmw-mcw/Parsing the spdf electron orbital model.htm;
a pdf version is available at http://gsjournal.net/Science-Journals/Essays/View/5032

Data Appendix

From Martin Chaplin, *Water Structure and Science*, http://www1.lsbu.ac.uk/water/hbond.html and http://www1.lsbu.ac.uk/water/molecule.html

- The experimental values for gaseous water molecule O—H length is 0.95718 Å
- The O—O distance in ice Ih varies between 2.75 Å (0 K) and 2.764 Å (253 K).
- In ambient atmosphere the O—O in the water dimer is 2.985 Å (calculated by JMW); the short O—H bond is 0.948Å and the long bond is 2.037Å

From U. Bergmann, A.Di Cicco, P. Wernet, E. Principi, P. Glatzel, and A. Nilsson, *Nearest-neighbor oxygen distances in liquid water and ice observed by x-ray Raman based extended x-ray absorption fine structure*, J Chem Phys. 2007 Nov 7;127(17):174504, http://www.ncbi.nlm.nih.gov/pubmed/17994824

- O—O of water average distance (2.81 Å for water and 2.76 Å for ice)
- And a slightly shorter peak position (2.70 Å for water and 2.71 Å for ice)

From C Chieh, http://www.science.uwaterloo.ca/~cchieh/cact/c120/bondel.html

- C—C 1.54 Å
- O—O 1.48 Å
- H—H 0.74 Å

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Chapter XIV

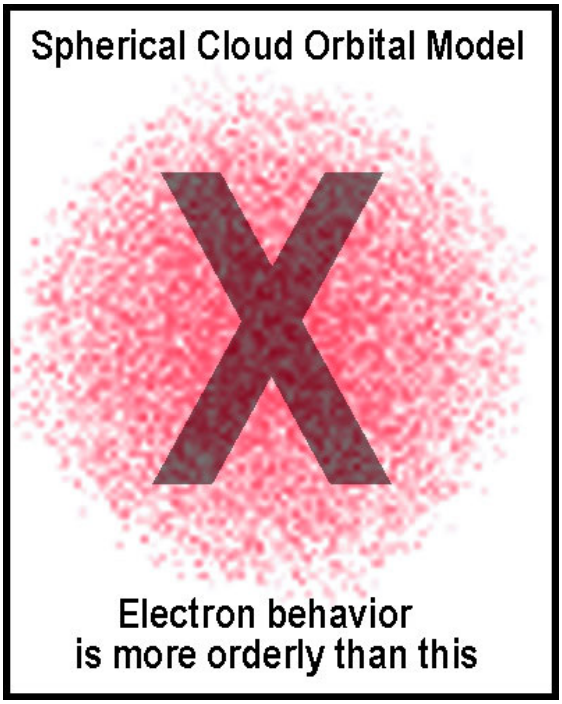
Nixing the 'Balloons-of-Electron-Dots' Atomic Orbital Models

Abstract

Experimental location data indicate that electrons are not distributed as 'balloons-of-electron-dots' depict. Spectral data constancies have always indicated that electrons behave quite orderly. Consequentially, atomic orbital models with center-concentrated dots are misleading and should be nixed. Likewise, the idea of molecular bonds as capsules filled with dots of 'non-repelling, spin-paired electrons" should also be nixed.

The Spherical Cloud Model of Electron Orbitals

Orbitals are intended to provide a handle on how electrons might be arranged around a nucleus. The data presented by Stodolna, et al[63] using a 'quantum microscope' technique indicate that electrons are not randomly dispersed. They suggest that their results might indicate "circular or spherical" orbitals for the hydrogen atom. While one might wonder about some induced artifacts, it is clear from their images that hydrogen orbitals are fairly well defined. "Dot-matrix" cloud representations[64] of electron orbitals, as depicted in the figure at the right, and their hybrid mixings are not and are, thus, misleading. Such representations are presumably efforts to convey probability distributions that are based loosely on static (no time factor) continuum calculations. They provide no information about how or why an electron got to a possible location or where it would go next.



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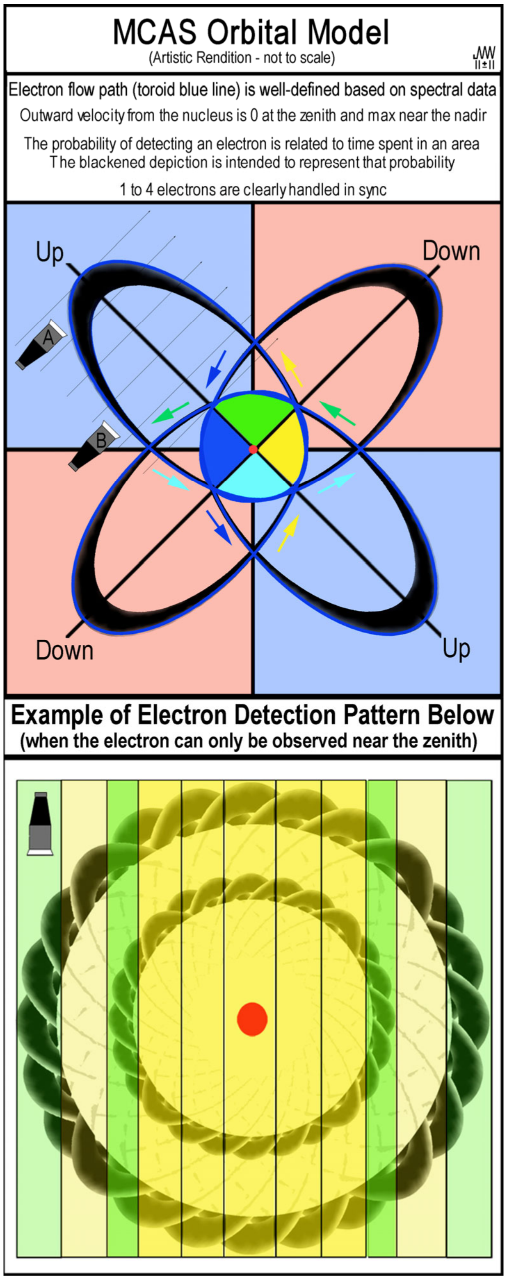
[63] A. S. Stodolna, A. Rouzée, F. Lépine, S. Cohen, F. Robicheaux, A. Gijsbertsen, J. H. Jungmann, C. Bordas, and M. J. J. Vrakking, *Hydrogen Atoms under Magnification: Direct Observation of the Nodal Structure of Stark States*, Phys. Rev. Lett. 110, 213001 (2013)

[64] For example, these images are displayed on the web and presumably taught (some images just show up to connect searchers to phishing websites):
http://www.chem.queensu.ca/people/faculty/mombourquette/firstyrchem/molecular/orbitals/SP.gif;
http://www.chem.queensu.ca/people/faculty/mombourquette/firstyrchem/molecular/orbitals/2sp.gif;
http://www.thestudentroom.co.uk/showthread.php?t=1539934;
http://upload.wikimedia.org/wikipedia/commons/thumb/9/9b/AOs-3D-dots.png/500px-AOs-3D-dots.png;
http://www.chemguide.co.uk/atoms/properties/porbital.GIF;
http://faculty.colostate-pueblo.edu/linda.wilkes/111/3c.10.jpg;
http://sun.menloschool.org/~dspence/chemistry/atomic/wave_mech.html;
http://homepages.gac.edu/~huber/chromatek/atomic.htm;
http://wps.prenhall.com/wps/media/objects/3311/3390683/imag0605/AAAUAWJ0.JPG

The ‘quantum microscope’ experimental data, also discussed further below, show that ELECTRONS BEHAVIOR IS QUITE ORDERLY. Indeed, the constancy and sharpness of SPECTRAL DATA HAVE ALWAYS INDICATED THIS. It is strange that the electron in a cloud model, which might be in any position, low near the nucleus or far from it, nevertheless jumps in response to the exact same photon into one precisely higher orbital position, regardless of the point from which it jumps. Unless there are significant qualifications to the observed experimental location and spectral data, “electrons-can-be-anywhere-and-everywhere” probability models make no sense! Thus, models such as that depicted in the figure above should be nixed!



Electron Orbitals as Generated by the MCAS Model

While the authors of the ‘quantum microscope’ data indicated that their results might indicate “circular/spherical” orbitals for the hydrogen atom, the data also supports non-spherical orbital shapes. Actually, the data may only represent the summation of the outer (zenith and nadir) limits of electron movement at each energy level.[65] These are the points of zero movement from the nucleus where the electron is most likely to be observed. Indeed, electrons are observed as particles whose “roundness” and dipole character are now being sought![66] Could they actually be too pudgy to be quantum changelings? *“Electron-spin predestined the predominant singular twist of natural molecules (e.g., DNA). With a singular spin, electrons flow chirally around nuclei. Thus, electronic orbitals possess built-in chirality. Atoms of the universe were the first to have a one-way traffic system.”*[67] Orbitals should be considered as defining where electrons travel alone on beaten “paths”, ruts, tubular conduit worm-holes or as in sync groups possibly like “necklace” beads on an orbital “string” wave. While it may be easier to draw orbitals with conical lobes, the actual paths may be more like twisted paddles. Spin-pairing occurs in the MCAS model with electrons flow in opposing orbitals in contrast to the current electron-spin reversal requirement.

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[65] See comment #14 (entitled “Circular averaged Nadir and Zenith - not orbitals”) to *Quantum microscope' peers into the hydrogen atom*, http://physicsworld.com/cws/article/news/2013/may/23/quantum-microscope-peers-into-the-hydrogen-atom

[66] H. Loh, K, etal., “Precision spectroscopy of polarized molecules in an ion trap”. Science (2013) Vol. 342 no. 6163 pp. 1220-1222; editor’s summary: “One of the signatures of this “new physics” would be a non-vanishing electric dipole moment of the electron - http://www.sciencemag.org/content/342/6163/1220.abstract

[67] Joel M Williams, “*The Electronic Structure of Atoms*”, in Challenging Science, AuthorHouse, 2005, p15

The following discussion demonstrates how electrons will be observed per the MCAS model. The figure at the right is a flattened MC tetrahedral orbital which the model would use for a hydrogen atom's simplest levels. The depiction is "not to-scale". The lobes in the blue quadrants were "Up", while those in the pink quadrants were "Down". Electron movement will be along very narrow paths as illustrated by the blue-lined toroid. The lobe dimensions are set by the energy of the electrons and their electrostatic interaction with the nucleus. The extent of the lobes is integer-based ($n^2 = 1, 4, 9$, etc); a simple demonstration of why this is so has been presented elsewhere[68]. Black areas inside the blue orbits are included to provide a rough indication of the probability of an electron being observed. At the orbital zenith, the electron is neither moving from nor towards the nucleus. Just before and afterwards, it is also slow in that regard; elsewhere, movement to/from the nucleus is quite rapid. Detecting an electron depends on the observing device's response time and sensitivity. While detection of an electron may be obtained with "sensor A", the same setting on "sensor B" (or a single sensor viewing the entirety) may show nothing as an electron speeds past its view. The situation becomes similar to the image in the figure at the lower right when many 'sightings' are made and the tetrahedral orbital's 3D movement is not anchored along with that of the nucleus. The vertical green strips indicate the perpendicular view that shows where the slowest movement to/from the nucleus occurs and is thus the most likely region for success in detecting electrons. The yellow strip areas are relatively similar to one another and provide much less chance of detecting an electron. With sufficient data merging, details become blurred and smooth rings are generated. Experimental electron detections will be for 3D tetrahedral orbitals; for illustrative purposes, the lobes are shown flattened here.

For a hydrogen atom, a single, particulate, electron can ONLY be at one place at any given moment in time. A second orbital level is shown to illustrate the cumulative effects of data summing. Depending on conditions, inter orbitals, which are of lower energy, could very well have a higher temporal concentration of that electron and thus show up more intense than outer ones. **Conclusion:** the probability of an electron being found at a location depends on temporal as well as non-temporal factors, such as electrostatic interactions and energy levels.

The MCAS Model and 'Quantum Microscope' Results

In order to evaluate how the MCAS model fits the 'quantum microscope' results[63], the images from that work have been inspected. That work is very elaborate and extensive. Holding the nucleus in a rigid location is quite impressive as is the detection of an electron's position. In the end, however, the accomplished effort simply provides a collection of singular results: projected 2D locations of the 3D locations of a single electron, in the case of a hydrogen atom, regardless of how the electron got there. Impressive numbers of singular results were required to indicate that the electron spends time in well-defined "orbitals".

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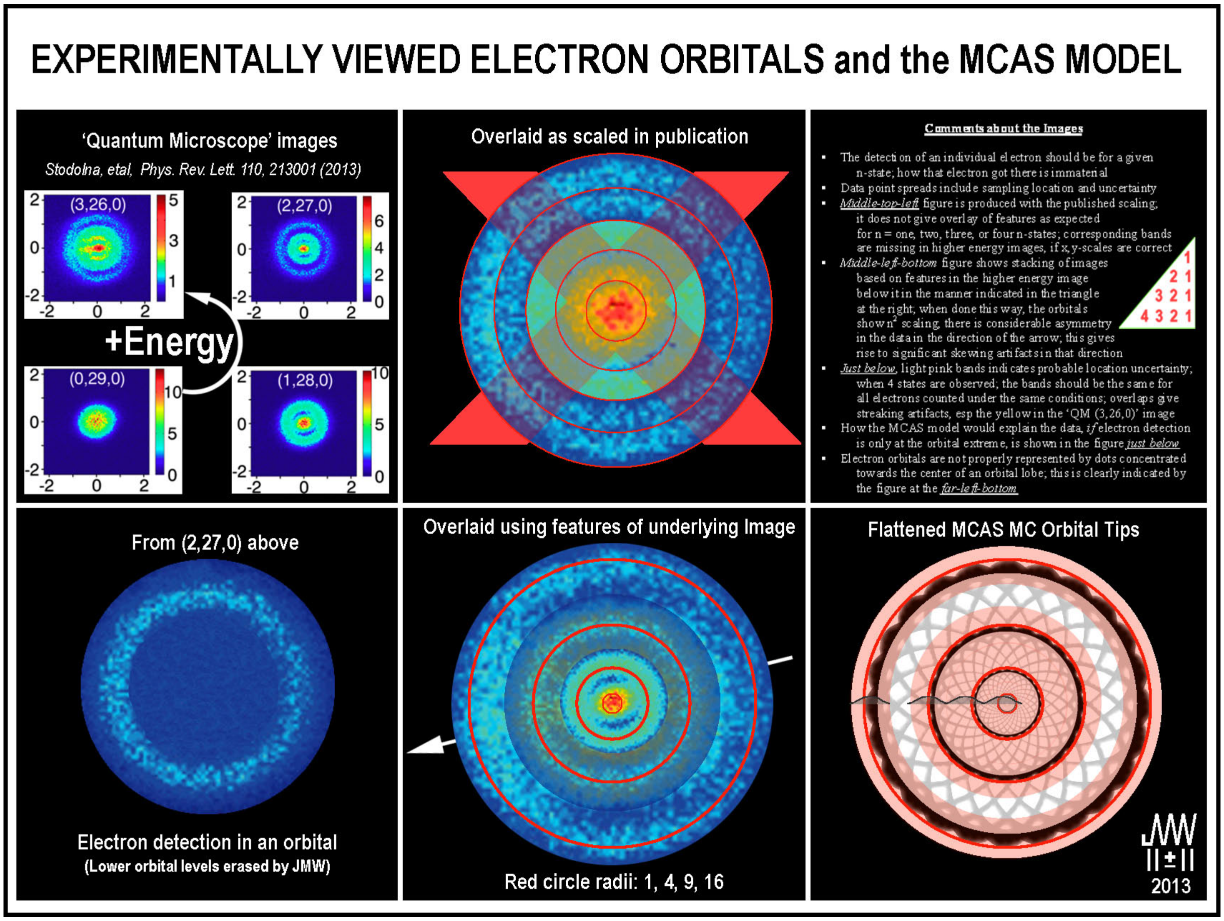
[68] Joel M Williams, "Why do electron orbitals have discrete quantum numbers?" - http://vixra.org/abs/1210.0133; or http://pages.swcp.com/~jmw-mcw/Quantum%20Numbers%20from%20a%20Simple%20Quantum%20Mechanics%20Machine.htm

The figure below has been created to interpret the ‘quantum microscope’ results and to relate the MCAS atomic orbital model to them.



EXPERIMENTALLY VIEWED ELECTRON ORBITALS and the MCAS MODEL

‘Quantum Microscope’ images

Stodolna, etal, Phys. Rev. Lett. 110, 213001 (2013)

Overlaid as scaled in publication

Comments about the Images

- The detection of an individual electron should be for a given n-state; how that electron got there is immaterial
- Data point spreads include sampling location and uncertainty
- *Middle-top-left* figure is produced with the published scaling; it does not give overlay of features as expected for n = one, two, three, or four n-states; corresponding bands are missing in higher energy images, if x, y-scales are correct
- *Middle-left-bottom* figure shows stacking of images based on features in the higher energy image below it in the manner indicated in the triangle at the right; when done this way, the orbitals shown n^2 scaling, there is considerable asymmetry in the data in the direction of the arrow; this gives rise to significant skewing artifacts in that direction
- *Just below*, light pink bands indicates probable location uncertainty; when 4 states are observed; the bands should be the same for all electrons counted under the same conditions; overlaps give streaking artifacts, esp the yellow in the ‘QM (3,26,0)’ image
- How the MCAS model would explain the data, *if* electron detection is only at the orbital extreme, is shown in the figure *just below*
- Electron orbitals are not properly represented by dots concentrated towards the center of an orbital lobe; this is clearly indicated by the figure at the *far-left-bottom*

From (2,27,0) above

Electron detection in an orbital

(Lower orbital levels erased by JMW)

Overlaid using features of underlying Image

Red circle radii: 1, 4, 9, 16

Flattened MCAS MC Orbital Tips

The original images (*upper-left set of images*) demonstrate cleanly separated, outer regions for the higher activated states. Delving into the inner orbital makeup is a bit difficult when the images are apart. To address this problem, the images, which were indicated in the published work to have the same scale, were stacked with the highest energy image at the bottom (*upper-middle image*). The outer region of each lower energy image was removed in order not to obscure that portion of the image below. Since the second lowest energy image indicated a tight center, that center was copied and placed on the top. Alternating rings would have to be missing in several of the published images, if the individual x-y scales are correct. Also, some image details, esp. those of the middle two energy level images, do not overlay. This overlay from the publication’s indicated scaling is inconsistent and therefore has been “**X**’d” out.

The published images are stacked differently in the *bottom-middle image*. Each lower energy image is scaled to the inner structure of the higher energy one placed just below in the manner indicated in the triangle in the *upper-right image*. Again, the outer portion of the next upper image is removed to show the outer region of the image below. Images higher in the stack have also been made more transparent to show some of the lower image’s details. While the rings are nearly circular, they are not uniform. An obvious bias (asymmetry in the detection or detector array?) in the populations is indicated by the arrow. This bias is likely a systematic issue in the data collection as it appears in all of images. The spread in the rings is likely from uncertainties in both actual electron locations and experimental error. Together, they will produce the artifacts that prevent the “dark blue” circular regions that separate the lower energy orbitals from being complete and the non-circular skewing in the ‘QM (0,29,0)’ image. More about this is discussed below.

The PhysRevLett article indicates that only four levels are present and that is clearly evident in the *bottom-middle image*. It is also clear that the levels scale closely to $n^2 = 1^2, 2^2, 3^2$, and 4^2 (see the red circles in the *bottom-middle image*) when stacked in this manner.

There is considerable asymmetry in the data in the direction of the arrow. This gives rise to significant skewing artifacts in that direction. The light pink circular bands in the *lower-right image* indicate the possible uncertainty in the characterization of the highest energy orbital of the ‘QM (3,26,0)’ image. It would be the same for all of the orbitals measured under the same conditions. (The second highest energy image (‘QM (2,27,0)’) appears to have a bit less uncertainty which would explain why it is sharper and more widely shown.) The uncertainty bands overlap for the lowest 3 energy orbital states in the ‘QM (3,26,0)’ image; this leads to streaking artifacts, notably, the yellow ones.

How the MCAS model would explain the data, *if* electron detection is only at the orbital extreme, is shown in the *lower-right-image*. The tip portions of the flattened MC-orbitals are placed at the mid-region of the various energy rings. This indicates zero movement towards or from the nucleus. While the electron will move through 3D-space in its journey to and from the nucleus, it is at these zeniths that the electron will most readily be detected. The probability of locating an electron has a time factor as well as the normal electrostatic ones that are typically considered.

The *lower-left image* shows an experimentally observed orbital – the outer orbital of the ‘QM (2,27,0)’ image – wherein the lower energy orbitals have been erased for clarity. This image clearly demonstrates that electron orbitals are not properly represented by dots concentrated towards the center of an orbital lobe. Dot representations are even more misleading when the lobes are not even nucleus-centered! One should also seriously question the imagery of molecular bonds as “capsules” whose space is filled with dots of ‘electrostatically non-repelling, spin-paired, electrons’.

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Chapter XIII

Changes in Avogadro's Number over Time

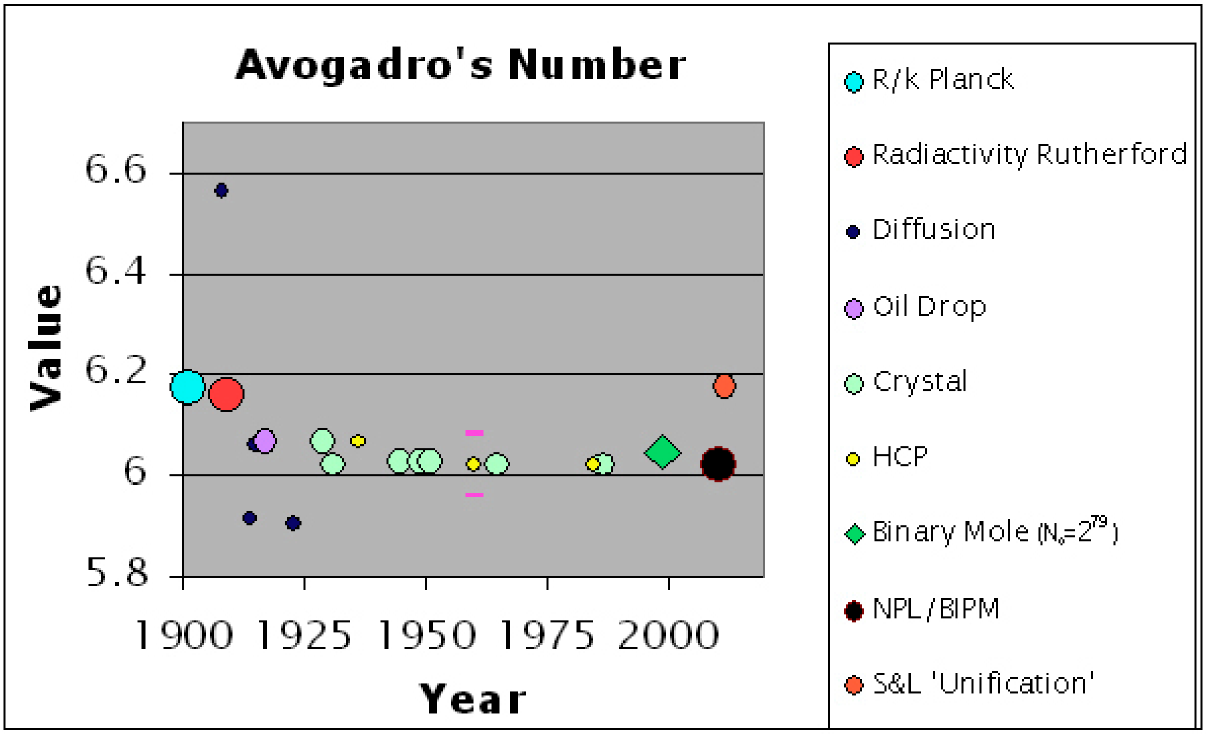
Abstract

ALL of the methods to determine Avogadro's Number should give the same value! The x-ray crystallography method has commanded the quest since the 1930's. Defining the ninth digit via x-ray crystallography when the second or third digit differs from that of other methods is counter to the scientific approach for seeking the correct answer.

DISCUSSION

Scientists strive for accuracy, but often mistake precision for it. Currently the effort is to look for the ninth or tenth decimal place of Avogadro's number while relating it to the arbitrarily defined mass of a chunk of metal in France. Better that they should base it on all scientific methods and look for the convergence of all to a single value at least to 4 digits.

A brief look at the changes in the value of Avogadro's number with time and methodology is given in the figure below with the sources listed in a table further down.



The crystal and NPL/BIPM values are driven by the definition of the kilogram with the HCP values following suit. Other than the widely variant diffusion values, the values from the other approaches indicate that the x-ray derived values are too low.

ALL of the methods should give the same value of Avogadro’s Number!

The numbers of 28Si atoms in those highly polished, “kilogram” spheres are certainly well-determined. With the “proper” value of Avogadro’s Number, a “proper” value of the kilogram can be obtained.

Redefining the kilogram via [Kilogram → x-ray Avogadro's Number → Kilogram] is circular reasoning.

A good history of Avogadro’s Number is at:
http://depa.fquim.unam.mx/amyd/archivero/Avogadro%5C's_Number_17614.pdf:
Also http://www.nist.gov/director/vcat/upload/International-Metrology-and-the-Redefinition-of-the-Kilogram.pdf
Consensus in this reference?

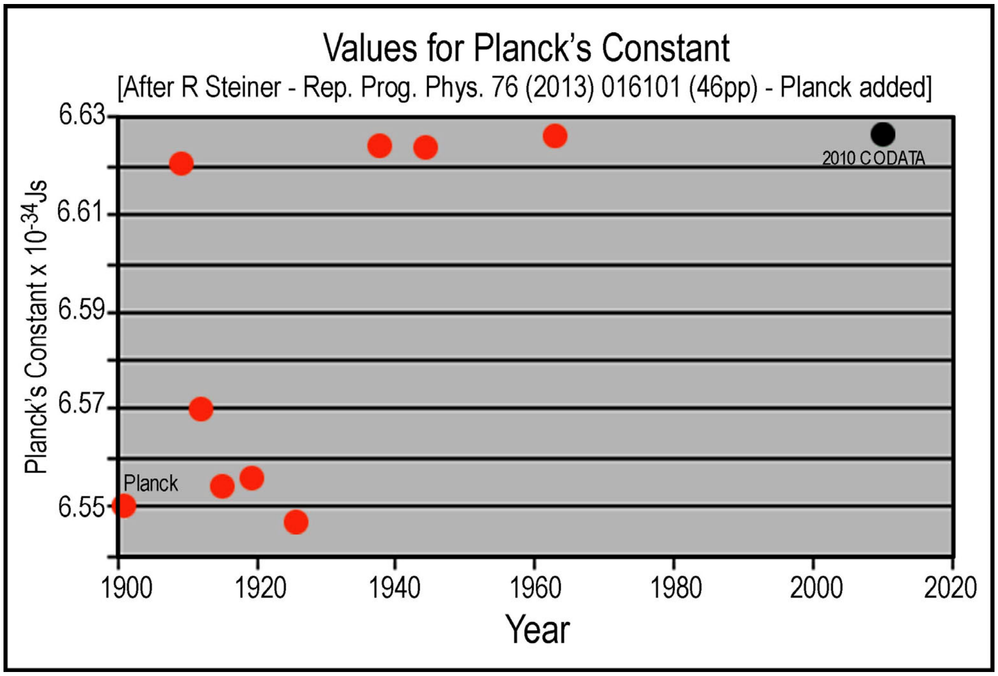
Year	**Source**	**Method**	**Value/10^23**
1873	J D van der Waals	Early	11
1908	J Perrin	Early	6.7
1914	T Fletcher	Early	6
1890	W RRontgen	Film	7
1890	J W S Rayleigh	Film	6.08
1924	PL du Nouy	Film	6.004
1901	M Planck	R/k	6.175
1909	E Rutherford	α-particle theory	6.16
1908	A Einstein	Diffusion theory	6.56
1914	I Nordlund	Diffusion in fluids	5.91
1915	A Westgreen	Diffusion in fluids	6.06
1923	TWShaxby	Diffusion in fluids	5.9
1903	HA Wilson	Oil drop method	9.3
1904	J JThomson	Oil drop method	8.7
1917	RA Millikan	Oil drop method	6.064
1929	R T Birge	Crystal	6.064 4
1931	J A Bearden	Crystal	6.019
1945	R T Birge	Crystal	6.023 38
1949	M E Straumanis	Crystal	6.024 03
1951	JWM DuMond	Crystal	6.025 44
1965	J A Bearden	Crystal	6.022 088
1987	R D Deslattes	Crystal	6.022 134
2011	NPL/BIPM	Crystal (kilogram & 28Si)	6.022 140 78
1936	Handbook Chem & Physics		6.064
1960	Handbook Chem & Physics		6.02
1985	Handbook Chem & Physics		6.022 045
1996	JM Williams Binary Mole	Halving decay to whole unit	6.044 629 098 073 145 873 530 88
2012	Seshavatharam & Lakshminarayan http://vixra.org/pdf/1209.0106v1.pdf	"Unification?" Rest mass - Gravity	6.174 407 621

Note the near identity of Millikan’s 6.064 1917 oil drop value, and Birge’s 6.0644 1929 crystal value; the 1936 HCP reflects these. Note, now, the 0.041 drop in Birge’s 6.0644 crystal value to 6.02338 in 1945. The change from the oxygen standard to carbon-12 did not occurred until 1967 with the International Committee for Weights and Measures and until 1971 with the General Conference on Weights and Measures. Avogadro’s Number then began to hone in on 6.0221. Not surprisingly, the current 2010 CODATA Faraday (coulombs/mole) divided by the current e-charge (coulombs/electron) give 6.022 141 293, as the mole is based on the current definition of the kilogram and thus circular reasoning.

There is much intertwining of physical property values with Avogadro's Number being common to many. Hence, "adopting a concrete value" for some properties forces other properties to have "preordained" values. Avogadro's Number has thus been "directed".

Planck's "constant" was "1.2% greater" in 2010 (6.62606957(29) $\times10^{-34}$ Js: 2010 CODATA) than it was in 1901 (6.55 $\times10^{-34}$ Js: copy of Planck's paper at http://bourabai.kz/articles/planck/planck1901.pdf); their ratio and the current Avogadro's Number give an Avogadro's Number of 6.092 that is in line with values (6.1; average of Planck, Rutherford, Millikan, Birge) until the 1930s. It is interesting that, while Planck's papers in the early 1900's are referenced in a history of Planck's Constant (http://iopscience.iop.org/0034-4885/76/1/016101/pdf/0034-4885_76_1_016101.pdf), Planck's 1901 Constant value is not plotted in Fig 2 of that reference that spans 1900 to 2020. I have reproduced Steiner's Fig 2 and added Planck's value in the following figure.

The plot of Planck's Constant (E=hc/λ) values in Js (m2kg/s) with time and the plot of Avogadro's Number earlier indicate that these two physical "constants" have simply been reciprocally changed: new product/old product = [(6.62606957*6.022141)/(6.55*6.1)] = 0.999. Did Planck also make a mistake as has been attributed to others before the jump in Planck's Constant around 1930 in the history account? Again, the issue is all about the definition of the kilogram.



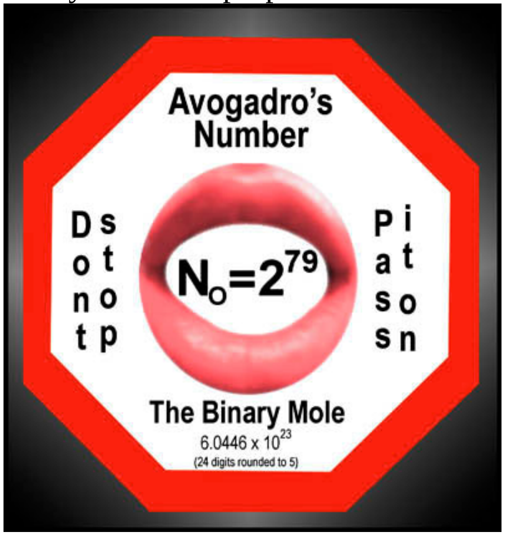
From the plot of Planck's Constant in Fig 2 of that reference and the plot of Avogadro's Number in this paper, it appears that these two physical "constants" have simply been reciprocally changed: [(new product)/(old product)] = [(**6.62606957*6.022141**)/(**6.55*6.1**)] = 0.999. Did Planck also make a mistake as has been attributed to others before the jump in Planck's Constant around 1930 in the history account? What was deemed so untouchable that these two were reciprocally treated?

Considering all of the changes in many of the physical units over the last century,
I suggest that Avogadro’s Number, thus the mole, be a very simple expression
and have a value between the old and current values.

$N_o = 2^{79}$ is such an expression.

Its full integer value is **$6.04462909807314587353088E^{23}$** for the fine stuff and standards
while **$6.0446E^{23}$** is good enough for the rough stuff.

Experimentally measured properties can then fall in step.



A note about integer quantities

A dozen is a set integer count of things - (12) - whether it is eggs, rolls, balls, screws, nuts, etc. Suggesting that the size of the eggs should influence the count in a dozen would get a response of rolling eyes and a shaking head from anyone with much of an IQ.
A dozen large eggs should be 12.5 while a dozen small eggs should be 11.5? Ludicrous.
The difference would be in weight not numbers.
In many ways, however, that is what has been occurring over the past century with the definition of the mole.

If the Binary Mole definition is not simple enough or good enough
for those making the decision, then I suggest that,
after having a number of numbers proffered during the last century,
the powers-to-be should just bite the bullet and define the mole simply as

$6.0000000000000000000000 \times 10^{23}$

be done with it and get on with the business of specifying those physical properties that have to be measured and related to it!

Polished 28Si marbles would be distributed to standards labs and balance manufacturers defining the "new K".

Chapter XII

The spdf Atomic Orbital Model
A Violation of Common Space Physics

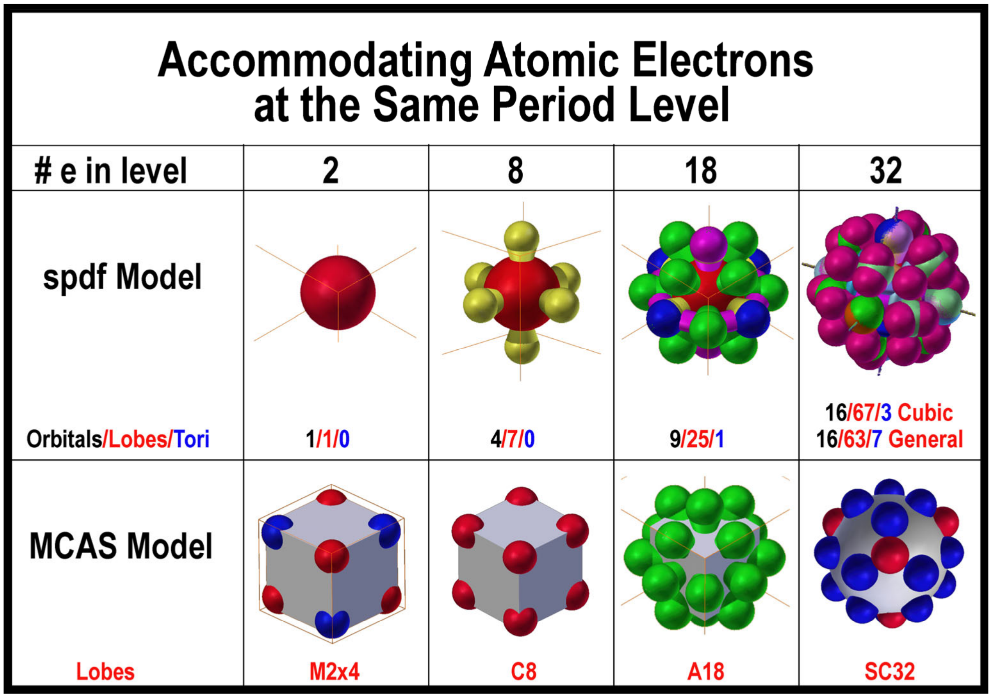
Aufbau Accommodation of Electrons around a Nucleus

Abstract

This brief has a single focus: the violation of common physical space by the spdf orbitals as they "collectively" accommodate electrons around a nucleus.

The currently espoused, spdf, electron orbital model is widely taught at all levels of education. A pyramidal chart of the orbitals is presented elsewhere[69]. The spdf orbitals are presented, studied, and applied in separate or hybridized forms, but seldom viewed from the perspective of their "collective physical totality" around a nucleus. This brief has a single focus: how do orbitals collectively accommodate electrons around a nucleus?

The top row in the figure[70] below illustrates how the spdf model accommodates electrons at the various loadings required by the elements that form the various n-levels of the periodic table.



Accommodating Atomic Electrons at the Same Period Level

# e in level	2	8	18	32
spdf Model Orbitals/Lobes/Tori	1/1/0	4/7/0	9/25/1	16/67/3 Cubic 16/63/7 General
MCAS Model Lobes	M2x4	C8	A18	SC32

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[69] Joel M Williams, http://pages.swcp.com/~jmw-mcw/spdf%20electron%20orbital%20models%20-%20inverted%20pyramidal%20stacking%20chart.jpg

[70] Joel M Williams, http://pages.swcp.com/~jmw-mcw/spdf%20versus%20MCAS%20orbitals%20for%20layers.jpg

The spdf model accommodates additional electrons of the same period by having them occupy some of the space already occupied by other electrons. Electrons are said to be able to coexist in an orbital of a set (s, p, d, or f) through “spin-reversed pairing”. Apparently, even more electrons can coexist in areas where the sets overlap. What counter-intuitive mechanism allows “two’s company, three’s a crowd” to become communal without any of them repelling any other? Note that this just addresses the agglomeration for one “n-level”. The situation is compounded when other n-levels are added to the mix. One would expect the “atomic machinery” to be more orderly than this.

Consider the logic of providing separate orbital space for each electron as the MCAS model does. Consider, too, that the MC orbitals are already in the “sp^3 form” needed for real molecules!

Details of both models are presented elsewhere[71]. The objective here is simply to encourage the reader to ponder the violation of common space physics on top of the other counter-intuitive physics assumptions that have been made in order to foster the spdf model.

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[71] Joel M Williams, http://pages.swcp.com/~jmw-mcw/Parsing%20the%20spdf%20electron%20orbital%20model.htm

Chapter XI

The spdf Electron Orbital Model Parsed

Abstract

The currently accepted, QM, spdf electron model is a collection of individual orbital sets designed to handle 1, 3, 5 and 7 groupings. For anyone who takes enough chemistry, these mathematically generated images are some of the most memorable – as separate presentations, that is. When combined in 3D space to contain 32 electrons, they are a mess as the sets are not orthogonal to one another; nor are they dynamic. The spdf orbital sets, their shapes, orientations, and spatial overlapping are addressed.

INTRODUCTION

The spdf orbital model of the electrons of the elements of the periodic table is now over a century old. As such, it is deeply entrenched in scientific studies. The individual components (s, p, d and f) are presented in graphic form for all to grasp. They form some of the most recognizable images of the scientific arena. Individually, that is. Images of them combined in 3D beyond the s+p level are seldom set forth. This paper has been prepared to address that issue and to illustrate how these individual components collectively handle 32 electrons.

THE spdf MODEL

The s, p, and d orbitals are quite familiar to anyone who has studied the electronic structure of atoms. The f-orbitals, on the other hand, are not so familiar. Interestingly, while the s, p, and d orbitals are presented as singular sets, there are two (2) sets in common usage for the f-orbitals: cubic and general[72]. Images of both sets are found on the web with the cubic[73] showing up more often than the general[74].

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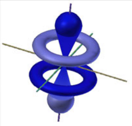
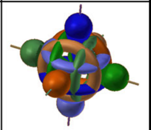
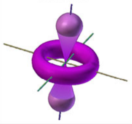
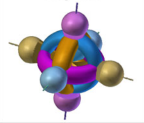
[72] Atomic orbitals: 5f (cubic set), University of Sheffield - http://winter.group.shef.ac.uk/orbitron/AOs/5f/

[73] a) Electronic Orbitals, UCDavis - http://chemwiki.ucdavis.edu/Physical_Chemistry/Quantum_Mechanics/Atomic_Theory/Electrons_in_Atoms/Electronic_Orbitals;
b) Electron Orbitals, http://www.angelfire.com/falcon2/dirgni/orbitals.html;
c) 4f Orbitals (General Setting) Department of Chemistry - University of Oxford - http://www.chem.ox.ac.uk/icl/heyes/LanthAct/I3.html;
d) f orbitals, WikiMedia Commons - https://commons.wikimedia.org/wiki/File:F_orbitals.png;
e) seven f orbital are less well understood, Los Alamos National Labotratory - http://www.lanl.gov/orgs/nmt/nmtdo/AQarchive/04spring/VO.html

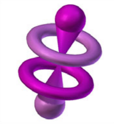
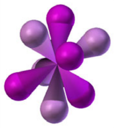
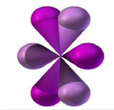
[74] a) Atomic Orbitals f orbitals, Delta School District British Columbia, Canada - https://fc.deltasd.bc.ca/~mannandale/oldchemsite/Chemistry11/Atomictheory/forbitals.htm;
b) f-orbital models on stands, University of Michigan SharePoint Portal - https://sharepoint.umich.edu/lsa/physics/demolab/DemoLab%20Asset%20Library/F%20Orbital%20Models_7B50.10.bmp

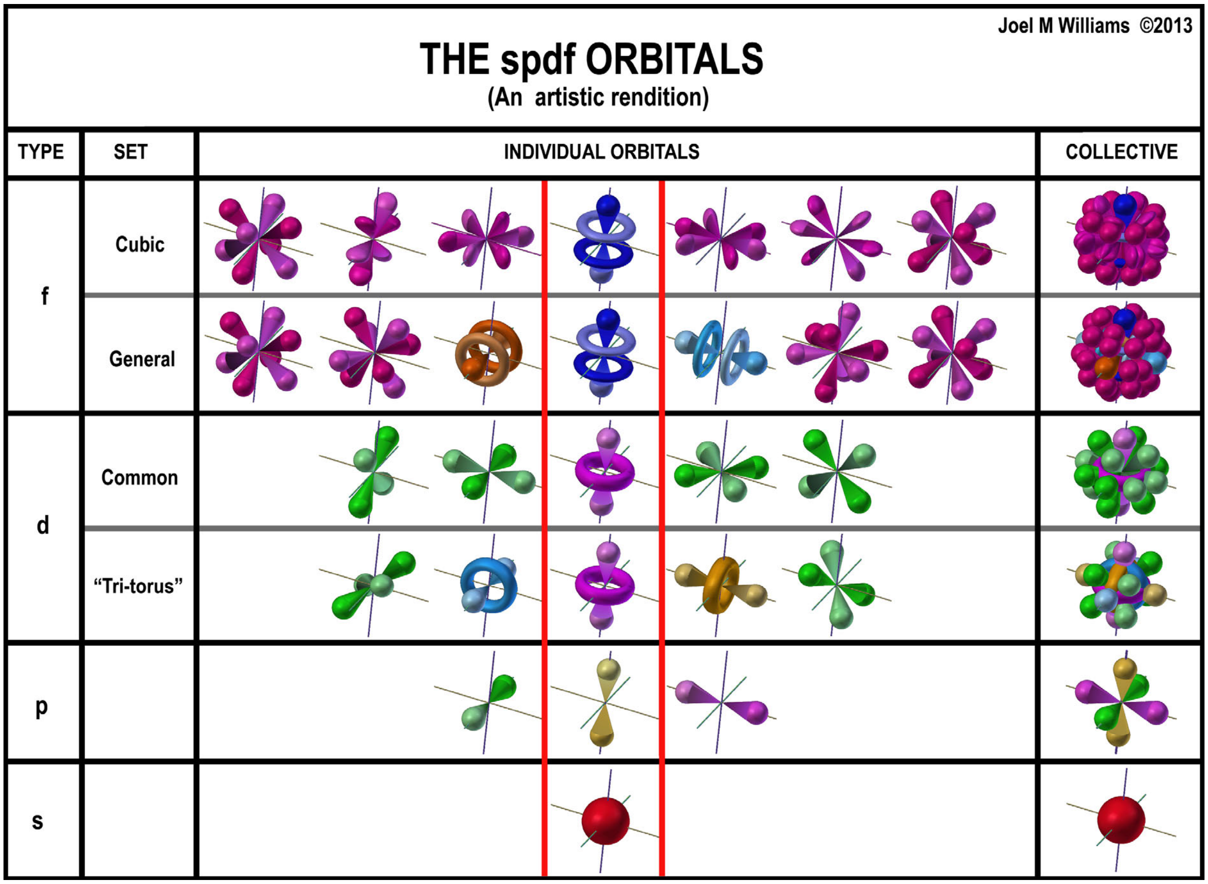
The two f-orbital sets use the three (3) orbital shapes shown in the figure at the right. Three are common to both sets[72]. The “cores” differ primarily in the number of “tori-orbitals” as shown in the figure on the left. The core of the general set gives the illusion of a “gyroscope”[75]. Why isn’t a similar set presented for the d-orbitals? The four common spdf orbital sets are presented as artistic representations in the following chart in typical, but inverted, “pyramidal” fashion along with d and f tri-torus sets.

d and f Orbital Set Cores

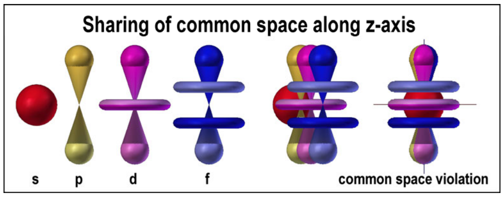
	Orbital set tori unit	
Orbitals	Cubic	General
f		
d	Current 	Why not? 

f-Orbital Shapes
(2 sets in current usage)

f-Orbital Shape	Number in Set	
	Cubic	General
	1	3
	2	4
	4	0



This layout of the spdf orbitals emphasizes what the orbitals are intended to do: model space for 1, 3, 5, and 7 pairs of electrons. What should be clear is that each set ignores the fact that it starts by occupying the space dedicated to the preceding one. This is seen in the center column of the above figure and emphasized in the figure at the right. Roughly, the electron density of ~6 electrons, out of 32,


Sharing of common space along z-axis

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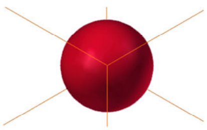
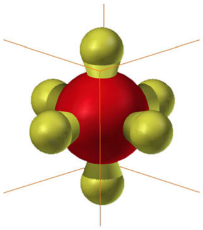
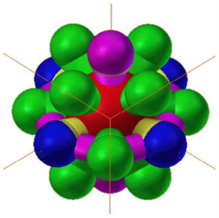
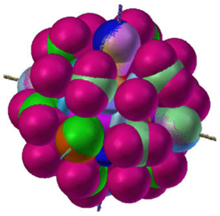
[75] Gyroscope, from collection at the National Museum of American History at the Smithsonian Institution, Department of Physics, Kenyon College - http://physics.kenyon.edu/EarlyApparatus/Mechanics/Bohnenbergers_Apparatus/Bohnenbergers_Apparatus.html

is concentrated along this axis. With similar overlaps along the x and y axes, ~60% of the total electron density of a period is concentrated in ~20% of the spherical volume! This may be nice for mathematics, but it is unlikely to occur in a real world situation.

While they can handle the 1, 3, 5, and 7 pairs separately, they do not present proper orbitals when the sums of the electrons are 2, 8, 18, and 32 as needed to address the periods of the periodic table of elements. The following figure illustrates how the spdf electron orbitals mesh to provide the number of electrons for a period in the periodic table. The spdf orbital model starts with a "mild" overlap as the s and p-orbitals combine to accommodate 8 electrons. The overlap is not so mild when the d-orbitals are added to the s/p group to handle 18 electrons. [The portions where the d-orbitals coexist with the p_x and p_y orbitals are tipped with blue; a bit of yellow can be seen where the p-orbitals are present. The p_z orbital coexists with the purple d_{x^2} orbital.] The overlap situation becomes extreme when the f-orbitals are added to the s/p/d sum. [The general f-orbital set is used in the figure.] Of note is the change in the number of lobes required to accommodate a pair of electrons: 1 for 2, 7 for 8, 25 for 18, and ~64 for 32 along with a few tori. Strange! Of course, it is, but they have been mathematically generated according to the precepts of the QM nlms numbers and fitting 5 or 7-component sets into 3D space.

Accommodating Atomic Electrons
at the Same Period Level

# e in level	2	8	18	32
spdf Model				
Orbitals/Lobes/Tori	1/1/0	4/7/0	9/25/1	16/67/3 Cubic 16/63/7 General

Conclusion: the spdf orbital models look neat and crisp when viewed as independent sets of orbitals, but become a garbled mess when combined beyond the simplest grouping of 8. This garbled mess becomes even worse as more periods are considered. The spdf model is simply a rigid orbital, "file cabinet" model, starting with a single drawer and stacking more on top. The spdf model is rather myopic when broad application is considered. Dogged adherence to its rigidity indicates either that little has been learned in the past century about the actual structure or that no one dares to disturb the sacred icon.

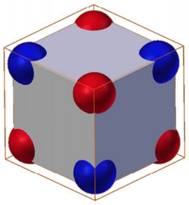
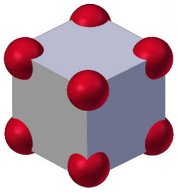
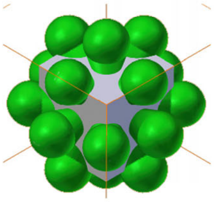
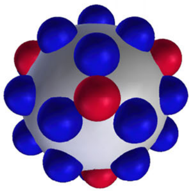
Caveat: lest the reader believe that I think very poorly of those scientists that developed the spdf/nlns model, let me assure you that I have great admiration for their reasoning and experimental efforts. The level of today's science is what it is because of their efforts and those of many, many others. It is attention to the continued adoration of a physical law-defying model to the exclusion and suppression of non-physical law-defying explanations that I give voice.

Think about alternative models that do not need the spdf assumptions.

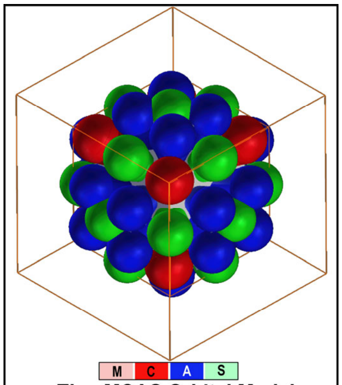
THE MCAS MODEL

Consider now the logic of starting from the standpoint of accommodating all of the electrons of each period in a symmetrical manner AND then seeing what subsets they contain. The MCAS model was developed with just this approach. The figure below shows how the MCAS model accommodates the differing numbers of electrons needed for each layer.

Accommodating Atomic Electrons at the Same Period Level

# e in level	2	8	18	32
MCAS Model Lobes	 M2x4	 C8	 A18	 SC32

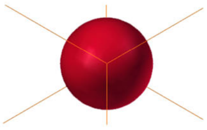
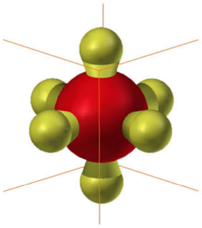
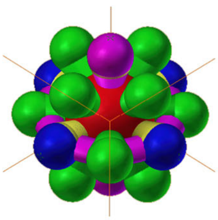
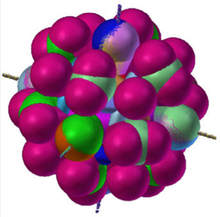
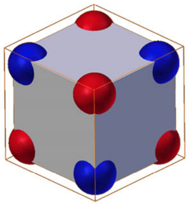
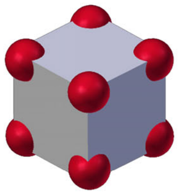
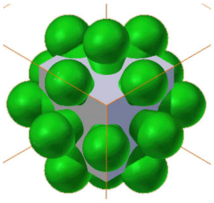
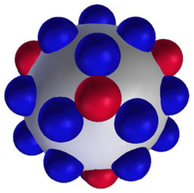
Nesting of the orbital types is clearly evident with each electron having a "dedicated" home abode. Sub-orbital units can be established to associate electrons into groups as required (that is demonstrated for the 2 electron case), but an overall symmetrical distribution of electron density (as defined by the lobes) must be maintained. The complete nesting symmetry of all of the MCAS orbital types is shown in the figure at the right.

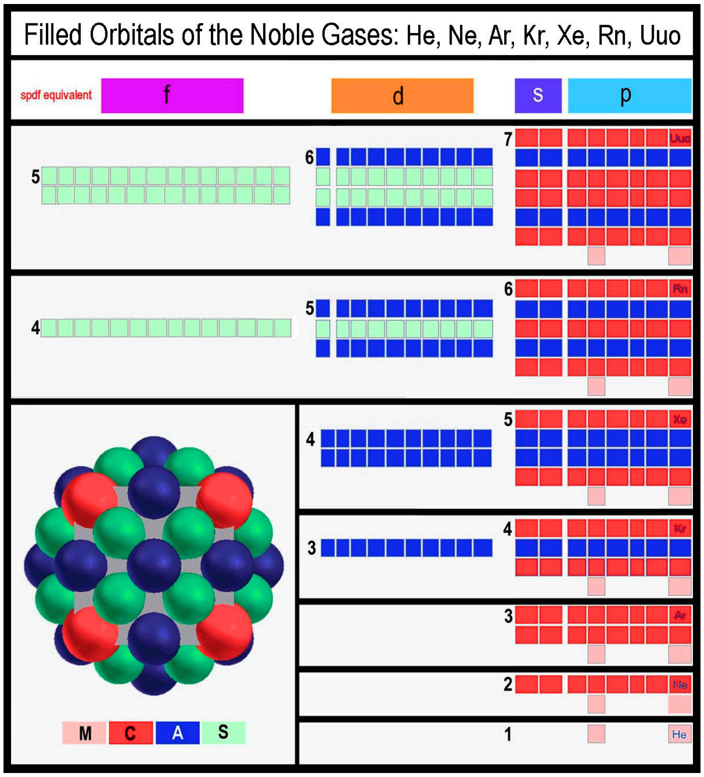


The MCAS Orbital Model

Layer nesting of orbitals is not a feature of the spdf model! Nor does the spdf model provide dedicated (orthogonal) space of the orbital sets as touted. The following figure provides a side-by-side comparison of how the spdf and MCAS models the 2, 8, 18, 32 electrons around an atom to provide an easier recognition of their differences.

Accommodating Atomic Electrons at the Same Period Level

# e in level	2	8	18	32
spdf Model Orbitals/Lobes/Tori	 1/1/0	 4/7/0	 9/25/1	 16/67/3 Cubic 16/63/7 General
MCAS Model Lobes	 M2x4	 C8	 A18	 SC32



So, what is so important about "nesting"? Consider that the currently known elements require seven (7) periods (levels) of electrons. The last element in the 7th period will contain 118 electrons in periods of 2, 8, 18, 32, 32, 18, and 8 electrons. These periods are not onion-skin layers independent of the layer above and below. "Nesting" provides the mechanism that allows electron orbitals to be placed in each period in a manner that provides the lowest energy for the total arrangement. "Nesting" of the orbitals is clearly seen in the orbital structure of the noble gases when modeling has been performed with MCAS orbitals (see figure below; its generation is presented elsewhere[76] - click here to connect).

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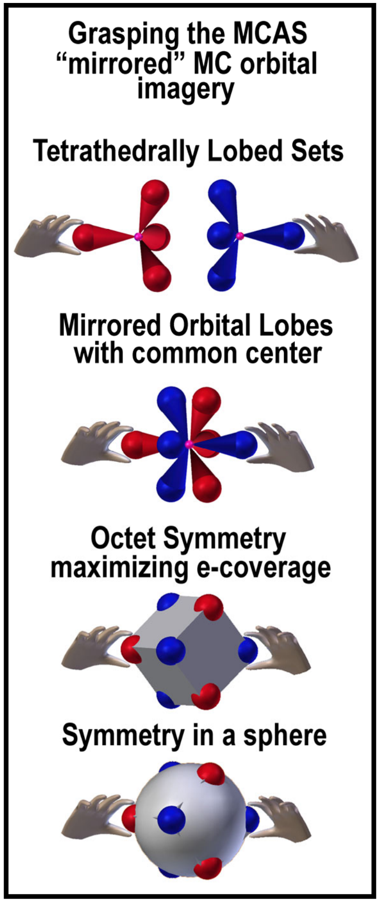
[76] Creating the Familiar Periodic Table via MCAS Electron Orbital Filling,, Joel M Williams - http://pages.swcp.com/~jmw-mcw/The%20Familiar%20Periodic%20Table%20of%20Elements%20and%20Electron%20Orbital%20Filling.htm

Note that only two levels of A or S sets ever need coordinating! Electrons in similar orbital types of different “periodic levels” are coordinated as orbital dimensions range from the nucleus outward to the farthemost extent of the orbital type. Dynamic coordination is an inherent feature of the MCAS model.

SUMMARY

The spdf model is a stoic mathematical model that is based on creating independent sets of orbitals containing 1, 3, 5 and 7 pairs of electrons. The resulting sets have memorable 3D images of their individual components. Individually, each set is aligned along the x, y, and z axes. When combined to handle 2, 8, 18, and 32 electrons in 1, 4, 9, 16 pairs, these sets are not orthogonal to one another and overlap from the very start. The noble elements require well-coordinated groups of 2, 8, 18, and 32 electrons. When the spdf orbitals are subjected to a 3D, visual summing, they present anything but a neat assemblage of the electron spaces needed to handle the required number of “periodic” electrons. It is not a matter of how the spdf orbital sets have been generated (the mathematical logic of the individual sets can clearly be followed and taught), but whether the summation logic follows the same constraints that are applied to the individual sets. When the orbital sets are combined, it is clear that the same constraints are not followed.

In contrast to the spdf electron orbital model, the MCAS electron orbital model provides simple, nesting, configurations to handle the electrons needed for the periods of the periodic table of elements.

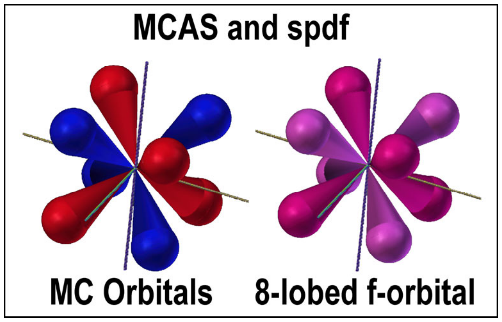


“*Comparing the Logic behind the spdf and MCAS Models*” also addresses the spd portion of the spdf model[77] - click here to connect.

ADDENDUM

The figure at the right is given to aid in understanding the MC “mirrored” orbital concept.

Stanch adherents to the spdf model who thus oppose tetrahedral orbitals in place of the spherical one should consider the similarity of one of their f-orbitals to the MC pair (see figure at right). Two electrons can occupy the f-orbital, but just how one or two of them can occupy those 8 lobes is not clear. How electrons occupy space in the MC orbitals is clear.



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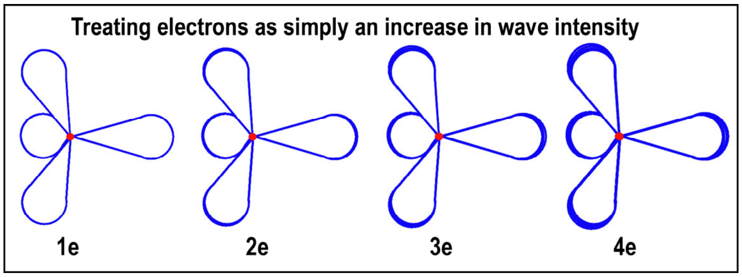
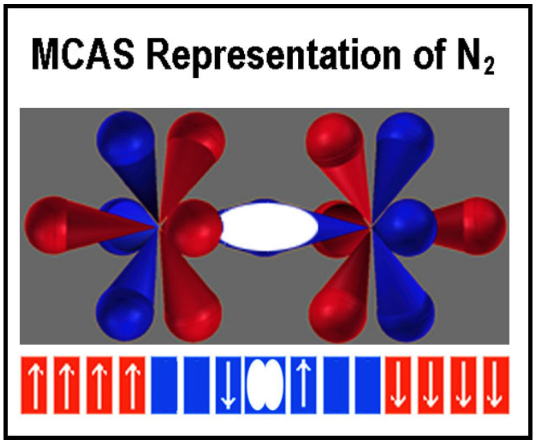
[77] Is the Logic Behind the Spdf Orbital Model Really Rational?, Joel M Williams - http://vixra.org/abs/1308.0012

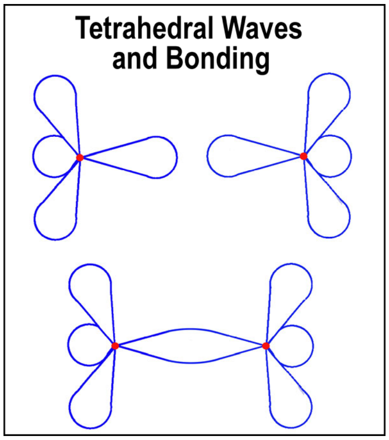
For adherents of the wave approach to electrons, think of the edges of the lobes of the tetrahedral orbital as defining the wave length. The number of electrons in the tetrahedral orbital can be thought of as the wave's intensity. This imagery is presented in the figure below. The size of the tetrahedral lobes determines how many electrons can be accommodated. The first tetrahedral unit is only large enough to handle a single electron. The wave intensity of a single tetrahedral orbital unit beyond that first level can scale to 4 (1 per lobe); the sum of the two mirrored tetrahedral orbitals can reach 8.



Bonding using the orbitals of the MCAS model has been presented elsewhere where electrostatic attracting and repelling of the electrons and nuclei are included[78]. The nitrogen molecule is shown at the right.



In keeping with the wave imagery above, the figure at the right shows the combination of tetrahedral waves from two separate atoms. Lower energy results from the longer (~doubled!) combined wave length. At the lowest orbital level, this would be one of the possibilities for H_2 (2 electrons). For the next level and a larger tetrahedral unit, the combined wave can accommodate up to 6 electrons (F_2). A 7th electron will not be accommodated as the combined wave would be more energetic than the two individual ones. Also, a "permanent" electron presence would occur between the nuclei. Think about Ne and F not forming a bond.



For those preferring a particulate model, the combined "wave lines" indicate coordinated passage of electrons around each nucleus and then onto the other giving greater mean coverage to the nuclei. There are electrostatic interactions of these orbitals with the other tetrahedral orbitals that are not shown here.

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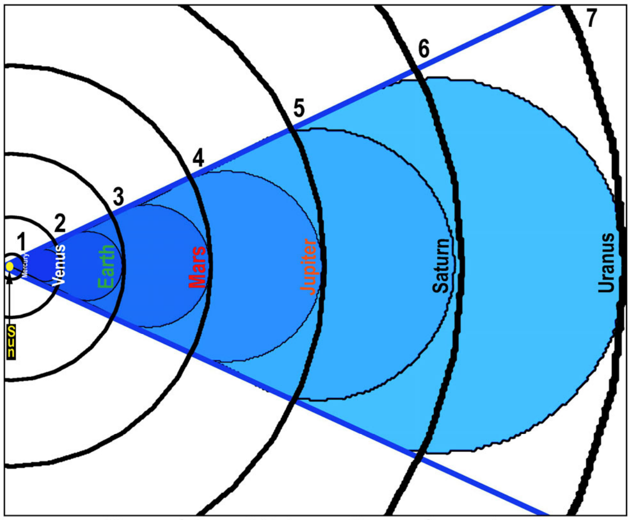
[78] a) Understanding the Bonding of Diatomic Molecules, Joel M Williams - http://vixra.org/abs/1305.0077:
b) Electron Orbital Models and the Hydrogen Molecule, Joel M Williams - http://vixra.org/abs/1305.0165;
c) Electronic Bonding of Atoms, Joel Mann Williams - http://gsjournal.net/Science-Journals/Essays/View/4043;
d) Modeling the MCAS Way, Joel M Williams - http://arxiv.org/html/physics/9902046v2 (sharper imagery at http://pages.swcp.com/~jmw-mcw/science)

For those preferring a probability model, the overlapped orbitals are simply a way of reducing the total orbital volume to be filled with the totality of electron density; 8 orbitals reduced to 7. A high concentration of electron negativity should NOT be expected in the overlap, however, as the other lobes have requirements, too. For N_2, 2 electrons would be distributed among the 7 and, as a first approximation, the overlapped region would have 0.29 electron; not 2. For F_2, it would have 0.86 electron.

Orbitals scale by n^2 (see the figure at the right). It is easy to see how a wave or moving particle could create such orbital spaces as they relate to defined energy levels. It takes a lot of energy to reach the outer limits. With sufficient energy an electron will escape the nuclear grip and leave a positively charge atom (ion). Otherwise, the electron remains associated with the nucleus in a *controlled* manner.

Electron Orbital Lobe Scaled by n^2



None of the orbitals are those of any planet
Planet names are used for emphasis of orbital magnitude

The definition of orbital space by electron probability (defined as the likelihood of finding an electron in a given spot) is less facile. Since the spdf model has electron densities concentrated in overlapped orbital spaces along the x, y, and z axes, what keeps the electrons in those overlapped probability clouds confined to a particular orbital?

Probability information reads like a census of the number of residents in tenement buildings of a complex without explaining why or how those residents got there. When thinking about forming bonds by overlapping e-rich orbitals - as is done in the current approach, consider the effect of stuffing more residents, especially hotheads, into the same tenement space while leaving other space vacant.

Chapter X

Comparing the Logic behind the spdf and MCAS Models
Is the Logic behind the spdf Orbital Model really rational?

Abstract

The currently accepted, QM, spdf electron model is a rigidly forced mathematical one. The MCAS model is dynamic and does not require that macro-physics ceases as atomic dimensions are approached. Conceived as a Newtonian model, it is just an orbital model. This essay provides a side-by-side comparison of these two models of atoms. spdf and MCAS refer to the orbital shapes in the two models. The orbital image renditions have been generated with 3D software. One should ponder about the logic behind the accepted spdf model

INTRODUCTION

Media sources relish in providing witty motivational quotes. SmartQuotes arrive daily from Sigma Xi.

> **"Do not go where the path may lead, go instead where there is no path and leave a trail."** -- Ralph Waldo Emerson[79]

Students and researchers are encouraged to explore, while accepting "established truths" without question. Don't venture too far from the beaten path, however, and definitely do not trash the superhighways.

John Dewey indicates[80], however, what often is required:

> **"Every great advance in science has issued from a new audacity of imagination".**

Max Planck indicates[81] the way things often happen in reality, however: **"A new scientific truth does not triumph by convincing its opponents and making them see the light, but rather because its opponents eventually die, and a new generation grows up that is familiar with it."**

Of course, "new scientific truths" must be "published" somewhere for that "new generation" to be aware of them. Challenging entrenched dogma meets stiff resistance. Established scientific publication houses simply ignore attempts to convey alternatives. While the Internet has its pros and cons, it does provide a venue to communicate ideas that are counter to or make significant, often unwanted, modifications to established teachings; especially to century-old ones.

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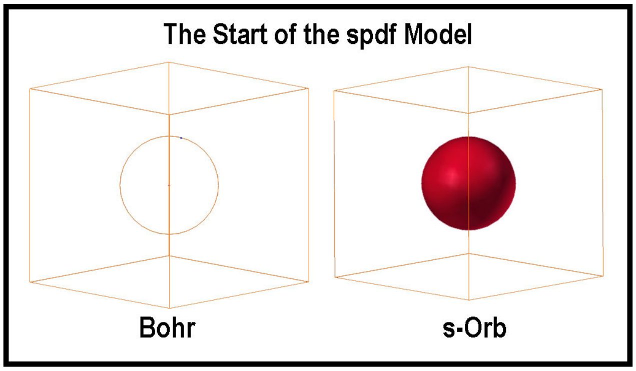
[79] Sigma Xi SmartBrief, July 3, 2013

[80] John Dewey, The Quest for Certainty: A Study of the Relation of Knowledge and Action, 1929, republished April 30th 2005 by Kessinger Publishing

[81] Max Planck, Scientific Autobiography and Other Papers, 1950

Occam's razor states that **among competing hypotheses, the hypothesis with the fewest assumptions should be selected. In other words, the simplest explanation is usually the correct one[82].**

In this essay, I exercise some audacity in challenging the current spdf model of the atom. The spdf model is neither the simplest explanation nor the correct “particulate” one as it requires that things are different at the atomic level. An abrupt change in physics near the atomic level is difficult to phantom, but widely preached. A side-by-side comparison, with 3D imagery, is presented for the spdf model versus the MCAS model. One may be surprised at their near convergence before diverging again.

COMPARING THE LOGIC BEHIND THE spdf and MCAS MODELS	
The spdf Model	**The MCAS Model**
The spdf model got off to a simple enough start with the Bohr circular representation of an electron moving around a nucleus at constant energy. This 2-D representation engendered the 3-D sphere.  It is at this point that the spdf model was “cast in concrete”, as the saying goes. Here, the definition of orbitals was decreed: an orbital contains only 1 or 2 electrons (therein the constant requirement of spin-pairing) regardless of the number of lobes or tori. Orbitals are fixed. That is, there is no hybridizing. This, of course, had to be changed when it came to addressing real molecules, but that view for the elements of the periodic table has never been changed in over a century. Thus, the spdf model for the elements is a rigid, non-conformal model. With that in mind, let us continue the logic of the model built on this circular orb-turned-sphere.	

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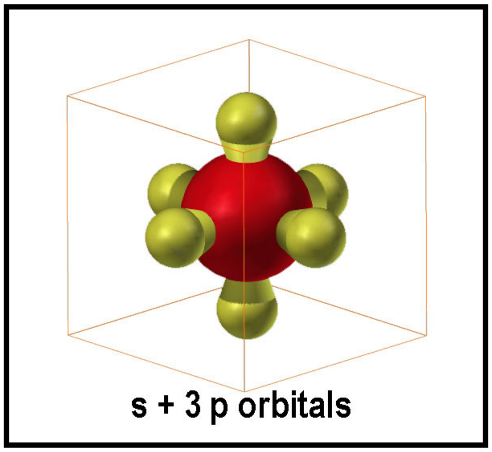
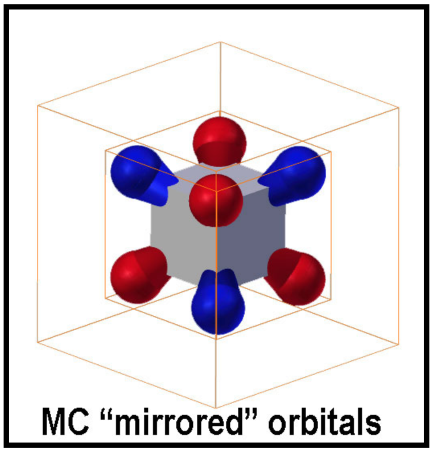
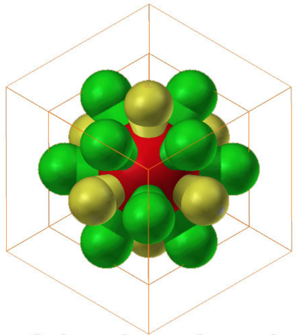
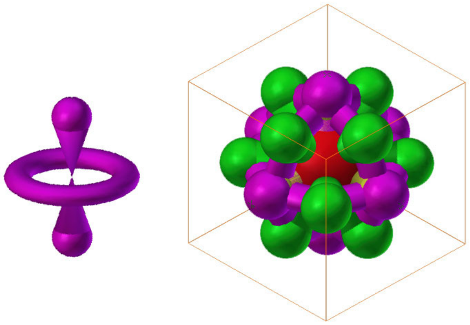
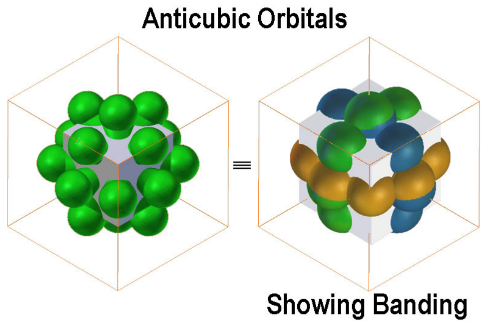
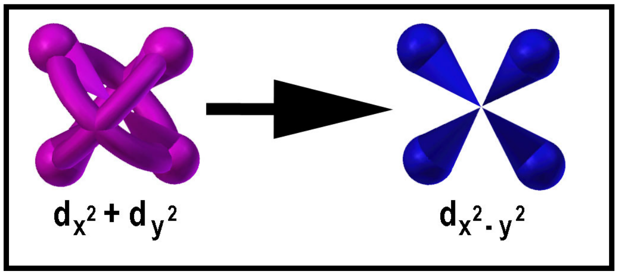
[82] http://en.wikipedia.org/wiki/Occam's_razor

The spdf Model	**The MCAS Model**
The periodic behavior of the elements next required enough orbitals to house 6 electrons (3 pairs). This was modeled with 3 orthogonal orbitals with 2 lobes each. They were given the monikers p_x, p_y, and p_z.	It is now time to introduce an alternative particulate model: the “mirrored orbital” MCAS model.
 s + 3 p orbitals	 MC “mirrored” orbitals
An interesting point here is that, while 2 electrons shared the same spherical, single-lobed space and thus had to be spin-paired, two electrons in a p-orbital could occupy opposing orbital lobes and thus be paired without spin-reversal. Reciprocal behavior would serve to “pair” them. Rigid adherence to the notion of electron spin-reversal stemmed that train of thought. Here we have completed the requirement to house 8 electrons, all-be-it in 7 lobes. The issue of why each p-orbital fills with a single electron before two could reside in one led to Hund’s rule as it was not clearly obvious why it had to be so. ⤴	The MC “mirrored” orbital sets provide 8 lobes for the 8 electrons that the s+3p orbitals do. An electron in each of the red and blue sets is equivalent to the s orbital without requiring spin-reversal and cohabitation in a single lobe. When there is only a single electron in a set, it is referred to as an “M” (mono-substituted) orbital. When all 8 lobes are filled, all 8 electrons are equivalent, unlike in the spdf model. It is easy to imagine why electrons fill in a certain pattern. First one goes into red or blue. Second goes into the other as balancing and pairing. The third goes into either and creates an unbalanced situation. The fourth and fifth go into the same and the orbital becomes center symmetric and balanced within itself. Electrons 6-8 go into the other set. In the case of oxygen, the 4-2 (triplet; normal) and 3-3 (singlet) loadings are sufficiently close in energy to have both observed.

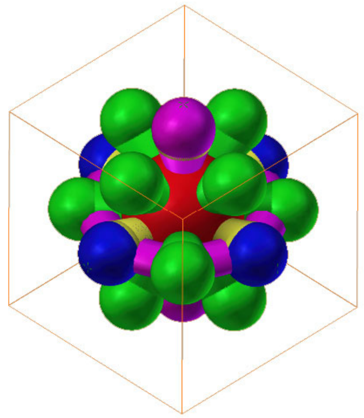
The spdf Model	**The MCAS Model**
When more electrons must be accommodated at a given level, more orbital spaces are required. The image below shows the symmetrical placement of 12 lobes in the p-orbital planes. These are designated as the d_{xy}, d_{xz} and d_{yz} orbitals with each having 4 lobes. At this stage, there are more lobes than the 18 slots required to match the number needed for the 4th period of the periodic table.  s + 3p's + dxy + dxz + dyz But, alas, the model is not flexible. Thus, the s and p-orbitals must be filled. And, by definition, a d-orbital can only house 2 electrons even with 4 lobes; so 4 electrons still need space The extra orbitals needed are provided with a new orbital shape. Enter d_{x2}, d_{y2} and d_{z2} orbitals with torus belts. These orbitals smother the p-orbitals, placing 4 electrons in the same general space. But the orbital distribution is nicely symmetrical.  d_{z^2} s + 6 d-orbitals	Below are shown the Anticubic orbitals of the MCAS model. Note the symmetry and banding. Note also that the lobes of the MCAS Anticubic orbitals are exactly the same as those of the 3p + 3d orbitals on the left that are also banded (alternating yellow and green). Unlike the spdf model, however, this arrangement is part of the flexibility of the MCAS model to accommodate 18 electrons without anything extra. 

The spdf Model

Of course, only 2 more orbitals are needed. Thus, 2 are declared “mathematically equivalent” and combined. Just how these two solutions are "equivalent" should raise some eyebrows! Posited today, this would not be acceptable. But it is "gospel" as written in text books.



This gives the correct number of orbitals with each containing 2 electrons, but the result is not spherically symmetric; only hemi-spherically. This is the currently accepted spd portion of the spdf model to accommodate 18 electrons.



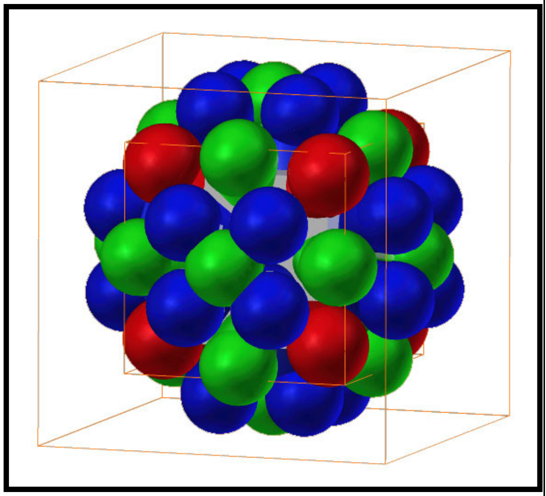
Current spd orbitals for same e-level
(Note the smothering of the p’s)

Considering the manipulation to force the rigid spdf model to just create orbital space for 18 electrons, the gyrations to accommodate 7 more doubly filled orbitals (14 more electrons) on top of this group is unwieldy. With the simplicity offered by the MCAS model, there seems little reason to spend the time doing the modeling. There are plenty of f-orbital individual models elsewhere, but few 3D spdf images as shown above for spd.

The MCAS Model

Note that the A (“**A**nticubic”) orbitals of the MCAS model handled 18 electrons with much less manipulation and with greater symmetry.

The full complement of orbitals for the MCAS model is quite simple. Orbital colors are **RED** (MC), **GREEN** (A) and **BLUE** (S).



SUMMARY

The current spdf electron orbital model is clearly not the simplest. Its uncompromising rigidity balks at the certainty that atoms will arrange their electrons in the lowest energy possible. Its premises about electron spin-reversal pairing[83] and far more lobes than necessary are not needed. The MCAS model, on the other hand, is a dynamic one requiring no electron spin-reversal and no extra lobes.

As the models address the elements of the periodic table, the reader might find the application of the MCAS model to the structure of the periodic table interesting: Creating the Familiar Periodic Table via MCAS Electron Orbital Filling.

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[83] Spin-pairing attributed to G.N. Lewis (1916) - Jean Maruani (1989). Molecules in Physics, Chemistry and Biology: v. 3: Electronic Structure and Chemical Reactivity. Springer. p. 73. ISBN 978-90-277-2598-1

Chapter IX

On Quarks, Nuclei and Boron-10 Neutron Capture

ABSTRACT

The quark make-up of protons and neutrons is discussed. Neutrons that give protons and electrons must be composed of "Combo Up or Down" quarks. The neutral baryons of stable nuclei do not contain "Combo quarks". An alpha particle containing a "Combo quark" is not the same as an electron-stripped He-4 atom which contains none. Since the mass of Up and Down quarks constitute less than 1% of the total mass of baryons, the remainder mass of these must be non-particulate mass, herein called "fat". Dumbbell models of the stable positive and neutral baryons are presented. Using these baryonic dumbbells, the extraordinary ability of the Boron-10 nucleus to capture neutrons is modeled.

Keywords: quarks, baryons, protons, neutrons, nuclei of elements, neutron capture, Standard Model, baryonic dumbbells, combination quarks, nuclear mass, quark mass, alpha particle

INTRODUCTION

After neutrons were discovered[84], it was soon found that they decayed into protons and electrons.

$$\mathbf{n = p^+ + e^- + energy} \qquad \textbf{(1)}$$

In 1956, Cowan and Reines[85] demonstrated that the energy was in the form of a neutrino. In 1964, Gell-Mann and Zweig[86] proposed that the basic components of protons and neutrons were quarks. The introduction of quarks, which have actually been detected[87], led to the Standard model[88]. While there have been many more particles introduced, neutrons and

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[84] J. Chadwick, Possible Existence of a Neutron, Nature 192, 312 (1932)

[85] (a) "Detection of the Free Neutrino: A Confirmation", C. L. Cowan, Jr., F. Reines, F. B. Harrison, H. W. Kruse and A. D. McGuire, Science 124, 103 (1956); (b) "The Neutrino", Frederick Reines and Clyde L. Cowan, Jr., Nature 178, 446 (1956).

[86] (a) M. Gell-Mann, Phys. Let. **8**, 214 (1964); (b) G. Zweig, "An SU3 Model for Strong Interaction Symmetry and Its Breaking," CERN Report No. TH 412 (Geneva, 1964); (c) Michael Riordan, The Discovery of Quarks, SLAC-PUB-5724, April 1992 (http://www.slac.stanford.edu/cgi-wrap/getdoc/slac-pub-5724.pdf)

[87] Up and Down quarks have been detected; others are suspect. Breidenbach M. et al. (1969) Observed Behavior of Highly Inelastic Electron-Proton Scattering, Phys. Rev. Let., Vol. 23, No. 16, 935-939.

[88] See Modern View (Standard Model) timeline: 1964 – present, http://pdg.web.cern.ch/pdg/cpep/history/smt.html

protons are still presented as combinations of Up and Down quarks[89]. Up quarks are designated as having +2/3 charge and Down quarks having -1/3 charge to make the mathematics work. The old equation now becomes more graphic with quarks and Feynman diagrams.

The imagery in still accepted after nearly half a century. So, what could be wrong?

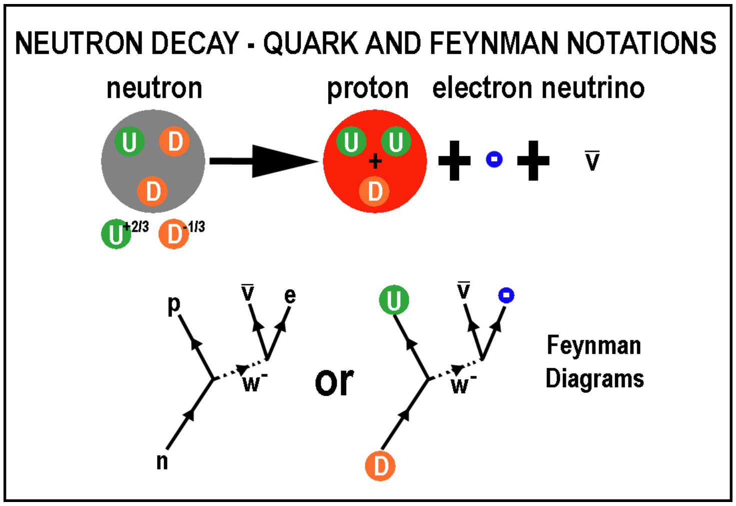

Figure 1. Current quark and Feynman notations for the decay of a neutron.

- Firstly, Up and Down quarks are supposed to be unique and singular. Thus, having a Down quark give an Up quark plus some other stuff is irrational.
- Secondly, why doesn't the Down quark of the proton decay? Unlike a neutron, which has a lifetime of ~880 seconds[90], a proton has a lifetime longer than 10^{34} years[91]. A proton's lifetime is therefore about 7×10^{23} times longer than the universe's estimated age[92], a number slightly greater than an Avogadro's binary mole (2^{79})[93]! The total mass of the earth's hydrosphere[94] is 1.4×10^{24} g and therefore about 10^{24} protons. You're not likely to be in the right place, if one should decay.
- Thirdly, many of the elements of the periodic table are quite stable, in spite of having many "neutrons".

Recent studies at Jefferson Lab indicate that two Up and Down quarks pair up in protons and neutrons and leave the 3rd dangling[95]. They indicate that paired quarks can have different behavior than the single. Diquarks have not been confirmed nor dismissed, yet, so the nature of the quarking of the baryons is still a bit unsettled. This paper will focus on the current Standard Model view and the application of the triad quarks to some nuclei and to neutron capture.

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[89] Protons and neutrons have recently been addressed with the 3-spaces model: The Mechanics of Neutron and Proton Creation in the 3-Spaces Model, André Michaud, http://www.ijerd.com/paper/vol7-issue9/E0709029053.pdf

[90] Fred E. Wietfeldt and Geoffrey L. Greene, The neutron lifetime, Rev. Mod. Phys. 83, 1173–1192 (2011); http://rmp.aps.org/abstract/RMP/v83/i4/p1173_1

[91] http://www-sk.icrr.u-tokyo.ac.jp/whatsnew/new-20091125-e.html

[92] How Old is the Universe? http://map.gsfc.nasa.gov/universe/uni_age.html

[93] J.M. Williams, The Binary Mole, http://arxiv.org/html/physics/9904016v1; http://pages.swcp.com/~jmw-mcw/binary_mole.htm

[94] http://nssdc.gsfc.nasa.gov/planetary/factsheet/earthfact.html

[95] (a) JLab 2013 News, Quarks Pair Up in Protons and Neutrons, https://www.jlab.org/news/stories/quarks-pair-protons-and-neutrons; (b) G. D. Cates, C. W. de Jager, S. Riordan, and B. Wojtsekhowsk, Flavor Decomposition of the Elastic Nucleon Electromagnetic Form Factors, Phys. Rev. Lett. 106, 252003 (2011), http://prl.aps.org/abstract/PRL/v106/i25/e252003

DISCUSSION

The current Standard Model as presented in Figure 1 must be wrong. A neutron must not be made up of an Up quark and 2 Down quarks. To be consistent with Up and Down quarks being “singular and unique”, a neutron must be made up either of 1 Up quark, 1 Down quark and a combo of an Up quark with an electron and a neutrino (Option A - closer to the current) or 2 Up quarks and a combo of a Down quark with an electron and a neutrino (Option B). The mathematically correct representations are shown in Figures 2 and 3. Up and Down quarks are stable as indicated by the stability of the proton. In neither case is the unstable quark a stable Down quark as implied in the Standard Model. This might be the reason for the JLab results. Of course, it also indicates the problem of being able to distinguish the difference between combo quarks and simple ones of the same charge.

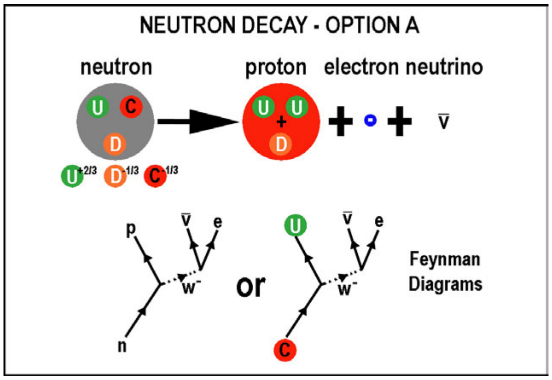

Figure 2. Neutron Decay Option A: Conversion of a combo component to an Up quark.

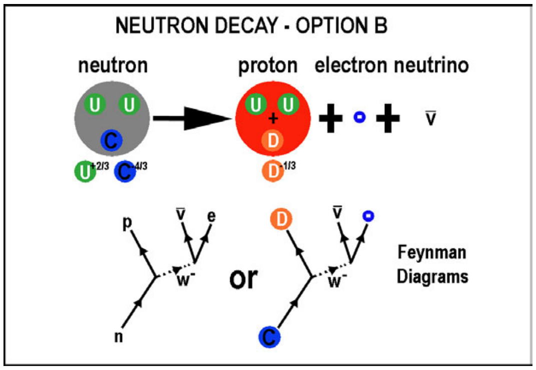

Figure 3. Neutron Decay Option B: Conversion of a combo component to a Down quark.

Both forms of the neutron would seem logical. The stability of the Up-combo and the Down-combo might be an issue, however. Why? Well, one could deliver the results when neutron decay is observed and the other could be the means to more stable, but still radioactive nuclei. Also, a Down-Up-Down assemblage of quarks, where the Downs are not combos with electrons, should give a stable neutral baryon, nee “nuclear neutron”.

RAMIFICATIONS FOR THE NUCLEI OF THE ELEMENTS

Assuming that Up and Down quarks[4] are the only “particle” constituents of a proton, it seems logical that they must surrounded by “fat” within the nuclear confinement. This can be represented by the following equation:

$$\mathbf{(U_{fat} + U_{fat} + D_{fat})}_{\text{proton nucleus}} \quad = \quad \mathbf{(U_{lean} + U_{lean} + D_{lean} + \text{“fat”})}_{\text{ proton nucleus}} \qquad \textbf{(2)}$$

And, if quarks can be fat and lean, then it is reasonable to assume that leptons can also be. Thus, neutron decay becomes

$$\mathbf{(U_{fat} + C_{fat} + D_{fat})}_{\text{neutron nucleus}} \rightarrow \mathbf{(U_{fat} + U_{fat} + D_{fat})}_{\text{proton nucleus}} + \mathbf{W_{fat}} \qquad \textbf{(3a)}$$

or

$$\mathbf{(U_{fat} + U_{fat} + C_{fat})}_{\text{neutron nucleus}} \rightarrow \mathbf{(U_{fat} + U_{fat} + D_{fat})}_{\text{proton nucleus}} + \mathbf{W_{fat}} \qquad \textbf{(3b)}$$

with

$$\mathbf{W_{fat} = (e_{fat} + \nu_{fat})} \sim\sim\sim\sim\sim\sim\sim\sim\sim\sim\sim\rightarrow \mathbf{e_{lean} + \nu_{lean} + \text{“fat”}} \qquad \textbf{(4)}$$

“Fat” must be non-particulate, non-descript “mass”. How much “fat”? For a proton, the “fat” is 106 times the mass of the quark sum (0.938% of the total and experimentally observed[96]!). Since a neutron’s mass is 0.001388 greater than that of a proton, this is W_{fat}. Thus, the “fat” around the electron adds 0.00084 or 53.1% to the mass of the electron when in the nucleus, assuming there is little fat around the neutrino. How that “fat’ is manifested is another matter.

The emphasis of high-energy research has been to delve deeper and deeper into the nucleus. Modeling has thus been on the simplest: proton and neutron and smaller. Most of the naturally occurring elements of the periodic table have very long lifetimes. Other than hydrogen, these elements have more mass than can be attributed to the protons alone. The extra mass is thus attributed to neutrons which add no charge. Considering the lifetime of a neutron, some other explanation is needed. Indeed, a “nuclear sphere” of proton and neutron balls seems rather far fetched anyway. Considering that a proton is quite stable with Up and Down quarks, it would seem that other stable nuclei are simply coordinated arrangements of these two stable quarks and their “fat” without the Combo with electrons. Extra “fat” is needed as the nuclear “body” grows. As an example, consider the nuclei of deuterium, tritium, helium, and mercury.

stable $(3U_{lean} + 3D_{lean} + \text{“fat”})_{\text{deuterium nucleus}}$ **(5)**

whereas

unstable $(4U_{lean} + C_{up\ lean} + 4D_{lean} + \text{“fat”})_{\text{tritium nucleus}} \rightarrow (5U + 4D + \text{“fat”})_{\text{He-3 nucleus}} + 1e$ **(6)**

or

$(5U_{lean} + 3D_{lean} + C_{down\ lean} + \text{“fat”})_{\text{tritium nucleus}} \rightarrow (5U + 4D + \text{“fat”})_{\text{He-3 nucleus}} + 1e$ **(7)**

stable $(6U_{lean} + 6D_{lean} + \text{“fat”})_{\text{He-4 nucleus}}$ **(8)**

stable $(280U_{lean} + 320D_{lean} + \text{“fat”})_{\text{Hg-80 nucleus for mass 200 (80p+120”stable n”)}}$ **(9)**

Consider that, if quarks are actually grouped in triads, the positive triads (protons) and neutral triads (“stable neutrons”) would likely be dumbbell-shaped as depicted in Figure 4. Can you imagine crystal–like networks – with and without flaws? Can you imagine how 80 UDU and 120 DUD dumbbells could be logically assembled for the Hg-200 nucleus? How about simple, minimal energy, arrangements of 600, individual, stable quarks? Since radioactive tritium has a half-life of 12.3 years[97] (441,000 x that of an “unstable neutron”), combo quarks can form pseudo stable nuclei. Can a non-radioactive H-3 (tritium) exist in analogy to He-3?

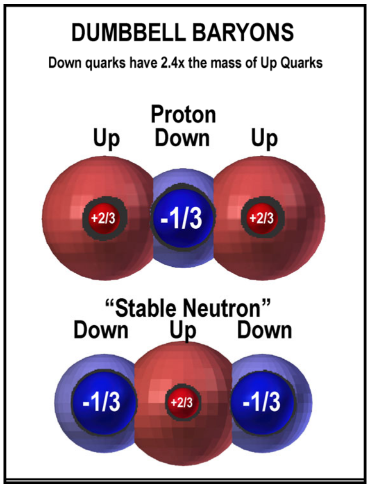

Figure 4: Dumbbell shapes for positive and neutral baryons.

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[96] (a) http://physics.info/standard/; (b) Adrian Cho, Mass of the Common Quark Finally Nailed Down, http://news.sciencemag.org/sciencenow/2010/04/mass-of-the-common-quark-finally.html

[97] http://www.epa.gov/radiation/radionuclides/tritium.html

NEUTRON CAPTURE

An interesting behavior of some nuclei is their ability to capture neutrons. In this realm, few nuclei rival that of Boron-10 and the only naturally occurring ones better at it are rare earth elements and Cadmium[98]. This light mass element has a neutron cross-section 1000 to 100,000 times bigger than a "barn" (a barn is the size of a Uranium nucleus[99]) when capturing low energy neutrons[100].

$$\textbf{Boron-10}^{5+} + \textbf{n} \quad \rightarrow \quad \textbf{Li-7}^{3+} + \textbf{Alpha Particle}^{2+} \tag{10}$$

The natural occurrence of Boron-10 and the facileness of this reaction allow it to be considered in low energy neutron cancer therapy[101].

The reaction seems simple enough, but what is the reason for Boron-10's unusual ability to capture neutrons? A low-energy transition pathway involving a loose and easily deformed nuclear mass would provide an excellent answer. The modeling in Figure 5 of the interaction of a possible Boron-10 nucleus with a neutron is based on the foregoing discussion of dumbbell baryons forming nuclei. With arrows to indicate baryon movement, it should be easy to follow the capture and conversion to observed products. Refer to Figure 4 for the shapes of the positive (proton) and negative (neutron) baryons, if necessary. The effectiveness of a softer punch (lower energy) by the approaching neutron should be clear. If the neutron is of the "combo" variety, the alpha particle will not be the same as He-4 stripped of its electrons. If it is of the "stable" Down variety, it will be.

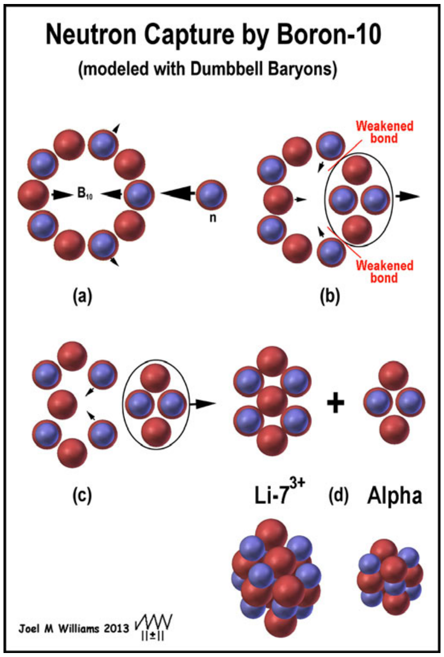

Figure 5. An explanation of the ease of neutron capture by a Boron-10 nucleus

Just as the electrons form orbital structures around a nucleus, a nucleus will have its components arranged in as minimal an energy configuration as possible. Whenever unstable "quark combos" or voids are formed to achieve these minimal-energy states, nuclear instability will follow. Also, a nuclear configuration will not emit a uniform field of electromagnetism. This will then influence the behavior of the electrons swarming around the nucleus.

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[98] http://environmentalchemistry.com/yogi/periodic/crosssection.html

[99] http://en.wikipedia.org/wiki/Barn_(unit)

[100] See plot at http://en.wikipedia.org/wiki/Boron

[101] (a) Neutron capture therapy of cancer, http://en.wikipedia.org/wiki/Neutron_capture_therapy_of_cancer#cite_note-Barth2012-45; (b) Barth, RF. Boron neutron capture therapy at the crossroads: challenges and opportunities. Applied Radiation and Isotopes 2009; 67:S3-S6; (c) The Basics of Boron Neutron Capture Therapy, http://web.mit.edu/nrl/www/bnct/info/description/description.html

SUMMARY

Neutrons that give protons and electrons must contain a “Combo Up or Down” quark. Neutral baryons of stable nuclei contain stable Up and Down quarks and no “Combo quarks”. An alpha particle containing a “Combo quark” is not the same as an electron-stripped He-4 atom. Up and Down quarks constitute less than 1% of the total mass of baryons; the remainder mass of these must be non-descript, non-particle mass, herein called “fat”. The triads of individual positive and neutral baryons form complementary barbell units with distribution of mass and electrostatic charge that facilitate nesting. The interaction of these dumbbells provides a mechanism for easy capture of neutrons by the Boron-10 nucleus.

Chapter VIII

Mirrored Orbitals Explain the Ortho/Para States of Helium

ABSTRACT

Helium provides the simplest, multi-electron, atomic situation. Quantum mechanics addresses the different magnetic and spectral properties of ortho and para helium with "mirrored twin" electrons. This paper addresses that difference with "mirrored rooms" and no electron spin-reversed pairing in the same orbital – a different implementation of parity. Models are provided to illustrate why each form of helium can not be converted to the other in a single photon-induced step. These models also illustrate the vastly greater orbital sizes of the excited states over the ground state. Included is a reference to a paper demonstrating that classical physics provides the physical mechanism that explains why an electron's energy levels scale with the square of integers. The mirror-room orbitals would also be appropriate for non-classical approaches without requiring spin-reverse pairing of electrons in the same orbital.

INTRODUCTION

Back a century ago, scientists worked diligently to explain the spectral data of excited atoms. These spectra included S(harp), P(rincipal), D(iffuse), and F(undamental) lines that were to be addressed. The main thrust of the physical model that continues to this day got its start with Bohr's circular-turned-spherical orb. From this "electron globe of a house", plans for larger electron families were drawn. Thus, basic, "1-room", spherical bungalows" were up gradable to "4-room split levels". With plans for adding 5 or 7-rooms, "electron condos" were created. The plans got labeled: s (1-room), s+3p (4-room split-levels), d (5-rooms), and f (7-rooms) - spdf for short. Those versed in the subject will, of course, note the Upper-lower S/s, P/p, D/d, F/f case connection. Double occupancy was required to satisfy the periodic table of elements, starting with helium.

Pauli mused that there was a problem of which occupant was which when the rooms were doubly occupied. Heisenberg, who made significant contributions to what became "quantum mechanics"[102], came to his rescue when he wrote to Pauli in 1926 that electron spin might be the solution to the ortho/para helium phenomenon[103] and thus to Pauli's exclusion problem.

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[102] Heisenberg was awarded the 1932 Nobel Prize "for the creation of quantum mechanics": Landsman, N.P. Getting even with Heisenberg. An Essay Review of P.L. Rose's, HEISENBERG and the Nazi Atomic Bomb Project: A Study in German Culture (Berkeley: University of California Press, 1998 http://philsci-archive.pitt.edu/9362/1/heisenberg.pdf

[103] (a) James, J. and Joas, C. http://quantum-history.mpiwg-berlin.mpg.de/news/workshops/hq3/hq3_talks/16_joas-james.pdf, **2010**; (b)Bloch, F. Reminiscences of Heisenberg and the early days of quantum mechanics, *Physics Today*, **1976**, Dec, 27; http://physics.clarku.edu/courses/171/sreading/HeisenbergW.pdf

So, “parity electron twins” that occupied the same room (cell, orbital) were created to give each twin a unique SS#[104]. Some would say that ortho/para helium proved the correctness of the quantum mechanics approach. In any case, endorsement of the QM approach certainly stifled alternative views while encouraging additional explanations that supported the basic, spdf, design.

The “quantum mechanical – spin-paired” model still is the accepted convention: n (floor level), ℓ (room shape), m (wing), and s (left or right-handed twin in the double bed) are the notations that define an electron’s place in the double-occupancy spdf rooms. While the mirroring of electrons (“mirrored twins”) can be handled by mathematics, it is still not clear just how it happens in our physical world where electrons repel one another and all free electrons appear with the same handedness. It is also significant that only an “upright twin” can occupy a room alone! Not only that, but other “upright twins” fill a common suite of rooms before their “downright twins” can start pairing up with them. It would have made more sense to have mirrored the rooms with single occupancy by “an electron”, but that option was eliminated when the lowest room in any condo had to be a doubly occupied, centered, sphere.

Scientists are now developing techniques to investigate electron levels at the sub-nanometer level[105]. Helium will likely be the next atom addressed. To provide an alternate particle approach to the current QM electron orbital model, a “mirrored room” model is herein described and applied to the differing spectra of ortho and para helium.

DISCUSSION

THE “MIRRORED ROOM” ELECTRON ORBITAL MODEL

A “mirrored room” equivalent of a sphere is easily envisioned. It is simply two, diametrically opposed, tetrahedral-lobed spaces with a common center (Figure 1). An electron moves progressively through each lobe of the quartet. When the orbitals (defined by the electron’s energy to make the circuitous journey) are so small (minimal energy to complete the circuit) that e-repulsions between electrons would make filling more than one of them prohibitive, only one electron occupies each quartet; this is the case for hydrogen and helium. As the

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http://www.slac.stanford.edu/th/mpeskin/stuff/mpeskin/SUSYspectrum.pdf - M. E. Peskin, Dec, 2001

[104] Many countries have SS numbering systems. A common one is the US’s social security system which is supposedly humanitarian. Nazi SS’s numbering, on the other hand, was hardly that.

[105] Stodolna, A.S., et al. Quantum microscope' peers into the hydrogen atom - Hydrogen Atoms under Magnification: Direct Observation of the Nodal Structure of Stark States. *Phys. Rev. Lett.* **2013**, 110, 213001; http://physicsworld.com/cws/article/news/2013/may/23/quantum-microscope-peers-into-the-hydrogen-atom. The results presented are based on averaging massive amounts of data points taken over time. While circular orbital structures are described as being observed, their images are best interpreted as simply showing the outer boundary of the orbitals and not the shape of the orbitals themselves. Electron movement to or from the nucleus is minimal (nearly stationary relative to the nucleus) at the outermost limit of the orbital and, thus, more easily detected.

orbital sizes increase (increased electron lap-energy), each orbital lobe can contain a single electron. When an electron occupies each of the eight orbitals, the filling is complete; e.g., for the second level this occurs with neon. Not only does this "mirrored room" equivalent replace a sphere, it is also equivalent to the doubly occupied, s+3p, split-level group, but with only a single type of orbital. This is the MC portion of the MCAS model[106].

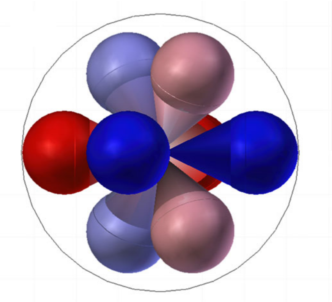
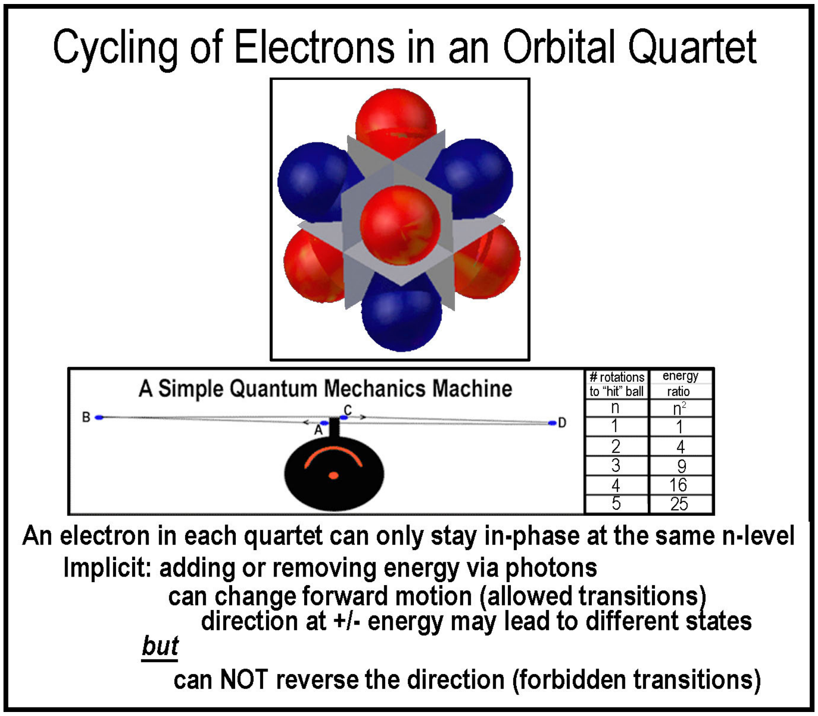


Figure 1: A "Mirrored room" electron orbital model

A simple quantum mechanics machine (shown in Figure 2, but discussed elsewhere[107]) indicates, a priori, why the excitation levels scale by n^2, where n is an integer. Implicit in the model is electron movement and coordination with the nucleus. The mirror-room" orbitals are simply that: orbitals; a different, but simpler set that explains the physical data and the periodic table. They would also be appropriate for non-classical approaches without electron-pairing should stanch adherents to the non-classical get past their objection to the fact that these orbitals can satisfy classical physics as well!



Cycling of Electrons in an Orbital Quartet

A Simple Quantum Mechanics Machine

# rotations to "hit" ball	energy ratio
n	n^2
1	1
2	4
3	9
4	16
5	25

An electron in each quartet can only stay in-phase at the same n-level

Implicit: adding or removing energy via photons

can change forward motion (allowed transitions)

direction at +/- energy may lead to different states

but

can NOT reverse the direction (forbidden transitions)

Figure 2: Electron levels scale by classical physics

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[106] (a)Williams, J.M. The MCAS Electron Orbital Model. http://vixra.org/abs/1205.0114 **2012** or http://pages.swcp.com/~jmw-mcw/MCAS/The_MCAS_Electron_Model_Booklet_for_web.pdf (booklet); (b) Modeling the MCAS Way. http://pages.swcp.com/~jmw-mcw/science or http://arxiv.org/html/physics/9902046v2 **1999**

[107] (a)Williams, J.M. The Bohr Model, Electron Transfer and Newtonian-derived Quantum Numbers. http://gsjournal.net/Science-Journals/Essays/View/4083 **2012**; (b) Why do Electrons (Orbitals) Have Discrete Quantum Numbers? http://vixra.org/abs/1210.0133 **2012**

At this point it is important to note the effect of adding and removing energy. Adding energy to or removing it from an electron's movement via photon addition or release is like accelerating and decelerating a car with the gas pedal – there is no effect on direction, per se. A reversal of direction by this action will not happen. Moving to a higher or lower lobe of similar shape is the norm. Moving to another orbital that has another orientation is possible, if the direction of the electron at the moment of energy change would send it there. Thus, an electron can NOT move from a **RED** orbital system to a diametrically opposed **BLUE** one or vice versa (Figure 2) by simply changing the energy level of the electron - this is a "forbidden" transition by photon action. To be "in-phase", two electrons must remain diametrically opposite one another or flowing in the same orbital group (Figure 3). To do this they need to be at the same energy level (n). Otherwise, the time to transverse the orbital lobes will be different. The "in-phase" state is the lowest for every energy level. Note that there are 3 non-diametric options even at the "same" energy level for the simple opposed quartets – these provide some fine structure before the unstable system moves to the more stable diametrically opposed position through energy changes. They provide staging points for transitions and may even make one electron appear more energetic than the other.

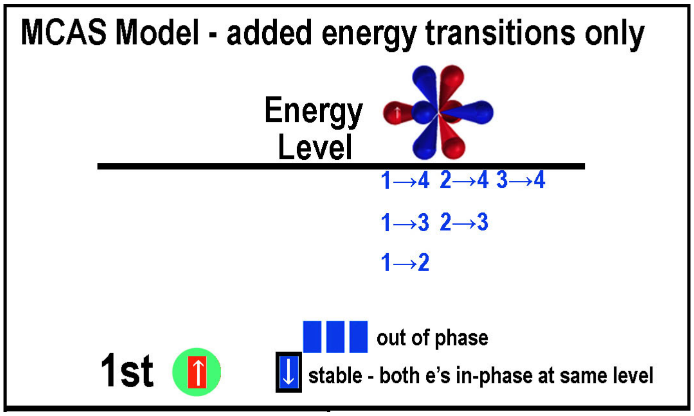
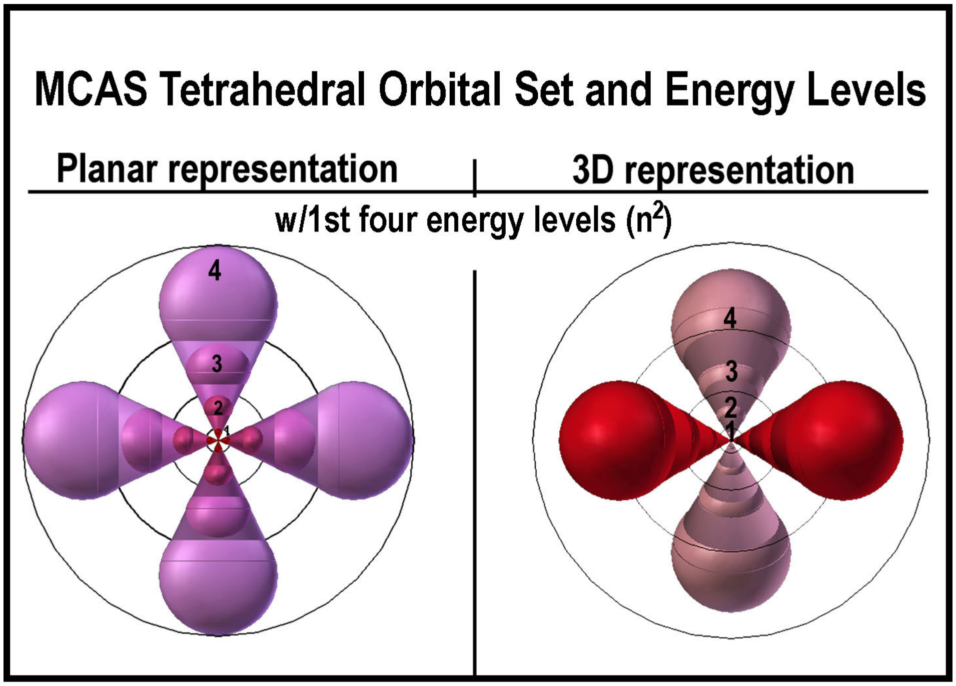


Figure 3: Orbital configurations for two electrons with one remaining at the lowest level

THE PHYSICAL SPACES OF ELECTRON TRANSITIONS



The Bohr circles that indicate simple one-electron n-state transitions do not indicate the magnitude of the energy involved in those transitions very well to students by my reckoning. Figure 4 is intended to provide a better feel. Note the tiny little first level.

Figure 4: Spatial-energy level relationships of the simplest electron orbitals

Orbital size is dictated by the energy-path of the electron that permits the electron to arrive back at the required appointment moment with the nuclear regulatory checkpoint and pass on to the next lobe. The nucleus keeps its electrons in line with firm discipline based on the constancy of the spectral data. This raises the question as to when energy is added to or removed from an electron: does it occur only when it passes the nucleus, at some other place, at many places, any or everywhere? Do atoms have fly-through pump and dump zones (“stations”)? Is photon energy actually input not to the electrons, but rather to the nucleus which then alters the movement of the surrounding electrons? Do electrons have to pass through nuclear magnetic “warping” zones as they orbit the nucleus? Knowing how electrons and nuclei interact is needed information for a more complete understanding of these miniature machines.

THE ENERGY STATES OF PARA AND ORTHO HELIUM

A composite of spectral energy levels for ortho and para helium from 3 web sources[108] is given in Figure 5. The data was consistent up to the 4th n-level, except for the 2nd level ortho “Principal”, where none agreed, but did not differ greatly. The Sharp and Principal notations are the spectral assignments and, of course, in the quantum mechanical model, they lower-case initial letter also represents that model’s orbital descriptions. Other energy levels are omitted here in order to focus attention on the first levels of energy changes. These spectral lines are handled by the C-orbitals of the “mirrored room”, MCAS model. helium

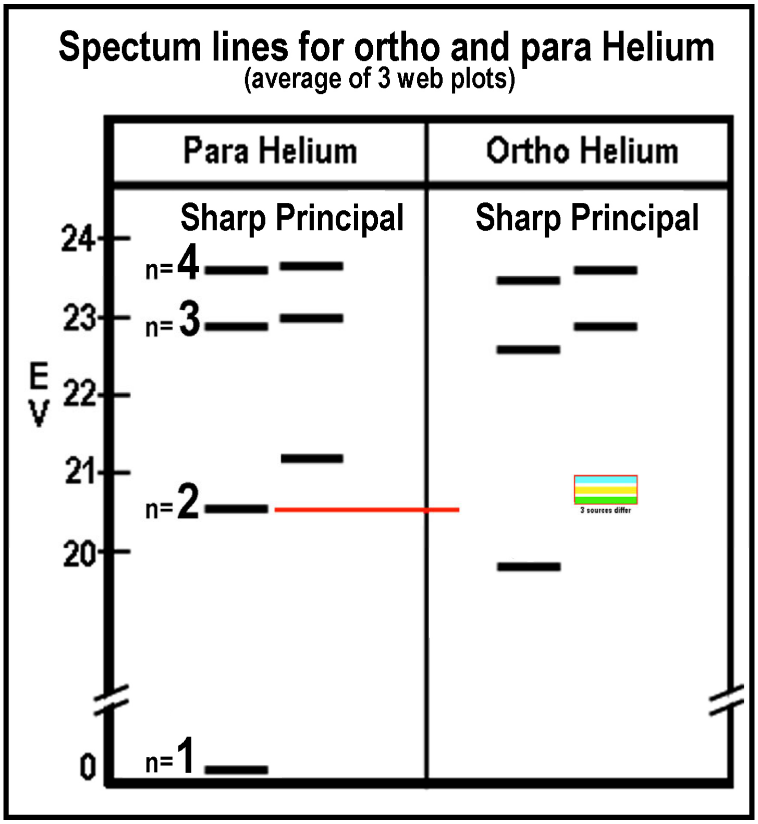


Figure 5: Spectral energy levels for ortho and para

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[108] Web sources for He excitation levels: (a)http://web.ift.uib.no/AMOS/PHYS261/2011_09_08/; (b) http://www.ipf.uni-stuttgart.de/lehre/online-skript/f40_03.html; (c)http://hyperphysics.phy-astr.gsu.edu/hbase/quantum/helium.html

The full MCAS model of orbitals is given in Figure 6 along with the s+3p orbitals of the spdf model: an M-orbital is a mono-occupied C-orbital quartet.

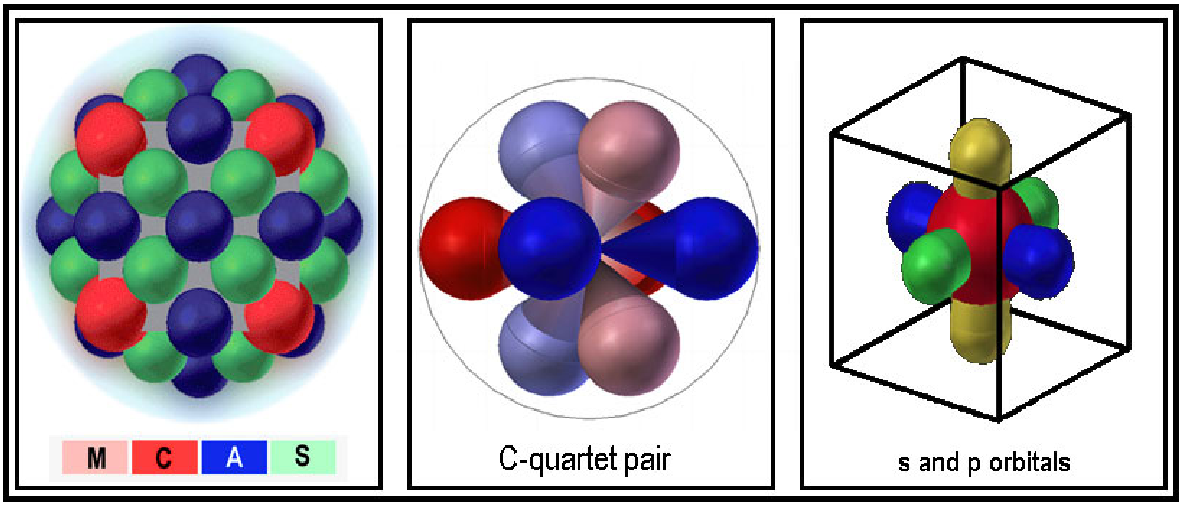

Figure 6: MCAS plus s and p orbitals

Elevation of the ground-state of para-helium to the next lowest energy level occurs in two steps without changes in electron spin (Figure 7).

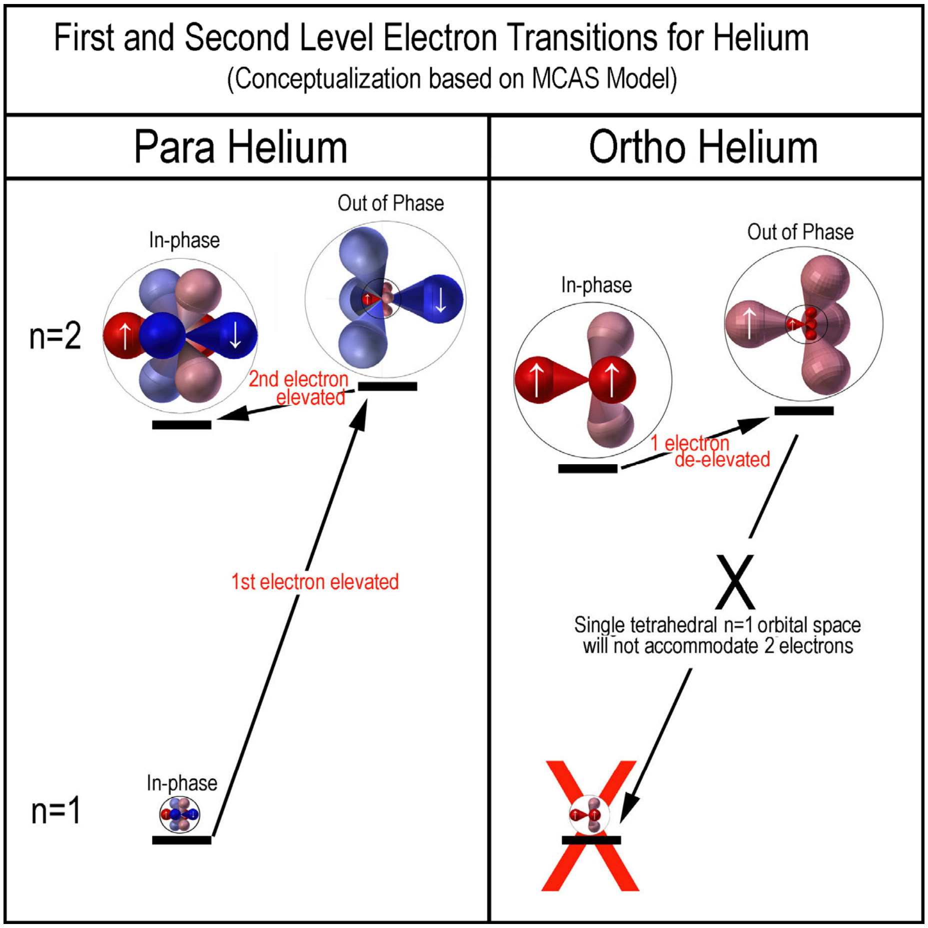

Figure 7: Electron excitation in orbitals for the first two energy levels of ortho and para helium

In the first step, one electron is elevated. This leads to a high energy, unbalanced (wobbly), out-of-phase, state. Part of the energy of this very unstable state is utilized in elevating the second electron. This gives rise to a balanced, in-phase state that has a lower total energy. Think about thermodynamics and chemical reactions. In the vernacular of chemical reaction mechanisms, the out-of-phase state is a high-energy, meta-stable state. In essence, the energy to promote the two electrons in the n=1 in-phase state to the n=2 in-phase state is less than that required to promote one electron from the n=1 state to the n=2 state. The process, however, must occur in two steps. The second step can only occur when the electrons are in diverging "pseudo" in-phase movement which allows a simple energy kick to put the second electron "in-phase" for a lower total energy. To return to the ground state, the process is reversed. Spectral lines indicate the energy of stable and meta-stable states; line intensities reflect the measurable quantity of these states. One should consider this when declaring that electrons are making "quantum leaps" from state to state.

With ortho-helium, the two electrons are in the same orbital quartet. Readers who are familiar with chemistry will recognize the ortho (adjacent) and para (opposite) placement of the arrows in the two "n=2 in-phase" images in Figure 7. Having two electrons in the same orbital quartet at the n=1 level is energetically prohibitive. Thus, the lowest state for two electrons in the same orbital quartet is at the n=2 level. This is the reason that lithium starts the second row of the periodic table[109]. As in the case with para-helium, a higher energy state can occur with one of the electrons dropping down to the n=1 level. Unlike in the para case, however, the second electron cannot drop down and this "out-of-phase, meta-stable" state simply reverts back to the more stable, but still high energy, in-phase state.

At first glance, it would seem strange that the n=2 ortho-state is lower in energy than the comparable n=2 para-state. Consider the relationships in Figure 8. The overall electron interactions and wobble are just greater in the para-state than in the ortho-state as they move through the orbitals and they are subjected to nuclear "supervision" on the way to the next lobe.

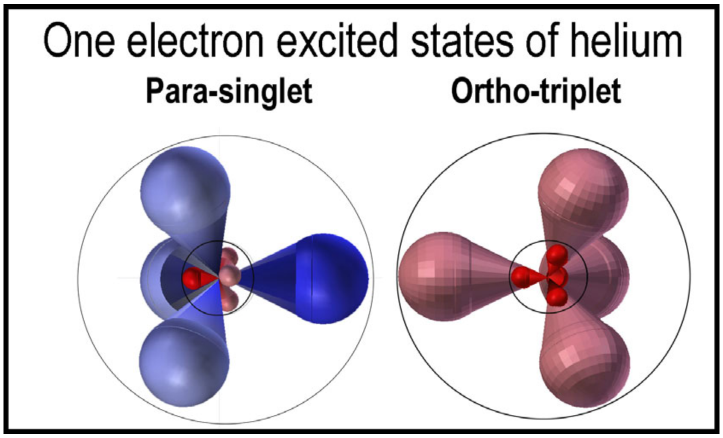

Figure 8: Orbital relationships of one electron excited in ortho and para helium

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[109] (a) Williams, J.M. Creating the Familiar Periodic Table via MCAS Electron Orbital Filling. http://pages.swcp.com/~jmw-mcw/The Familiar Periodic Table of Elements and Electron Orbital Filling.htm; (b) The MCAS Electron Orbital Model as the Underlying System of the Periodic Table. http://gsjournal.net/Science-Journals/Essays/View/4268 **2012**; (c) The Periodic Table and the MCAS Electron Orbital Model. http://vixra.org/abs/1208.0068 **2012**

The second electron in ortho-helium can not reverse direction under photon action and, thus, be converted to the para arrangement. The conversion of ortho to para of vice versa will not occur with the simple addition or removal of photon energy as a reversal of direction is needed. Strong magnetic fields are needed to align the movement of the electrons (orbitals) and thus pair electron flow; collision impacts are needed to reverse them.

SUMMARY

The “mirrored room”, MCAS, orbital model provides an excellent explanation for the difference between ortho and para helium. Spin-pairing is accomplished through movement through opposing orbital units rather than through the “mirroring of electrons” in the same orbital space as is done in the spdf model. The MCAS model clearly demonstrates why ortho and para helium are not converted from one to another with photon energy. The model also demonstrates that electrons are operationally connected to one another as they pass by and coordinate with the nucleus. They do not exist as clouds of negativity, although they emit negative fields. Energy levels are related to “coordinated junctions” near the nucleus and scale according to classical acceleration and deceleration laws of electron velocity and their related electrostatic attractions (and repulsions?) with the nucleus and repulsions with other electrons[110]. The MCAS model demonstrates that the lowest (n=1) energy level of atoms can only have two electrons moving in opposite directions (paired) and can not have electrons flowing in the same orbital quartet. This explains why the periodic table begins a new period after helium with a higher energy, more spatially expanded, set of orbitals which does allow additional electrons to occupy the same quartet. The rationale for G.N. Lewis’ “rule of eight” is quite clear with the eight-equivalent lobes of the “mirrored room” model. The MCAS “mirrored room” electron orbital model offers the simplest explanation for this and many other atom-atom interactions and does so without having to “hybridize” orbitals to make compounds and “reverse” the actual spin of electrons to effect pairing.

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[110] Some might say that electrons “talk” to one another. Since electrons emit electromagnetic fields, they certainly “influence” each other. The nucleus is doing the major controlling, however. The electron “drones” are just responding to its “warping” and the total electrostatic and magnetic fields generated by all of the atomic components. How the nucleus implements its warping influence would be very useful for understanding how these tiny atomic machines operate.

Chapter VII

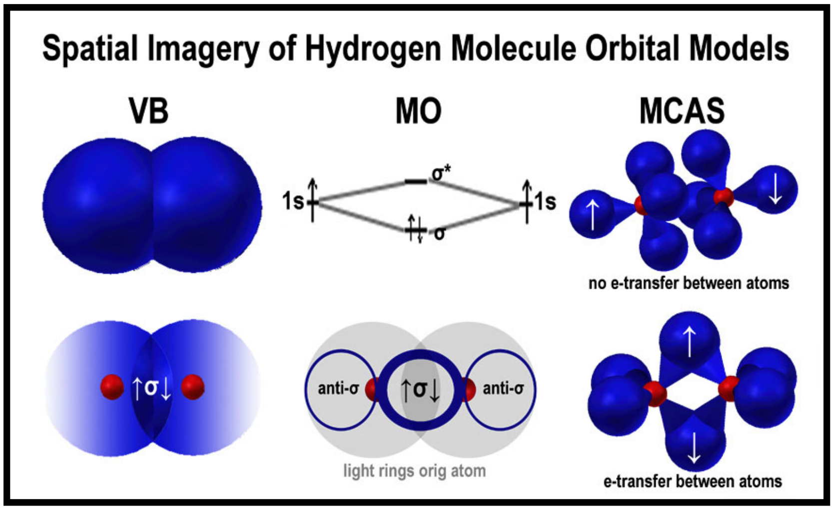
Electron Orbital Models and the Hydrogen

Comparing Several Orbital Approaches to the Hydrogen Molecule

Abstract

The current spdf and MO modeling of chemical molecules are well-established, but do so by continuing to assume that non-classical physics is operating. The MCAS electron orbital model is an alternate particulate model based on classical physics. This paper compares these models as applied to the hydrogen molecule.

The Molecular Orbital approach to the bonding of molecules is touted to be the proper one to address the bonding issue and maybe the hybrid atomic orbitals need to be archived[111]. While MOs might address energy levels and presumably bond order better, they have substantial shortcomings when it comes to addressing reaction mechanisms and molecular spatial arrangements. In many ways, the tinker toy/simple VB approaches to molecules and their interactions gave and will continue to give students and practitioners a hands-on mental grasp of what might be occurring at the femto-level. It is this 3D spatial appreciation of molecules that is sacrificed in the MO effort to emphasize energy levels. This short paper takes a look at the spatial implications of the MO approach compared to those of the Valence Bond (VB) and MCAS[112] models.


Spatial Imagery of Hydrogen Molecule Orbital Models

The figure at the right presents conceptual imageries of the Valence-Bond (VB), Molecular Orbital (MO) and MCAS approaches to the hydrogen molecule. This allows the three to be compared in the simplest molecular case. The VB and MO representations are illustrated tightly as implied by having two electrons located between the nuclei. Some readers would probably prefer that the e-fields be rather wide-spread to bath the nuclei with negativity - just how this occurs given the implied proximal constraint on the electron pair requires some imagination.

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[111] "Is It Time To Retire the Hybrid Atomic Orbital?",Alexander Grushow, http://pubs.acs.org/doi/full/10.1021/ed100155c, J. Chem. Educ., 2011, 88 (7), pp 860–862

[112] "Modeling the MCAS Way" (http://arxiv.org/html/physics/9902046v2); shaper image version at http://pages.swcp.com/~jmw-mcw/science; "The MCAS Electron Orbital Model" - http://vixra.org/abs/1205.0114 or http://pages.swcp.com/~jmw-mcw/MCAS/The_MCAS_Electron_Model_Booklet_for_web.pdf (booklet); all by the author

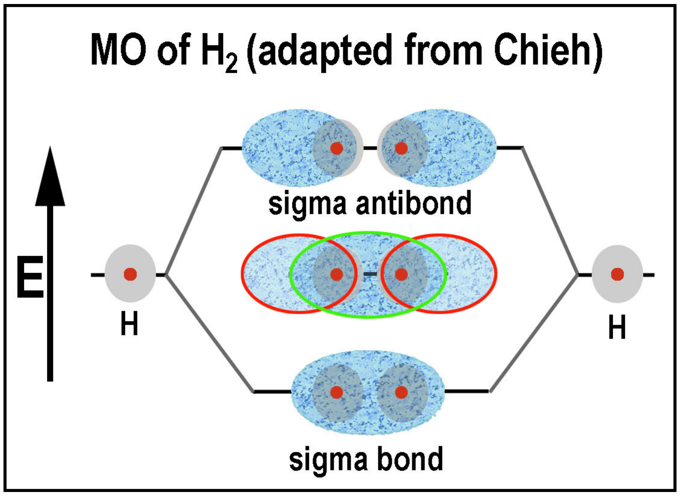
The bond strength of H-H (436 KJ/mole) is almost equal to that of O=O (497 KJ/mole). Thus, the two electrons provide significant coupling. The data tell us how much; what makes it happen is a different matter.

Two MCAS possibilities are given in the figure. The "no e-transfer" version is purely electrostatic with the electrons on each atom paired in motion with that of the other. Note that there all no antibonding electrons to destabilize the bond. The "e-transfer" version has the two electrons flow through the joined M-orbitals in concerted opposition; they are thus paired. The latter would provide synchronous looping from one nucleus to the other. Resonance energy? Both MCAS versions provide significant negativity around both nuclei as the electrons are free flowing through the orbital quartets. Which version is correct would take more detailed analyses.

The VB and MO treatments, on the other hand, call for both electrons to be cloistered between the nuclei to effect bonding. The commonly shown VB model in the upper left of the figure is hardly an accurate portrayal of the negativity with the electrons so cloistered. If fact, what is the basis for assuming that the electron cloud has nearly the same "probability distribution" of negativity (i.e., electron presence!) when the electrons are cloistered between the nuclei as when they are not? The bottom VB illustration is probably more accurate although it probably still shows too much negativity on the axis exo to the bond. The MO model is more explicit in its bonding/antibonding orbital assignment which leaves the ends bare-naked with unfilled antibonding orbitals. Such exposure of the nuclei as indicated by the VB and MO orbital models is hardly what one would expect for a molecule as stable as diatomic hydrogen.

Of course, O+O might equal ∞ (a conjunction?), but now we are talking MCAS and orbital pathways through which electron particles and their associated negativity flow while avoiding others with like attributes. As long as electrons are considered particles, it is reasonable to assume that their negativity is an inherent property that they carry with them and not something strewn in their wake. Whether they leave a persistent "charge-related" effect in the orbital space as they rapidly and repeatedly pass through is a different matter.

Serious consideration of spatial placements and e-e repulsions should raise major concerns, indeed, about the spdf-hybrid system and its MO offshoot. Some (many?) would say I have taken too narrow a view of the VB and MO models. I would counter that the VB and MO models take matters too loosely. For example, what is the mechanism for the MO sigma bond/antibonds orbitals for the hydrogen molecule covering so much space as indicated in a typical MO figure [see the figure on the right (adapted from ref [113])]. The appearance is that the electron clouds are just nebulous ovules drawn around points



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[113] “Molecular Orbitals of H_2”, http://www.science.uwaterloo.ca/~cchieh/cact/fig/sigma1s.gif; http://www.science.uwaterloo.ca/~cchieh/cact/c120/mo.html

and squished together. If there is any probability of an electron being somewhere, there needs to be a rational reason (path) for its getting there. In fact, what are those spin-paired electrons doing while they are in the sigma bond? If there is so much force to have them concentrate on the axis between the nuclei, how can there be much extended coverage exo the bond. The image in the center gives a composite of all the components. The packaging is tidy with bands demarking some limit of probability, but it gives no indication about the machine inside or how it works. The extent of the bonding zone should be tighter in the molecule than in the atom since the 1st ionization of the atom is 13.6 eV[114] whereas that of the molecule is 13% higher at 15.4 eV[115]. In this particular representation, I am not trying to single out Chieh by any means, but rather critiquing the vagaries of the MO concept!

MO imagery is much like the statement that "two is company, but three is a crowd" – why that is so requires more delving than simply making the observation. MO diagrams are like observing that stable marriages, wherein two can live together cheaper than two separately, become quite unstable and break up when an interfering third comes along – just a tabulation of the average costs of people or electrons bonding and debonding.

The MCAS model, on the other hand, provides a physical representation that does not resort to e-e non-repelling couplets and stresses coverage of the nuclei on all fronts, rears, and sides. As long as electrons are considered particles and move rapidly, they need "flyways"!

VB and MO approaches do not define how and where electrons move very well. In fact, the MO approach just treats the electrons as "blue hazes". Somehow, body parts and the world around us seem more substantial and orderly connected than this. Considering their reproducible atomic and molecular electronic spectra, their constant physical properties, etc, etc, etc, electrons are certainly operating in well-defined manners and NOT in "blue hazes"! After a century of thinking about them, we should have a clearer notion of how these little atomic machines juggle their electrons so consistently; especially considering that scientists seem ready to claim they know all about what is happening in the nucleus which occupies orders of magnitude smaller volume. Instead of thinking fuzzier and fuzzier orbital spaces, we should be thinking more refined orbital spaces. The MCAS model is an effort in that direction.

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[114] http://chemwiki.ucdavis.edu/Inorganic_Chemistry/Descriptive_Chemistry/Periodic_Table_of_the_Elements/Ionization_Energy

[115] Walker Bleakney, Phys. Rev. 40, 496–501 (1932) Walker Bleakney, http://prola.aps.org/abstract/PR/v40/i4/p496_1;
and A. G. Khrapak, W. F. Schmidt, and K. Yoshino (published after 2003) http://www.researchgate.net/publication/4163009_Ionization_potential_and_nature_of_charge_carriers_of_fluid_hydrogen_in_wide_pressure_interval/file/79e4150bb42806fb8f.pdf

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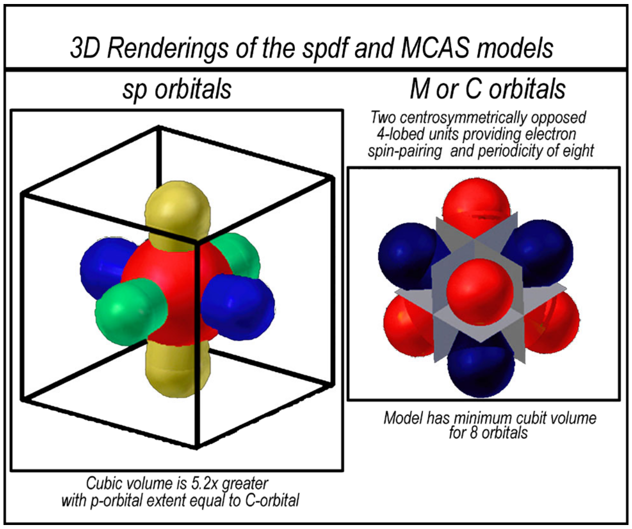
Chapter VI

Understanding the Bonding of Second Period Diatomic Molecules (Spdf vs MCAS)

Abstract

The current spdf and MO modeling of chemical molecules are well-established, but do so by continuing to assume that non-classical physics is operating. The MCAS electron orbital model is an alternate particulate model based on classical physics. This paper describes its application to the diatomic molecules of the second period of the periodic table. In doing so, it addresses their molecular electrostatics, bond strengths, and electron affinities. Particular attention is given to the anomalies of the carbon diatom. Questions are raised about the sensibleness of the spdf model's spatial ability to contain two electrons on an axis between diatoms and its ability to form π-bonds from parallel p-orbitals located over the nuclei of each atom. Nitrogen, oxygen, and fluorine all have the same inter-nuclei bonding: all "triple bonds" of varying strength caused by non-bonding electrons.

The spdf model was devised for single atoms by physicists and mathematicians. Kowtowing to them, chemists produce hybrid orbitals to explain how atoms could actually form molecules. Drawing these hybrids and meshing them on paper might look great, but, constrained to measured interatomic physical dimensions and electrostatic interactions, bonding based on the spdf-hybrids (sp, sp2, sp3) is illogical. To have even one electron occupy the "bond" region between the nuclei of diatomic molecules, at the expense of reduced coverage elsewhere, does not make sense for stable molecules. To have two repelling electrons in the area is nonsensical. To a third object, the perceived influence of two electrons may be additive, but the influence perceived by those two electrons of each other will hardly be congenial or neutral, as implied in the "duality" concept! While some question whether electrons are particulate, I have chosen to accept the fact that electrons have mass and, if the mass is a string, for example, it must at least be a ball of twine when fired at something. My qualms have to do with the spdf model and the history of forcing it to "meet" the experimental with mathematics ruling over common application of physical limitations, like e-e repulsion, and chemical properties, like the position of hydrogen in the periodic table. The MCAS model for bonding that is discussed below easily explains why hydrogen has the characteristics of carbon and thus belongs over carbon in the familiar periodic table.[116] This article is about bonding in simple diatomic molecules, however.


3D Renderings of the spdf and MCAS models

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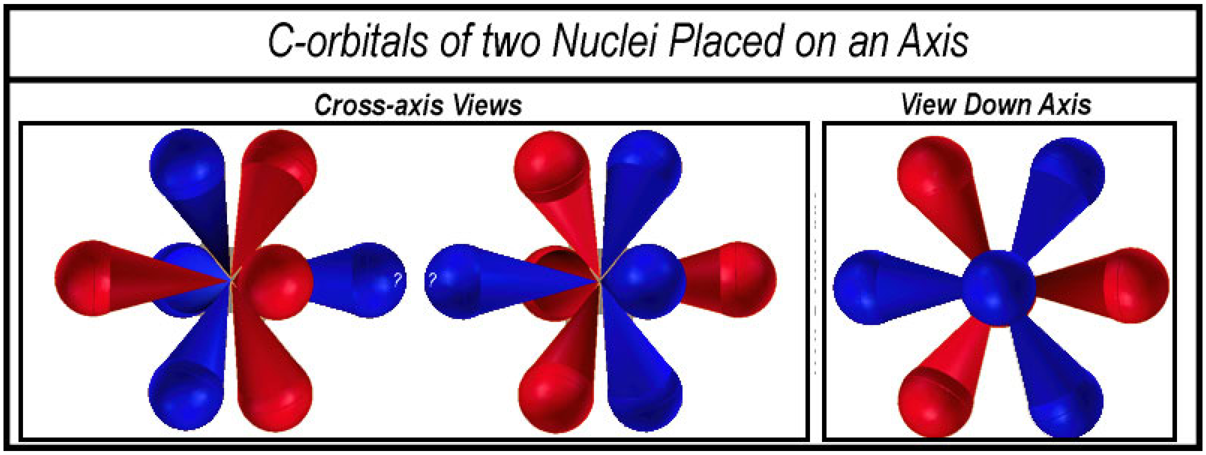
[116] "Creating the Familiar Periodic Table via MCAS Electron Orbital Filling" - http://pages.swcp.com/~jmw-mcw/The%20Familiar%20Periodic%20Table%20of%20Elements%20and%20Electron%20Orbital%20Filling.htm; "The MCAS Electron Orbital Model as the Underlying System of the Periodic Table" - http://gsjournal.net/Science-Journals/Essays/View/4268; "The Periodic Table and the MCAS Electron Orbital Model" - http://vixra.org/abs/1208.0068; all by the author

The MCAS model will be used to inspect the bonding interactions of simple diatomic molecules. The second period diatomic molecules use just the sp orbitals of the currently accepted spdf model or the M/C orbitals of the MCAS model.[117] The image to the right is an artistic rendition of how the two models place the electron orbitals about the atoms. The spdf model has 7 lobes for an eventual 8 electrons, thus, the requirement to "pair" electrons in the "red" s-orbital – achieved mathematically by spin-reversal. The 8 lobes of the MCAS model easily accommodated 8 electrons with "pairing" by reciprocal motion. For Neon, its 8, second period, electrons are not all uniformly packed around the nucleus with the spdf model. With the MCAS model, they are. Note that for equal orbital extent, the spdf model uses 5.2x the cubic volume of the MCAS model; i.e., the spdf model is not compact as one might expect the electron structure around a nucleus to be. For the purposes of forming diatomic molecules of the second period, the spdf model must be modified to sp, sp^2, or sp^3 hybrids although some MO treatments just make bond-antibond lattices without prehybridizing. No such hybridization is needed with the MCAS model. Since hybridized spdf modeling is so extensively taught in all levels of chemistry text, the reader is assumed to be well acquainted with them.

Atoms of the second period elements cover 8 positions with electrons as they are available. The following figure shows 2 MCAS-model nuclei placed on an axis in close proximity to one another.


C-orbitals of two Nuclei Placed on an Axis

Consider a case wherein 8 electrons fill the 8 lobes; such as with a fluoride ion. With all of the orbital lobes filled, the nucleus is symmetrically surrounded with "guarding" electrons. Consequently, it has no unguarded "posts" that need protecting. On the other hand, fluorine atoms have only 7 electrons. So, how can the unguarded "post" (see small "?'s" in the above figure) be protected? Without an available "free electron", another atom with a similar deficiency participates. The deficiencies merge and a bond is born. There is neither a need to spin-reverse an electron nor to ignore electron-electron repulsion as occurs in the mathematical treatment of the current spdf-hybrid modeling. In the way the orbitals are arranged in this paper, the red ones are "bonding" and the blue ones are "antibonding". Note that the bonding quartets include the exo-positions.

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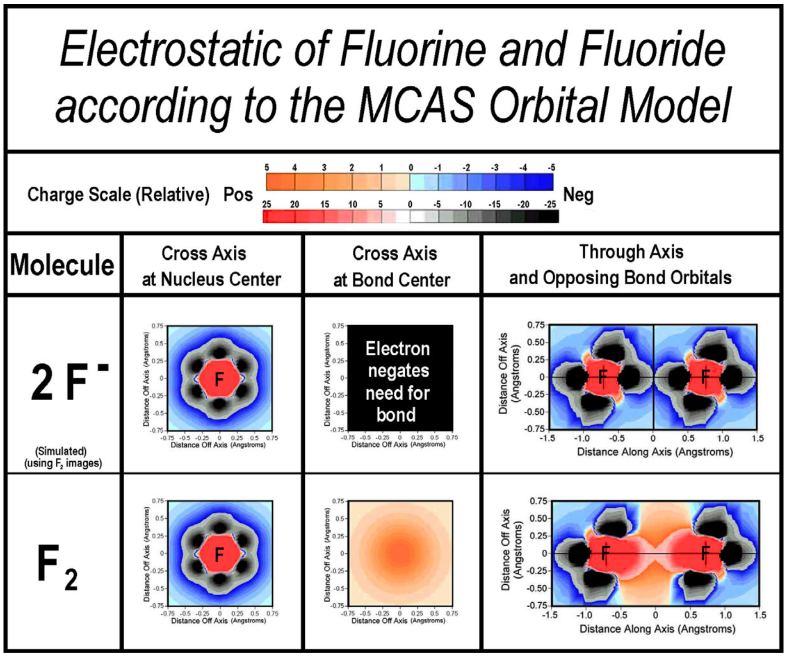
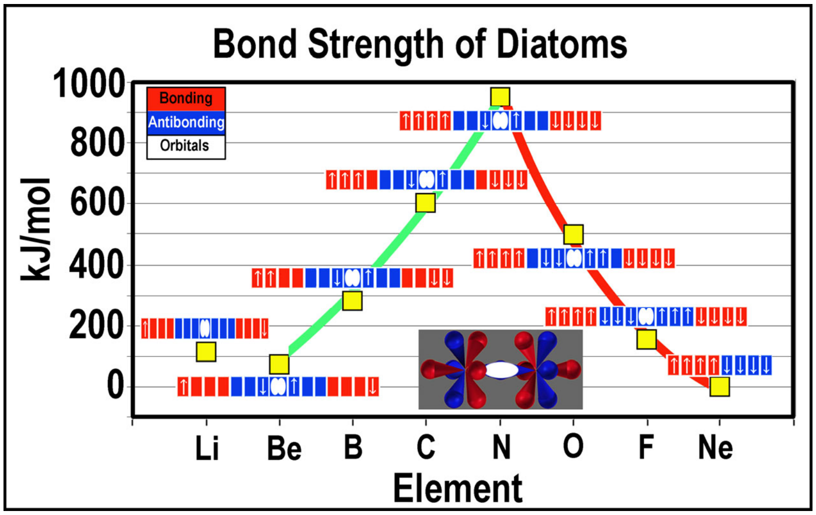
[117] "The MCAS Electron Orbital Model" - http://vixra.org/abs/1205.0114 or http://pages.swcp.com/~jmw-mcw/MCAS/The_MCAS_Electron_Model_Booklet_for_web.pdf (booklet); "Modeling the MCAS Way" - http://pages.swcp.com/~jmw-mcw/science or http://arxiv.org/html/physics/9902046v2; all by the author



The figure at the right illustrates the situation with accompanying electrostatic interactions. The electrostatic contours were determined with the nuclei at their experimental distance apart and with the electrons at the orbital extremes. Non-bonding electron charge was distributed uniformly to each lobe. Classical electrostatic attractions and repulsions with were used. The electrostatic images clearly demonstrate the surrounding symmetry of the 8-electron fluoride ion. They also demonstrate the weakness of the bond in the fluorine molecule. There is little negativeness (blue in the figure) protecting the molecule in this area. Consequently, fluorine is a very reactive electron-acceptor. Thus, while "neighboring" atoms may join to lower their individual vulnerabilities, this is inferior to having a full-time electron do the job. The current practice of putting electrons between the nuclei at the expense of de-shielding in other areas may be mathematically attractive, but it is illogical from standard electrostatic interactions. That is why physics had to be different at the atomic level. A bond represents electron-deficiency NOT electron-abundance. Orbital overlap may, however, provide a conduit for transient flow (!) of electrons from the antibonding quartet of one atom to another.



Consider now the bonding in some simple diatom molecules as given by the MCAS model. The figure at the right shows a plot of the experimental bond strength[118] of the diatomic molecules of the second period of the periodic table. Li-Li has a modest bond strength with a single "bonding" electron on each atom and no antibonding. There is an "antibonding" electron on each Be atom (this gives symmetry to the individual atom). The greater nuclear positive charge attractions for the bonding electrons is countered by greater nuclei repulsion and repelling of the opposite nucleus' antibonding electron by the nucleus' bonding electron and the bond is weaker. As nuclear charges increase and more "bonding" electrons surround the nuclei, bond strength

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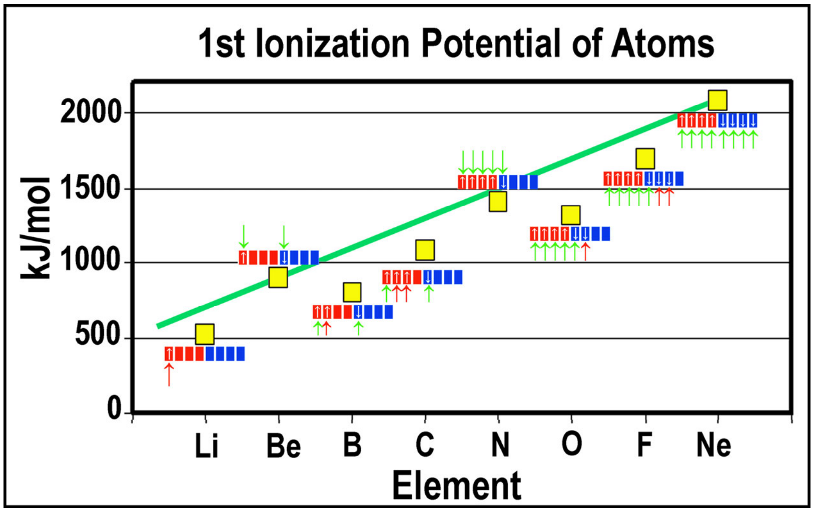
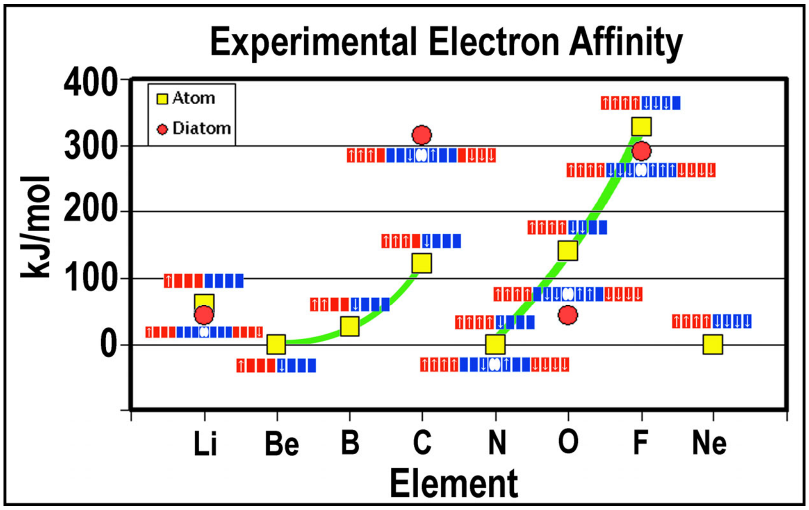
[118] "Diatomic Molecules as Examples of Bonding" - http://www.enigmatic-consulting.com/semiconductor_processing/CVD_Fundamentals/chemistry/diatomic_molecules.html

increases greatly (note green line). Maximum bond strength is obtained when there are maximum "bonding" electrons and minimum "antibonding" electrons. This occurs with nitrogen. Beyond nitrogen, "antibonding" electrons are added. Increasing interatomic "bonding-antibonding electron repulsion" and increasing repulsion of the nuclei overshadow increasing nucleus-bonding electron attractions. The MCAS model demonstrates the observed results without altering the disposition of the electrons around the nuclei. Contrast this with the ever changing hybridization required for the spdf-model to do the same.



The 1st ionization potential of a single atom is now addressed. The figure at the right shows the experimental data[119] of the second period elements. Ionization potential is the difference in the energy level of the original state and that of the generated state. The green line indicates ionization from "optimal" bonding-antibonding electron configurations (Be, N, and Ne; all green arrows) to "less optimal" configurations. Red arrows indicate electrons in "non-optimal" configurations. For Li, B, and O, their removal gives an "optimal" configuration. For C and F, removal of an electron from a "non-optimal" configuration just gives another "non-optimal" one. The N-value is slightly lower than expected.



The electron affinity of a single atom and its diatomic molecule is now addressed. The figure at the right shows the experimental data[120] of the second period elements. Consider first the single atom e-affinities (yellow squares and accompanying single dual 4-lobe C-orbitals). Li has an affinity to add an electron to provide symmetry. Adding one to Be destroys its inherent symmetry. Increased nuclear charge and improved symmetry occur with B and C. Adding an electron to N destroys its symmetry which counters its higher nuclear charge. Improved symmetry occurs again with O

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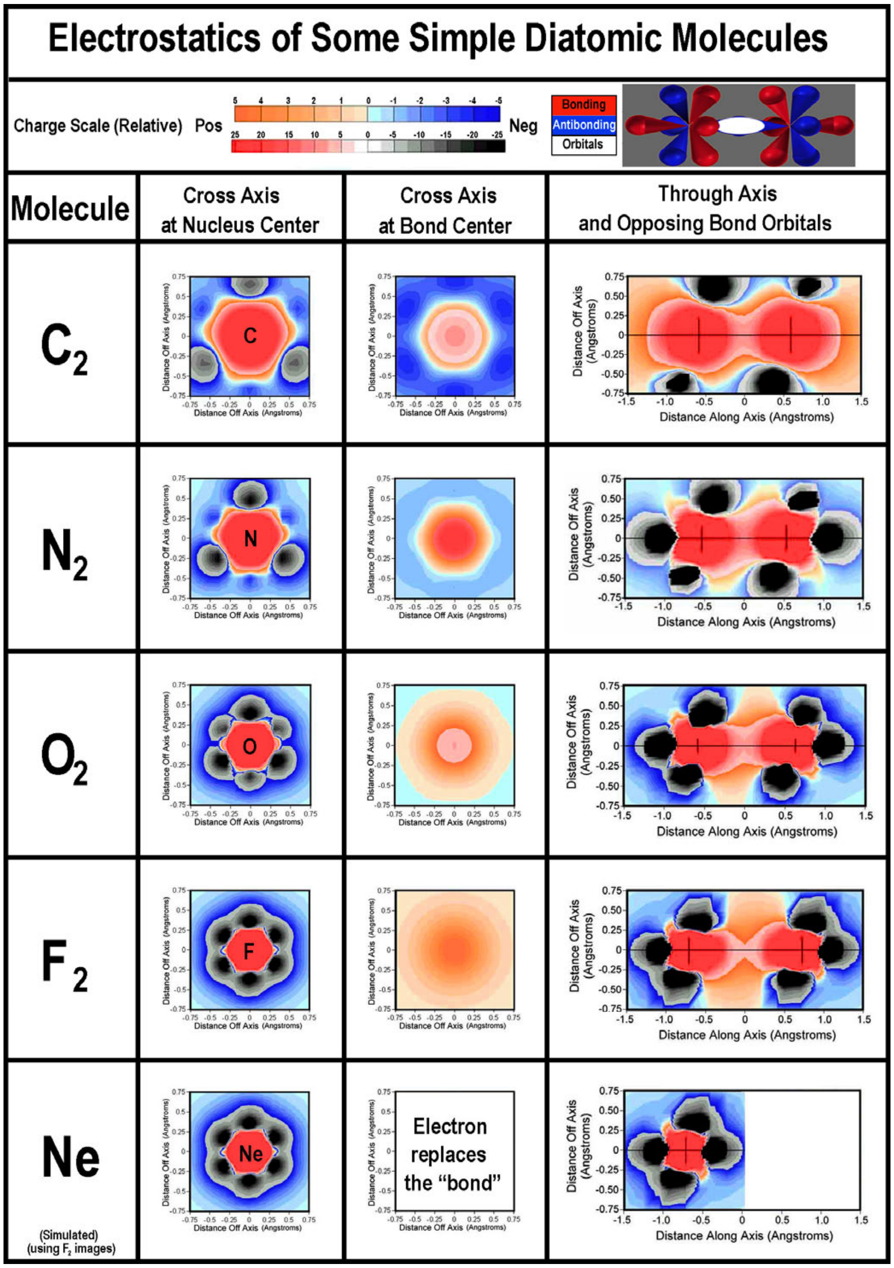
[119] "Ionization Potentials …………..'' - http://www.nist.gov/data/nsrds/NSRDS-NBS34.pdf

[120] "Atomic and Molecular Electron Affinities"http://www.colorado.edu/chem/ellison/papers/Rienstra-K_ChemRev_102,2002.pdf

and F with increased nuclear charge having a dramatic effect. For Ne, the 8-lobes are filled and, consequently, there is no need for an additional electron at this level.

The electron affinity of the diatomic molecules is a bit different (red circle and overlapped C-orbitals in the preceding figure). Li-Li has a slightly lower e-affinity than Li as the addition of an electron to the antibonding lobes would destabilize the Li-Li bond. No data for Be-Be and B-B are given in the reference. The C-C molecule has a much greater e-affinity than atomic C! The N-N molecule would not be expected to have much of a difference in e-affinity than the corresponding single atom which has none. The O-O molecule has a much lower e-affinity than a single O atom. Similarly, the F-F molecule has a lower one than the F atom, but not much lower.



The reason for the deviant electron affinities of the diatomic molecules becomes clear when the electrostatic interactions are considered, especially the enormously greater e-affinity of C-C. The figure at the right shows the calculated positive and negative charge levels around the molecules in the MCAS style with electrons at maximum orbital extension.

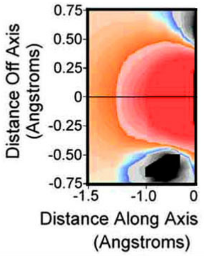
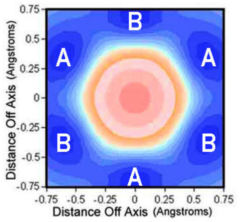
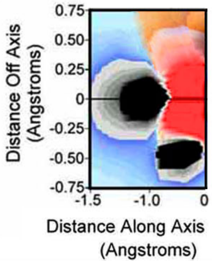
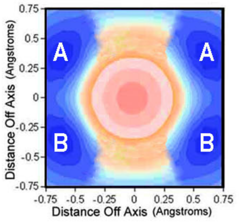
First, note that, as the nuclear charge increases (C to Ne), the surround electrons become more tightly bound (compact) and uniform, but always as symmetrical as possible.

Next, note the electrostatics of the diatomic molecules in the bonding area. The images are for 6 bonding electrons between the nuclei; required for N_2 to F_2 as the bonding orbital quartets are filled. For C_2, it is only one of its options and is shown here to emphasize the molecule's great need for an exo-electron.

The nitrogen diatom is the most uniformly bathed in negativeness. As nuclei-repulsion and interatomic bonding-antibonding repulsions increase, the bond lengthens and bond energy decreases. In the case of F_2, the bond is greatly weakened, even with the nuclei tugging on the opposite's electrons. At Ne, the need for a bond is replaced by an electron and the atom is more highly bathed in negativeness than is the nitrogen molecule.

Valence bond theory would require 4 bonds between the carbon nuclei to give 8 shared – this was never taught that I remember; but apparently is getting some press[121]. The exo-deficient image above for carbon is like **•C≡C•** with just 7 electrons for each and the lone electrons non-bonding, yet paired (by opposite movement).

There are 2 MO versions: sp+2p version (3 bonds between the nuclei; equivalent to the above: **•C≡C•**) and s +3p version (2 bonds, thus **:C=C:**).[122] One of the electrons outside the nuclei pair is in the non-bonding quartet; the other is in the bonding quartet. They are not paired in the same orbital as is usually implied. The MO model lumps the non-bonding together; here that is clearly not the case.

Electron Locations in the Bonding Orbitals of Carbon Diatom		
Time Bonding Electrons in Exo Orbital	Cross-section thru exo and anti-Bonding Orbital	Cross-section mid-Bond
1/4 time No Exo Cover •C≡C• Max Bond Strength		
3/4 time Exo Cover :C=C: Max Bond Strength	Artistic Rendition 	Artistic Rendition  One of 3 120°-Positions

Unlike the cases of N_2, O_2, and F_2, there are only 3 electrons to fill the 4 bonding quartet lobes. They can be placed in 1 of 4 ways with 3 being energetically equivalent. The two different options are shown in the figure to the right. Whether electrons are "paired" or not between the two nuclei will depend on how they move in the bonding quartets.

Does the mid-bond cross-section for the exo-covered option look like 2, side-by-side, A-B π-bonds for the exo coverage? How about 3 A-B π-bonds for the "no exo cover" option? Unlike the spdf/MO model, there is no connection; just proximity.

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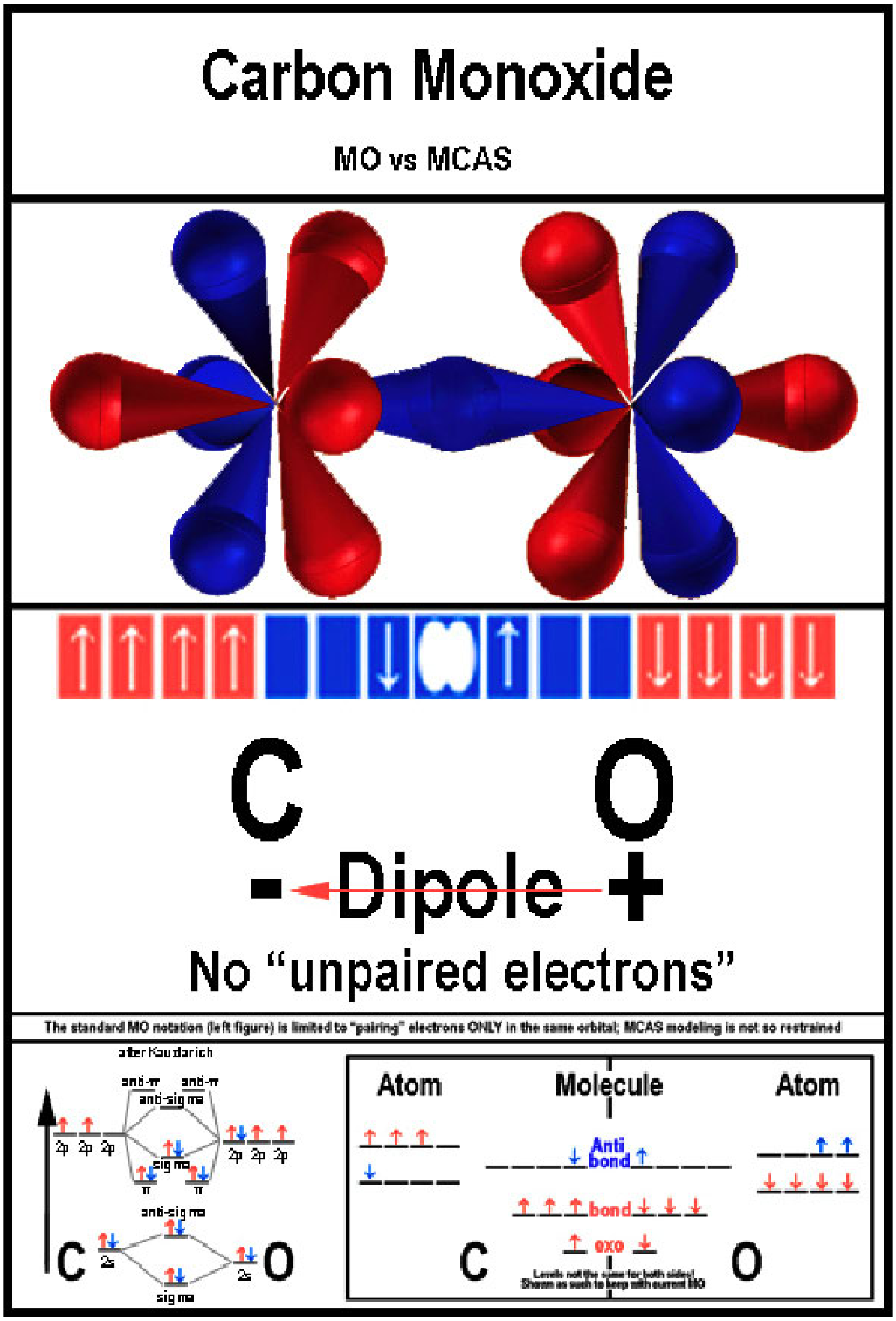
[121] http://www.rsc.org/chemistryworld/2013/05/quadruple-bond-carbon-debate-shaik-hoffmann-frenking

[122] "Diatomic carbon" - http://en.wikipedia.org/wiki/Diatomic_carbon

Now consider the carbon monoxide case. CO has the same number of electrons as does nitrogen: 10. Unlike the case with nitrogen where each atom has the same oxygen has 6. The figure at the right shows how the electrons are redistributed formed. According to the MCAS modeling, an electron from the "antibonding" orbital unit of oxygen is transferred to carbon. This results in a permanent dipole. With an electron arrangement like that of N_2, CO should have a bond strength attributed to a triple bond; actually it should be stronger (experimentally observed) with the higher charge on oxygen tugging on the carbon bonding electrons.



I have included an MO description[123] of what is happening for comparison. The bonding and anti-bonding sigma and pi orbitals/levels are easily formed schematically, if not envisioned physically. Seems like the four 2s electrons form two exo non-bonding orbitals instead of a sigma/anti-sigma pair! Since there are no unpaired electrons, MO requires (Hund's rule) that two electrons occupy each "bond" orbital. The MCAS model has no such restriction as each orbital has a complementary opposite; thus, there are no "unpaired" electrons, even if they are at opposite ends of the molecule.

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[123] chemwiki.ucdavis.edu/Wikitexts/UC_Davis/UCD_Chem_124A%3A_Kauzlarich/ChemWiki_Module_Topics/MO_Theory%3A_CO

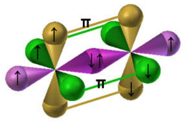
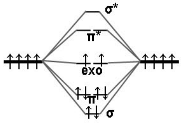
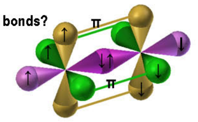
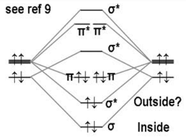
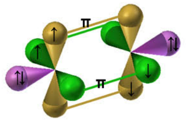
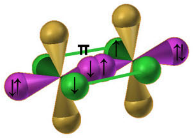
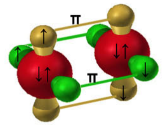
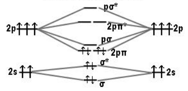
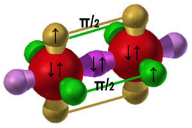
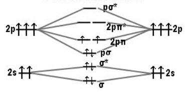
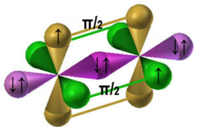
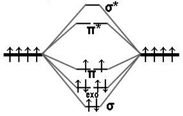
Students can learn to follow the teaching and textbook presentations of the spdf/MO model, but there are some serious questions about these models. For example,

- What is the great driving force to make a C-C molecule have much larger e-affinity (~ equal to F atom) than a C-atom in the visual form of the spdf-model?

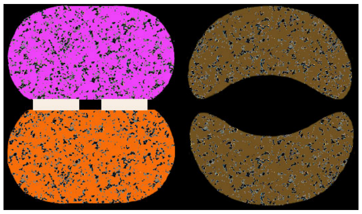
- Is there really enough space for two permanent electrons in a sigma bond between the two nuclei, even if the electrons could comingle as required in the mathematical treatment? If these electrons are located between the nuclei, as claimed in many models, why is there much electrostatic negativity outside the internuclear region as is usually illustrated in the hydrogen molecule case; esp. on the exo-nuclear axis?

- Does the "σ*- outside bond" from the p-orbitals[121] (as indicated in "ref 9" of the figure) constitute a bond and thus giving rise to a 4th bond? It does cover the molecule's ends. Having the two anti-bond lobes be a paired unit does get around Hund! The MO also gets around the problems that arise with the often used, very simplistic, boiler-plate, MO notations for C_2. These are illustrated in the bottom of the figure as "A traditional MO"![124] One is left to wonder why C_2 is so unstable when viewing the "4-bond" MO!

What is proper sp-Hybrid for C_2?

V-bond	Corresponding sp?	Correct MO?
Unpaired ·C≡C·		
All paired	4 bonds? 	see ref 9 
All paired :C=C:	  	A traditional MO 
Unpaired :C=C:		A traditional MO 
		s and p e's treated the same 

- Where is the overlap that would even provide a p-bond? What make these p-bonds strong? Some have proposed bent-bonds to provide overlap. Loops might work with reciprocal motion for pairing. Clouds connecting the tops and bottoms of the p-orbitals are also envisioned[124], but what would create e-pairing. Overlap is not implied in simple spdf-modelings when nuclei are placed apart and the p-orbitals are pear-shaped; spherical shaped p-orbital lobes would be better, but that is not what the mathematicians decree to my understanding. What keeps the electrons "floating"? MO modeling just indicates bonds and antibonds are formed without regard to spatial requirements. What is a filled p-bond + a filled anti-p-bond level but two, filled, nonbonding, p-orbitals – one on each atom? What is a filled s-bond + a filed anti-s-bond level but two, filled s-orbitals ala helium? What is the repulsion between these filled non-bonding s and p-orbitals? Also, s/s* from an s-orbital should definitely be different than s/s* from a p-orbital. Hence, the need to



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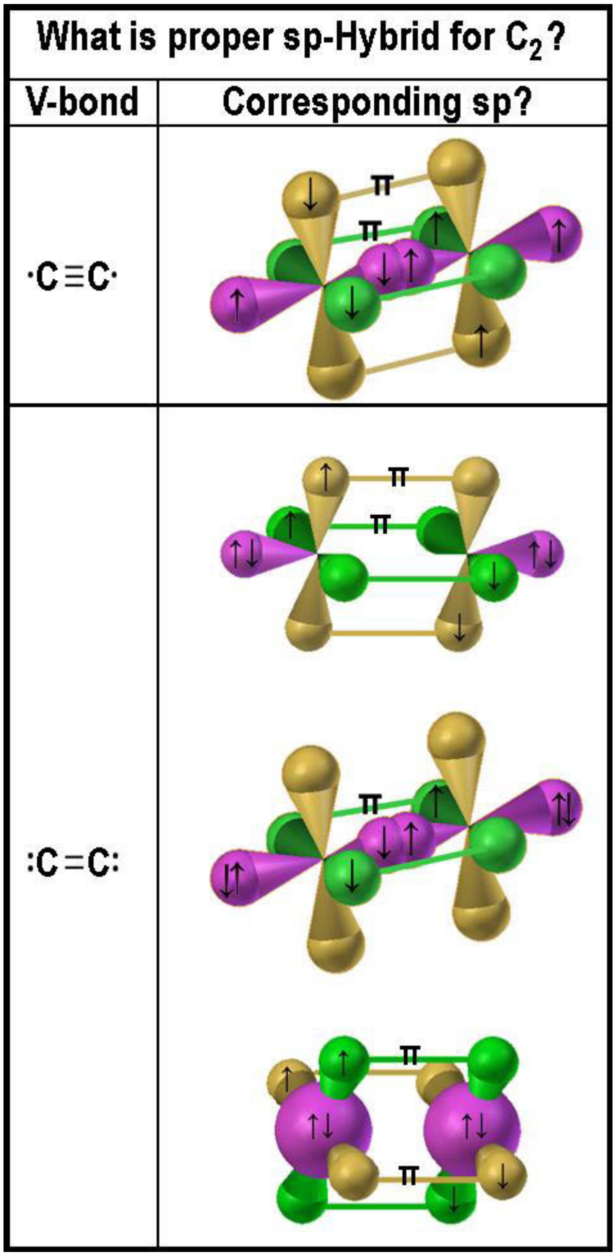
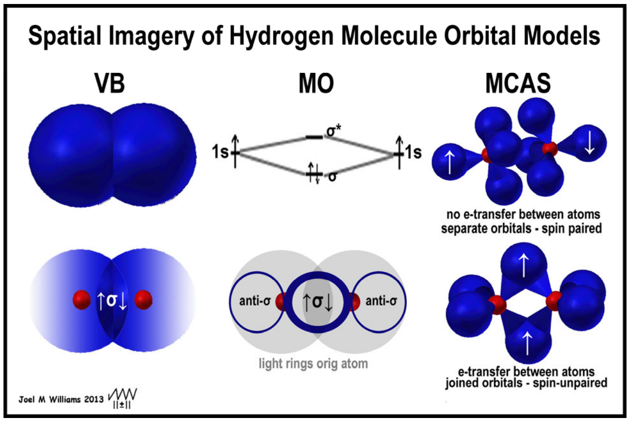
[124] http://www.meta-synthesis.com/webbook/39_diatomics/diatomics.html

have the p-orbitals form a 2-electron s* MO in two separate lobes at either end of the C-C axis[124] rather than from the two 2-s orbitals. MOs that assume that sp-hybridization occurs before bonding can get around this. Simply indicating that all the electrons of each atom are the same and then placing them in the needed MOs as I have done in several MO diagrams eliminates the problem. Of course, the real problem is determining what MOs are needed rather than where the electrons started. Carbon monoxide clearly demonstrated that electrons in a molecule go where they are needed - just as they do in the atoms of the periodic table.[116]

- C_2 should have two unpaired electrons in the triple bond case (•C≡C•), if Hund's rule is to be obeyed; like the top figure on the right? Is the no-sigma bond image logical, as near the bottom of the figure on the right, if there are paired electrons in the exo-bonds, as indicated in the double bond case (:C=C:), which has no unpaired electrons? Or are there two empty p-orbitals with one sigma bond and one p-bond? The filled s-orbital spheres (red) near the bottom are more in line with "traditionally presented MO diagrams". If they look a bit strange, one might consider that the "simple 'serves-all' MO approach" does not serve all! This "red sphere" illustration of anti-bonding negating bonding to yield an s-orbital emphasizes the shortcomings of the simple MO treatment. The bottom MO might make sense, if, in fact, p-orbitals can form p-bonds; especially 1-electron p-bonds! The reader is sure to find some others. No wonder some teachers might want to forget the Bohr-orb descendants. Of course, some of the learned might want something more tangible than some energy level lines on paper. I did as I tried to understand chemical reaction mechanisms, etc.



- 3-D images of the bonding and antibonding orbitals should be presented for students to grasp what is being presented in the MO diagrams. The figure does not show antibonding sigma and anti-p-bonds. MO for C_2 has an anti-sigma. Where? Seems a lot of extra stuff to explain what is going on, when the MCAS does so uncomplicatedly.



The figure at the right presents conceptual imagery of the Valence-Bond (VB), Molecular Orbital (MO) and MCAS approaches to the hydrogen molecule. This allows the three to be compared in the simplest molecular case. The bond strength of H-H is 436 KJ/mol which is almost equal to that of O=O which is 497 KJ/mol. Two MCAS possibilities are given. The "no e-transfer" version is purely electrostatic bonding with the electrons on each atom paired in motion with that of the other. The "e-transfer" version has the two electrons flowing through the joined M-orbitals in concerted opposition and so they are thus paired. Both MCAS versions provide significant negativity around both nuclei. The VB and MO treatments, on the other hand, call for both electrons to be between the nuclei to effect bonding. The commonly shown VB model in the upper left is hardly an accurate portrayal of the negativity with the electrons cloistered between the nuclei. The bottom VB illustration is likely more accurate with even it showing too much end exposure. The MO model is more explicit in its bonding/antibonding orbital assignment which leaves the ends bare-naked with unfilled antibonding orbitals. Such exposure of the nuclei as indicated by the VB and MO orbital models is hardly what one would expect for a molecule as stable as diatomic hydrogen.

Serious consideration of spatial placements and e-e repulsions should raise major concerns, indeed, about the spdf-hybrid system and its MO offshoot. The MCAS model, on the other hand, provides a physical representation that does not resort to e-e non-repelling couplets and stresses coverage of the nuclei on all fronts, rears, and sides.

Students can learn to follow the teaching and textbook presentations of the spdf/MO model. However, the learned, having demonstrated they can recite and apply what has been taught for nearly a century in the same manner, do not validate the model. Most accept it as workable and move on. Very few ever question the model further. The longer the hiatus, the more entrenched it becomes. Scholarly journals resist giving air to voices opposing ingrained models. The web gives exposure, but has little effect on the establishment as much is perceived as not having passed “establishment-peer review” and appeared in establishment, peer-reviewed, publications – Catch 22[125].

Summary

The MCAS electron orbital model provides a compact orbital arrangement which explains bond strength, 1st ionization potential, and electron affinity behavior of the diatomic molecules of the second period of the periodic table. It does so without hybridizing (reconfiguring) the orbitals as the spdf model is required to do. It does so while obeying classical physics; something the spdf approach has to declare invalid to operate. Hence, the MCAS model demonstrates that classical physics operates down to and includes the electron orbitals nanospace.

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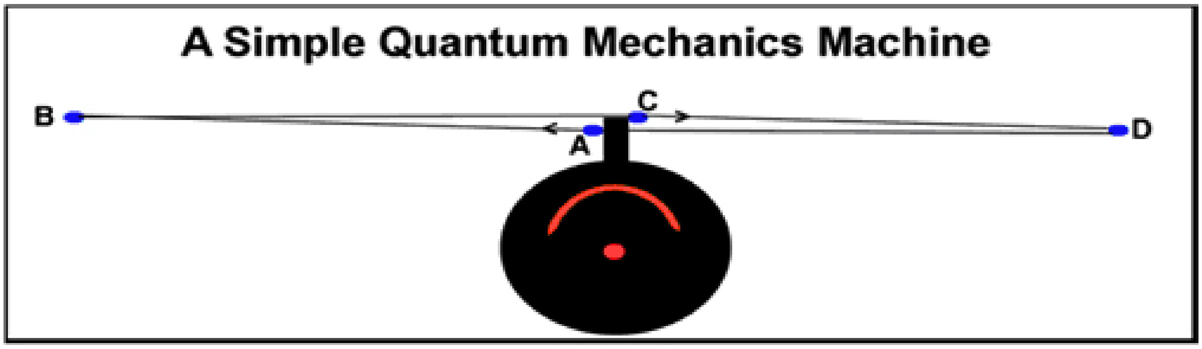
[125] http://en.wikipedia.org/wiki/Catch-22_(logic)

Chapter V

Why do Electron Orbitals have Discrete Quantum Numbers?

In other words, why do electrons generate the Balmer series? In the MCAS model, they do so because the nuclei and electrons have different motion parameters, but their interaction must coincide when the electron approaches the nucleus. It is not clear how a nucleus interacts with and directs the electron, but it must. Passing close to the nucleus allows the necessary intimacy, whereas the distant circular Bohr orbits never seemed to provide any such mechanism. Higher mathematical treatments have not provided a logical physical explanation either; just parameters to make it so as did the refinement of the Bohr model. Retrofitting has met resistance even when the nucleus is being shown to be a highly structured assemblage of entities.

As a thought process about why energy character around a nucleus is "quantum" and not "continuum", I present the following discussion of a simple quantum-mechanics machine. It consists of a robotic batter and a moving ball. Shortly, you will see how it generates a "ball-mer" (sic) series.



The ball, *moving with velocity V_o at point A*, receives positive, but discrete, energy input from the bat, if not perpetual motion, and continues on to max point B as governed by a constant decelerating force. Reversing, it accelerates to point C where it receives the same, discrete, positive energy input from the bat and continues on to max point D, again exposed to the same decelerating force. Returning to point A, the ball repeats the cycle. The robotic batter reverses rotation with each hit in this thought experiment (in order to "touch" the ball from behind in both directions), but comes back to point AC, as set by its constant rate of rotation, in integer time-quantities of t.

# rotations to "hit" ball	V after "hit"	Ball-mer Series	H atom Bohr r	Bohr r ratio
n(t)	V	d_x	Å	
1	1 a(t/2)	**1** $(a/2)(t/2)^2$	53	**1**
2	2 a(t/2)	**4** $(a/2)(t/2)^2$	212	**4**
3	3 a(t/2)	**9** $(a/2)(t/2)^2$	476	**9**
4	4 a(t/2)	**16** $(a/2)(t/2)^2$	846	**16**
5	5 a(t/2)	**25** $(a/2)(t/2)^2$	1322	**25**

The bat and the ball operate under different parameters/forces, but must arrive at point AC at precisely the same moment.

$V = V_A = V_C = V_o +$ energy from bat
$V_B = V_D = 0 = V – a(nt/2)$
$d_{A\text{-}B} = d_{C\text{-}D} = V^*(t/2) - 1/2a(nt/2)^2$
$d_{B\text{-}C} = d_{D\text{-}A} = 1/2a(nt/2)^2$
$a =$ constant
t is set by the batter’s constant rate of rotation and bat arrival at point AC

The “Ball-mer” series indicates what was needed to generate the Balmer Series with the Bohr model; adding “principal quantum numbers” (***n***) to produce discretely separated orbits rather than an infinite continuum of orbits. The energies differences are just that needed to achieve each timing-sequence of correlated interactions. Designating the “quantum” energy size does not indicate how it is applied or removed from the action; only that it is. Ball-mer behavior can occur in a multitude of similar situations as the accelerating-decelerating forces involved are not specified. The quantum-phenomenon is not size dependent as was used to justify why Newtonian physics did not work at the atomic level and, therefore, new physics was necessary. Quite clearly, Newtonian physics does apply in the electron-nuclear realm to define the parameters, ***if*** the physical model is appropriate.

Arnold Sommerfeld, who attended the first of the 1911 Solvay conference, had these "Nobel" students [Werner Heisenberg (uncertainty), Wolfgang Pauli (exclusion), Peter Debye, Linus Pauling], but never got a Nobel himself. It was Sommerfeld, however, who introduced "elliptical orbits" (quantum ***ℓ***) in 1916 to replace Bohr's circular ones and then the quantum ***m*** in 1920 that led to the spin-factor (***ς***). If Sommerfeld had connected his elliptical orbits to form a continuous 3-D spatial one, he surely would have come up with the MCAS model. BUT, the “Rutherford-Bohr” mold had “hardening”.

There has been great resistance to modifying the “corner stone of quantum physics”, now 100-years old. There are too many texts, teachers, “science bureaucrats”, benefactors, etc, etc that emphasize “livelihood through stability; not change”. The situation is much as if the original deed to NYC was a scam and the Indians are now legally entitled to raze it for a different “look” – mucho resistance!

Question: how does the probability orbital model generate quantum behavior? Starting with quantum behavior (numbers) and using it to predict probable electron density is not the same. Thus, while all agree that the BOHR model might be at least “a little wrong”, ***all*** “acceptable” models are based on it! The models are spdf / nlms, where the **s** orbitals are ***n***(iels) BOHR!

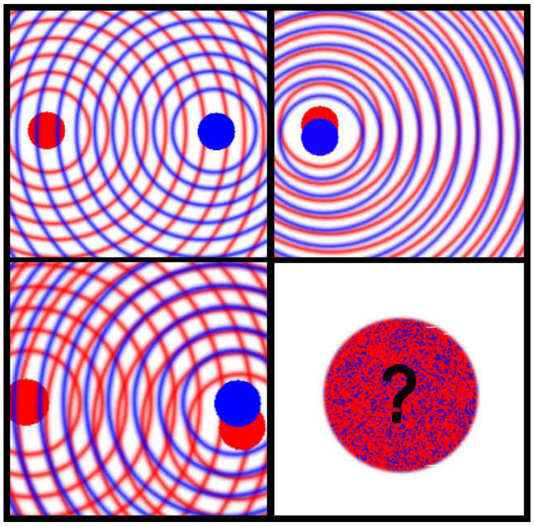
Chapter IV

The BIG BAND Gravity Theory[126]

An explanation for gravity was listed as one of the 11 greatest unanswered questions of physics in 2002 [Discover Vol. 23 No. 2 (February 2002)] and still remains a hot issue. Many have tried; none has successfully succeeded. Einstein spent much of his later life trying. The quantum theorists have proceeded under two hypotheses: that gravity is a separate force from other forces and that it fits the quantum theory ideal (thus, the proposed "graviton"). After a fruitless 80-year attempt to explain gravity with these restrictions and make it fit a grand unification theory, it should strike most that these tenets are faulty. That the premises were not changed long ago testifies to just how completely quantum theory has dominated science, crushing or simply ignoring thought perceived to be inconsistent with its tenets. No one dares challenge this religion1 for fear of being ostracized or more importantly admitting that one's own high IQ was insufficient to see its fallacies. It is doubtful that venerable peers would welcome changes that would make their thinking no better that that of an undergraduate. Peer review by the establishment becomes self-aggrandizing while claiming impartiality. Only now are novel ideas beginning to become widespread from unorthodox thinkers who pen non-peer-reviewed "papers" and "publish" on the world wide web.

Consider the simple equations for electronic and gravity interactions as the starting point for pondering what causes gravity.

Electrostatics	**Gravity**
$\mathbf{E = F(q_1q_2)/r^2}$	$\mathbf{E=G(m_1m_2)/r^2}$



Gravity would not be an unanswered question if it could be shown that an object emits an omni-directional, electrostatically neutral, wave that maximally combines with other like waves. The existence of such a neutral wave has been the difficulty. This contrasts with like-charge electrostatic waves. The electrostatic effect of a solitary particle flows outward from the particle in every direction at mathematically defined levels. Classical physics has demonstrated that similar effects are additive and that a NULL occurs when the sum of the positives equals the sum of the negatives and NOT because the components vanish. The figure at the right illustrates several of the points.

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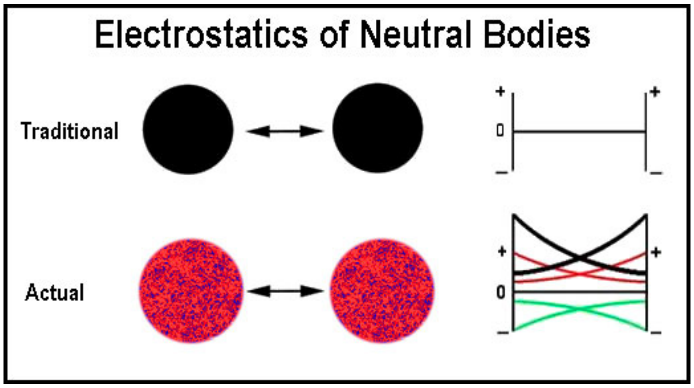
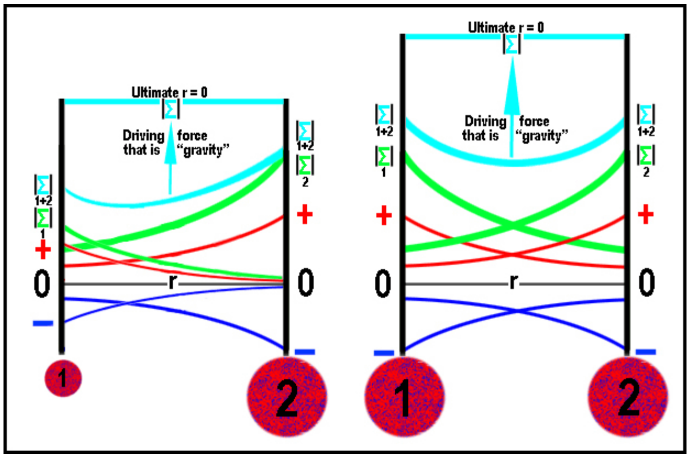
[126] Concept originally penned in 2002, partially included in "Challenging Science", Joel M Williams, AuthorHouse (2005)



The traditional view of a neutral body has a single component, electrostatic field that is zero at all distances from the object (see figure at right). Neglected in this view are the ever-present positive and negative fields generated by the many charged entities that form the objects. Opposing electrostatic fields from an object do not cancel, but nullify by opposition. The intensity of the resulting "neutral field" is the sum of the absolute intensity of all the individual electrostatic fields. Since most matter is made up of very tiny, charged species, the intensity of the neutral field will also be directly related to mass[127]; hence the similarity of the gravity mass-formula to the electrostatic charge-formula. In the quantum theory vernacular, the interaction of two neutral electrostatic fields is equivalent to orbital overlap with no net electrostatic repulsion or attraction from the sources. Here, the positive (dextral?) components combine; so do the negative (sinistral?) ones.



Electrostatic fields of a neutral object string out a dual, three-dimensional fabric (mesh or solid?) out to infinity. The summation of opposing components remains neutral, but the crescendo rises as the overlap like-components maximizes -- halting only when the two masses slam together. The force constant (G) is weak, but positive, for the overlap. Electrostatic repulsion/attraction is zero when the bodies are neutrally charged.

If the electrostatic "fabric" (solid, mesh?) of the universe is an electrostatically neutral double-weave formed from two like-charged fields, gravity is simply the propensity of like-charge fields to maximize overlap. Any unification theory that includes electrostatic charge forces already provides the means for handling the gravity force. Gravity does not require, nor have, an independent source. For over three-quarters of a century, some of our most intellectual scientists have searched for an independent source of gravity for their grand unification of forces. All have failed, as there is none. Gravity is a force subset, not an independent set.

The BIG BAND theory describes a law of the universe: "'Neutral' bodies attune" to provide maximum crescendo of the charges -- order from chaos, even as the 2nd Law of Thermodynamics grinds away to create more chaos. This explains the scientific dilemma of why we have any order at all. Gravity -- the tuning of the universe crescendo to the max.

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[127] To the extent that the charge/mass value of the smallest charge subatomic particles may be different, so will the gravitational force; achieving a normalized value as the average charge/mass value grays through astronomical numbers of each different entity. Does a hydrogen star have the same gravitational constant as a neutron star with the same mass? Closer to home, does the sun have precisely the same gravitational constant as the earth? Would a vastly non-spherical body (increased surface area, less shielding) behave differently than a spherical one?

Conclusion: it is not gravity that needs explaining, but rather what is the nature of the "fishbowl 'fluid/fabric'" in which all the "universes" are floating?" More specifically, "what is the medium that allows "matter as we perceive it" to communicate through what seems like void space (nothingness) with one another via gravity, light transmission, etc?"

ADDENDUM

The BIG BAND theory describes a law of the universe: "'Neutral' bodies attune" to provide maximum crescendo of the charges -- order from chaos, even as the 2nd Law of Thermodynamics grinds away to create more chaos. This explains the scientific dilemma of why we have any order at all. That electrons have spin allows another kind of order (spiral) to occur.

The following is offered to add a bit of levity to the issue:

A crowd gathered as the fiddler strummed the strings to set the tone. The trumpet blared to signal the spot and the sax blew a nostalgic note. The base and drums kept the beat, while the piano spewed out a catchy tune. Sound, in through the head -- out through the foot, induced the audience to hum. Some joined the instrumental gig and the band played on with a bit more gain. Few could pass by without being drawn near to check it out. Unfretted by time or space the band grew unbounded. Eventually the entire world heard the sound - a harmonious beat - and clustered around.

A musician might deem this "primal urge" -- this scientist deems it "gravity"!

Gravity -- the tuning of the universe crescendo to the max. Tuning is lost to generations that have only auto-tuned.

BIG BANDS play on to ever growing crowds even while they "sweat" (mass to energy).

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Chapter III

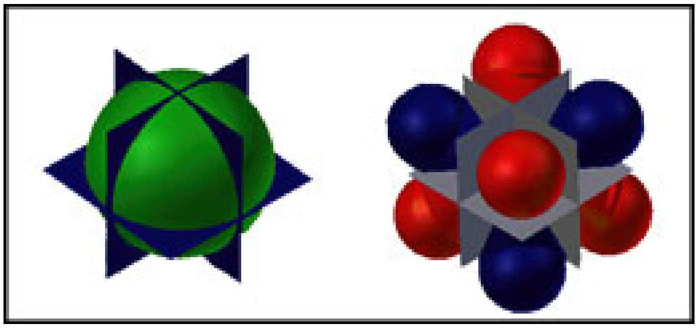
Creating the Familiar Periodic Table Via Electron Orbital Filling

Abstract

While the periodic table arrangement is usefully interpreted in columns of similar behavior, it is erroneous to imply that the underlying orbitals are all the same for all the elements in the columns of a block. Sub-orbital information has been excluded! From the standpoint of chemistry, the "rule of eight" would have provided better imagery on which to build an orbital system than was Bohr's orb turned-sphere. A sphere is useless from a chemical standpoint. Hybridization should not have to occur to explain the simplest of molecules. Simplicity would have the electrons occupying orbital spaces that are similar in shape. Only three orbital types are actually needed to describe the electron packing of the elements. Octahedral, square-planar, and pyramidal coordination complexes of the transition elements follow logically without the need to hybridize. This brief paper describes a rational packing of electrons around a nucleus that ends up mimicking the familiar periodic table when compressed to similar behavior.

Electron Orbitals and the Aufbau of the Elements

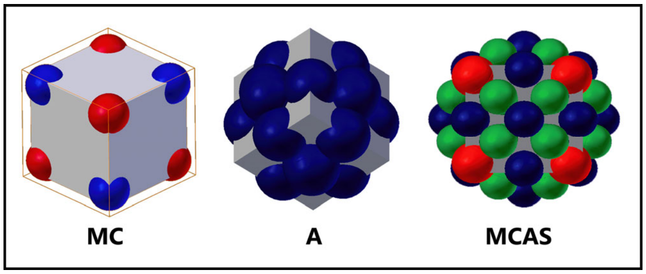
The currently accepted electron orbital structure of atoms is a concession to Bohr's circular orb. To this orb-turned sphere, the modelers added 3 more orbitals, then 5 more, and then 7 more of various shapes. Explanations of everything related to the electron behavior of atoms was forced to fit this accepted model. When the stoic orbitals could not explain observed behavior, as was the case for even simple molecules, the orbital types were "hybridized" to create even more orbital types, e.g., sp, sp^2, etc, etc. There was no looking back for models that needed less massaging to explain reality.



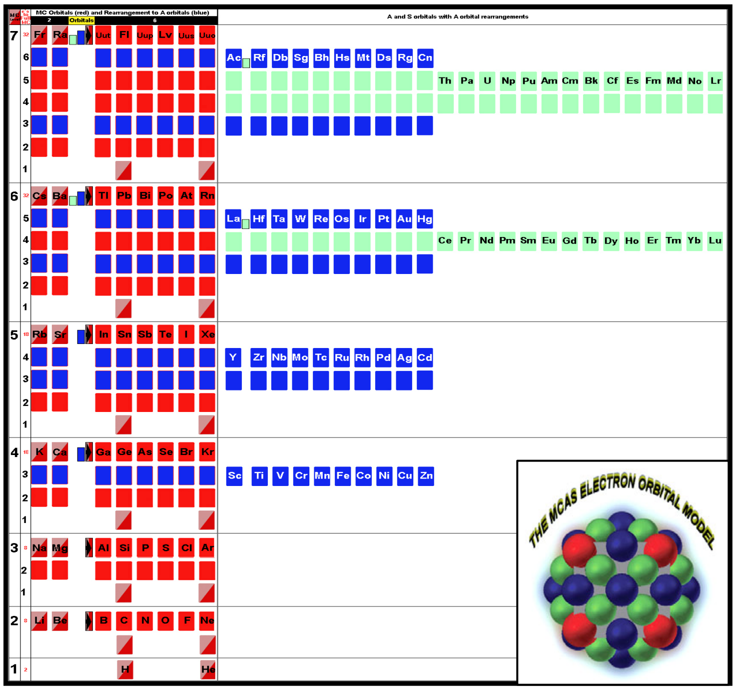
From the standpoint of chemistry, the "rule of eight" would have provided far better imagery on which to build an orbital system than was Bohr's orb which is useless from a molecular standpoint. The image on the right shows how non-intersecting orbital spaces are implemented utilizing this "rule of eight" concept.

As seen in the image to the right, there can be two opposing units with four-lobes each. When a single electron is in each of the "red" and "blue" sets, they can move counter to one another and thus be "paired"; this special case of the model negates the need for the spherical orbital type of the current spdf model. More electrons can be added until each lobe is occupied. Oxygen is of note, because its 6 electrons can be arranged in two ways, thus giving rise to the singlet/triplet phenomenon; something that required more massaging of the spdf model. Thus, this single 8-lobed model incorporates several of the points that must be addressed in the lowest electron loading and does so without the need for several types of orbitals (spherical and hourglass) and without the need to "hybridize". Unlike Bohr's orbs which are scaled to fit the observed spectral data, but have no other rationale, a single electron in one of the 4-lobed orbital scales according to simple classical physics motion and electrostatics to produce the observed spectral data.[128]

When the number of electrons is too large to be accommodated by the two quartets (8 total lobes), additional orbital space must be occupied. Simplicity would have the next order of orbitals distributed uniformly amongst the 8 occupied lobes. Simplicity would also have the electrons occupying orbital space not too dissimilar in shape. This is not the case with the spdf model which has increasingly more complex spaces. Symmetrical space-filling arrangements of orbitals around the original 8 are shown on the right.



Only three orbital types are needed to describe the electron packing of the elements of the periodic table: **C**ubic (designated **M** when only 1 or 2 electrons occupy it and **C** when more than 2 do so), **A**nticubic (18 orbitals in neat symmetry), and **S** square-faced (for lack of a better term; 24 orbitals with 8 more to get 32 via tetrahedral space). These orbitals will now be used to demonstrate the aufbau of the elements.



The image on the right demonstrates how the elements are formed via the **MCAS** model starting with the smallest (H) at the bottom and building electron numbers upwards. The unlabeled orbitals below indicated elements are those when all the **C**-orbitals of a period are filled to create the "inert" gas elements. Breaks in the packing of various orbital sets are shown with gaps and markers.

The following discourse describes some of the salient features of the **MCAS** aufbau.

1. The energetics of adding more electrons than opposing 2 (He) to the 8 **C**ubic lobes at the lowest (1st) energy level is far greater than starting a new level. This is much like the situation of landing patterns being able to handle only 2 planes and, thus, all others are placed in more distant patterns. Hydrogen is in mid (1/2-filled) position. Helium has 2 "paired" electrons. The partially filled 8-lobed space should provide some additional behavior that is not available to the other "inert" gases whose lobes are completely filled.
2. At the 2nd level (period), the first two electrons go into opposing 4-lobed **C**ubic orbital sets and are thus paired; electron movement is opposite that of those in the first level.

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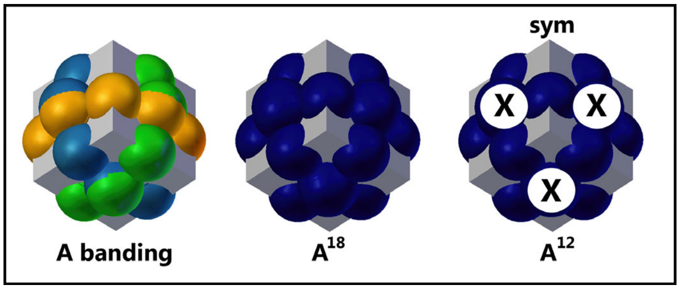
[128] Why do Electrons (Orbitals) Have Discrete Quantum Numbers?, http://vixra.org/abs/1210.0133, Joel M Williams

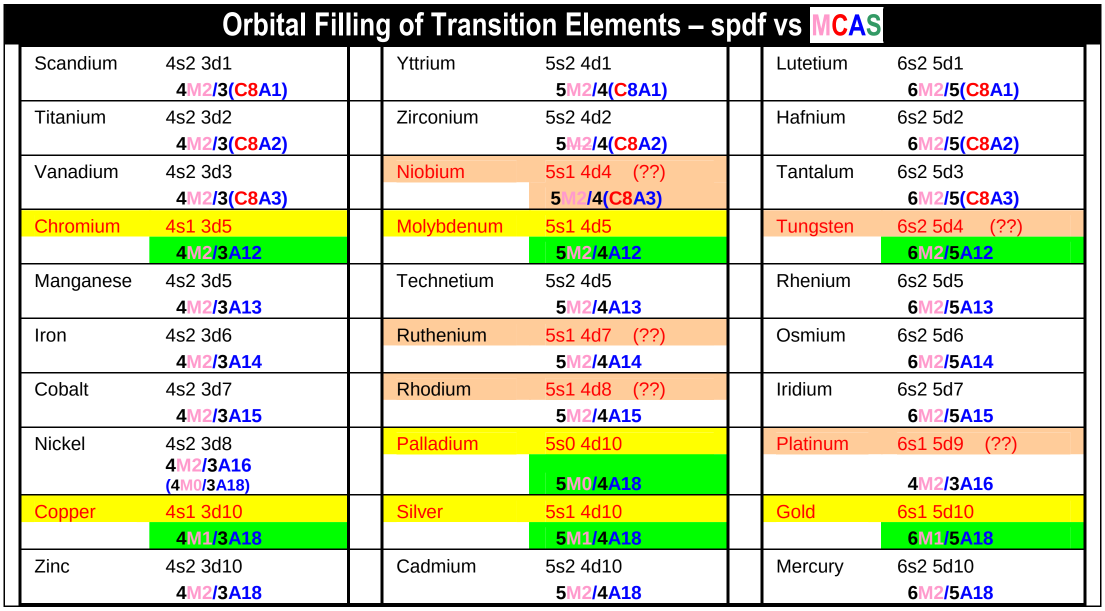
Further additions of electrons continue with the filling of one 4-lobed unit first. Thus, B (C^2M^1), C (C^3M^1), N (C^4M^1), O (C^4C^2), F (C^4C^3) and Ne (C^4C^4). The C^4C^0 state (4-unpaired electrons) of carbon, which facilitates tetrahedral bonding, is not the ground state, but an elevated one. The C^3C^3 state of oxygen provides the second state that allows O_2 to have both singlet and triplet states.

3. Electron filling at the 3rd period follows the scheme of the 2nd. Again the orbitals to be filled are the two 4-lobed **C**ubic orbital sets; electron movement is opposite that of those in the 2nd level whose orbital spaces are filled symmetrically (C^4C^4). This contrasts with the current spdf model that has two different types.
4. At the 4th period, two electrons can be placed oppose one another in the two 4-lobed **C**ubic orbital sets. Additional electrons, however, can be accommodated in **A**nticubic orbitals more favorably than adding them to the remaining **C**ubic orbitals. The image on the right should help in understanding the filling that gives the "transition series" its properties.



The **A**nticubic arrangement bands the **C**ubic alignment symmetrically. The first few electrons will be in one of the 3 bands. Eventually all 18 lobes will be occupied. Since only 10 electrons are added before the remaining **C**ubic lobes are filled, 8 electrons must be obtained from elsewhere. These are provided by what would have been the previous **C**ubic electrons of the same level. Favorable energetics are derived when the **A**nticubic lobes are filled symmetrically: **A**18 (completely) and **A**12 (face-deficient). The **A**nticubic arrangement easily promotes octahedral, square-planar, and pyramidal coordination complexes without hybridizing as required with the spdf model.

The table below explains the orbital filling further. Spdf fillings in red are non-Madelung[129].



Orbital Filling of Transition Elements – spdf vs MCAS

Scandium	4s2 3d1 4M2/3(C8A1)	Yttrium	5s2 4d1 5M2/4(C8A1)	Lutetium	6s2 5d1 6M2/5(C8A1)
Titanium	4s2 3d2 4M2/3(C8A2)	Zirconium	5s2 4d2 5M2/4(C8A2)	Hafnium	6s2 5d2 6M2/5(C8A2)
Vanadium	4s2 3d3 4M2/3(C8A3)	Niobium	5s1 4d4 (??) 5M2/4(C8A3)	Tantalum	6s2 5d3 6M2/5(C8A3)
Chromium	4s1 3d5 4M2/3A12	Molybdenum	5s1 4d5 5M2/4A12	Tungsten	6s2 5d4 (??) 6M2/5A12
Manganese	4s2 3d5 4M2/3A13	Technetium	5s2 4d5 5M2/4A13	Rhenium	6s2 5d5 6M2/5A13
Iron	4s2 3d6 4M2/3A14	Ruthenium	5s1 4d7 (??) 5M2/4A14	Osmium	6s2 5d6 6M2/5A14
Cobalt	4s2 3d7 4M2/3A15	Rhodium	5s1 4d8 (??) 5M2/4A15	Iridium	6s2 5d7 6M2/5A15
Nickel	4s2 3d8 4M2/3A16 (4M0/3A18)	Palladium	5s0 4d10 5M0/4A18	Platinum	6s1 5d9 (??) 4M2/3A16
Copper	4s1 3d10 4M1/3A18	Silver	5s1 4d10 5M1/4A18	Gold	6s1 5d10 6M1/5A18
Zinc	4s2 3d10 4M2/3A18	Cadmium	5s2 4d10 5M2/4A18	Mercury	6s2 5d10 6M2/5A18

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[129] http://en.wikipedia.org/wiki/Electron_configuration

For the transition elements of the 4 period, the **A**-orbital filling with the **MCAS** model is fairly straight forward. Unlike the spdf model, where the only way to have 6-unpaired electrons is to shift a 4-s to a 3-d orbital, the **MCAS** filling is normal to a symmetrical **A**12. The symmetrical **A**12 has one electron missing from each face. The absence of 6-unpaired electrons indicates that this configuration has six 3-electron sub-orbital sets. While the Nickel ground state is standard with 4M2/3A16, it reconfigures to 4M0/3A18 for the tetrahedral $Ni(CO)_4$ with bonding through a now vacant **C**-orbital. Copper does not follow the pattern as completing the **A**nticubic orbitals (3A18) with electron pairing provides a lower energy state than pairing an electron in the 4M orbitals. Silver and gold follow suit, in higher periods, with each having a primary valence of 1. Note that each of these has only one of the **C**ubic sets occupied! These elements are also unique in having fully occupied sub layers. The **MCAS** **C**ubic orbitals of Cu, Ag, and Au provide a donor (one electron in a high-energy tetrahedral orbital)-receptor (vacant tetrahedral orbital hole) network that is unrivaled. They, thus, conduct electricity (flowing electrons) nicely.

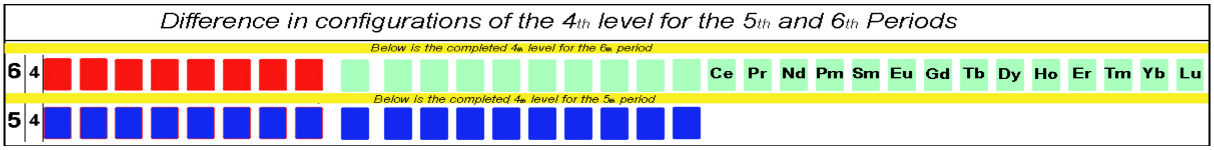
A word about the energy of “added” electrons. Internally packed electrons are not easily removed as they are part of a larger structure that would require reordering of others. Thus, while an electron may be “added”, in the sense that one more is needed to balance the nuclear charge, it is not necessarily of higher energy than all of those “added” before it as related to the previous element! Indeed, the “last electron added” is a common misconception produced by the drop-in, aufbau method of the stoic spdf model. Rather, all of an element’s electrons are arranged to give the lowest energy configuration. If one were filling from low-to-high energy, the last electrons loaded would be those in the outermost level! Thus, these are the first removed to form ionic species.

5. The transition elements of the 5th period have their 4th level **A**nticubic orbitals overlaying those of the filled 3rd level **A**nticubic orbitals. As such, they must coordinate with them; phased oppositely. This adds an additional factor to the aufbau and the likelihood of packing anomalies. The series according to the **MCAS** model starts like that of the 4th period (Yttrium and Zirconium) with the **A**12 and **A**18 symmetry drivers holding (Molybdenum and Silver). Palladium also has the **A**18 allotment and thus no 5M electrons. Niobium, Ruthenium and Rhodium are problematic for the spdf model. I have presented the **MCAS** configuration of all three that corresponds to those of the 4th and 6th period transition elements.

6. The transition elements of the 6th period have their 5th level **A**nticubic orbitals overlaying those of the filled 3rd level **A**nticubic orbitals. With the greater level (energy) separation than that in the 5th period, the aufbau is more similar to that of the 4th period. The electrons in the 4th level **A**nticubic orbitals now occupy 4th level **C** or **S** orbitals (see below). The spdf anomalies are Tungsten and Platinum. The expected **MCAS** filling is given for both with the knowledge that the **A**nticubic orbitals can load asymmetrically, although it appears this rarely happens.

7. When more electrons must be managed than the **A**nticubic 18 orbitals can handle, another arrangement of the electrons is necessary. After the 5th **A**nticubic level is begun in the 6th period, electrons are then added to the 4th level. Now, however, unlike the 18-lobes of the **A**nticubic configuration of the 4th level that sufficed for the 5th period, a

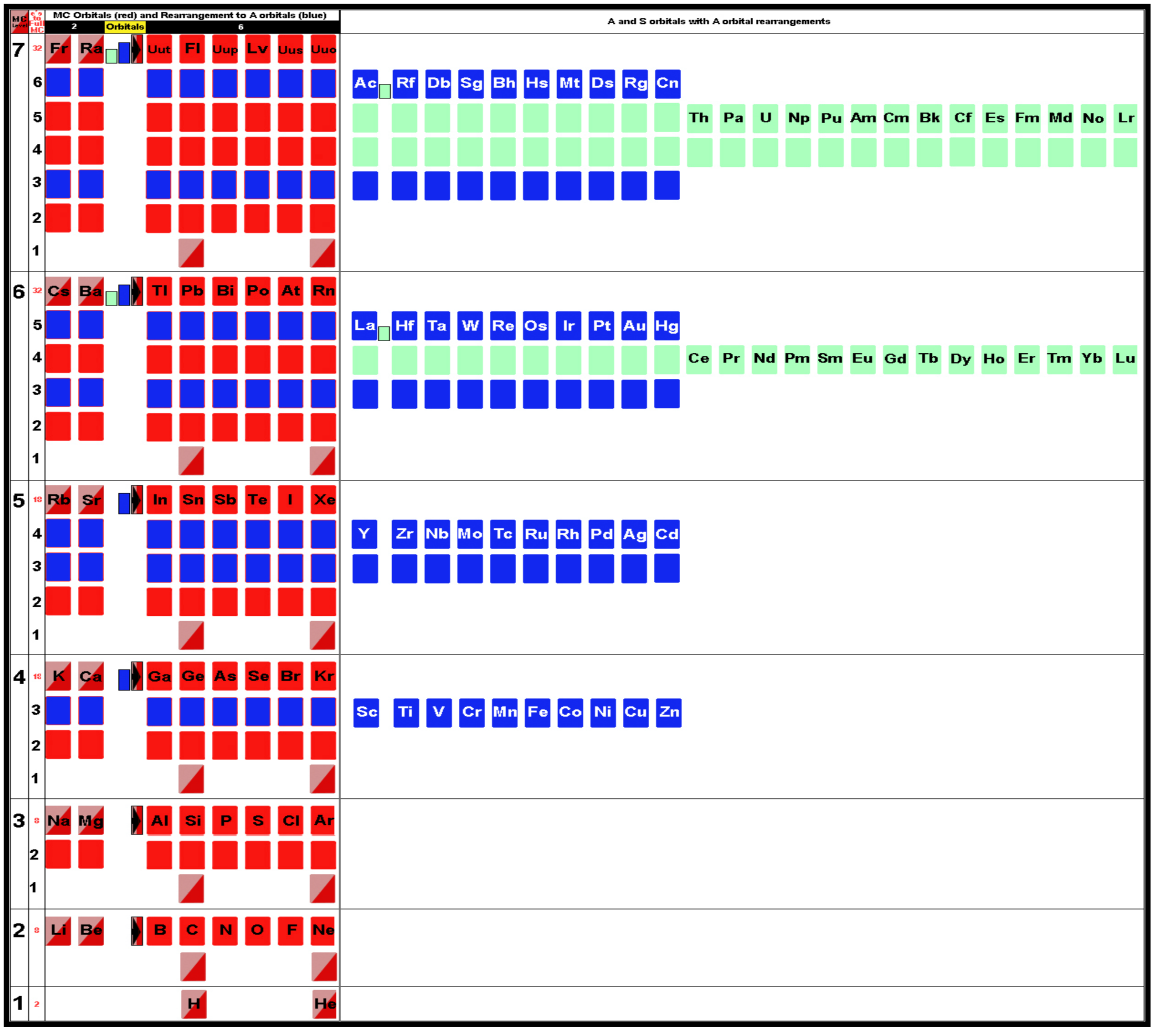
32-lobed configuration (24 **S** + 8 **C**) is required. The image below indicates how this is accomplished.



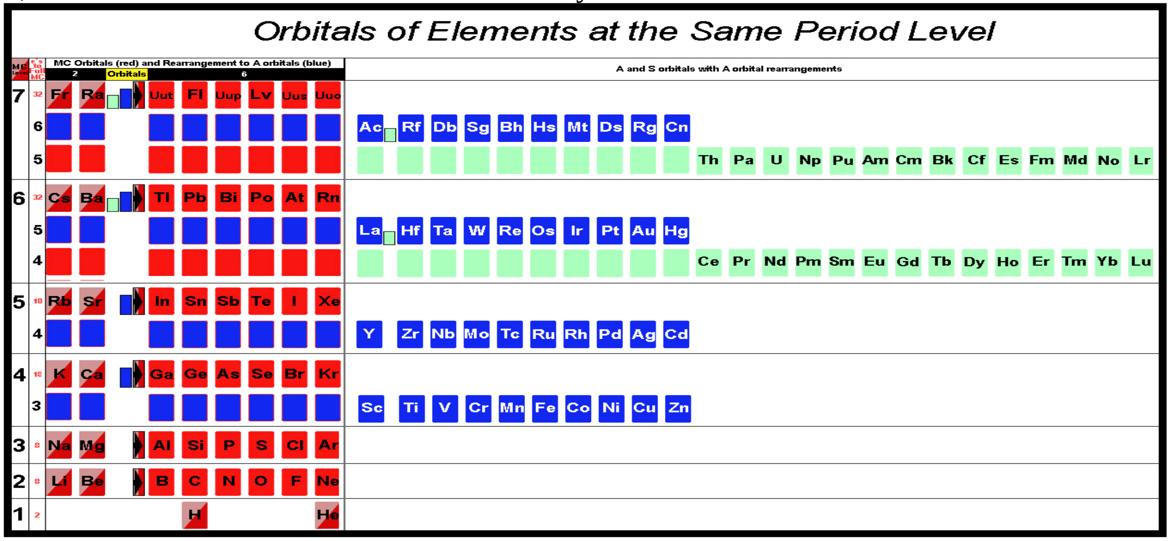
8. A similar situation occurs for the 7th period and the 5th level.

From Orbital Filling to the Familiar Periodic Table

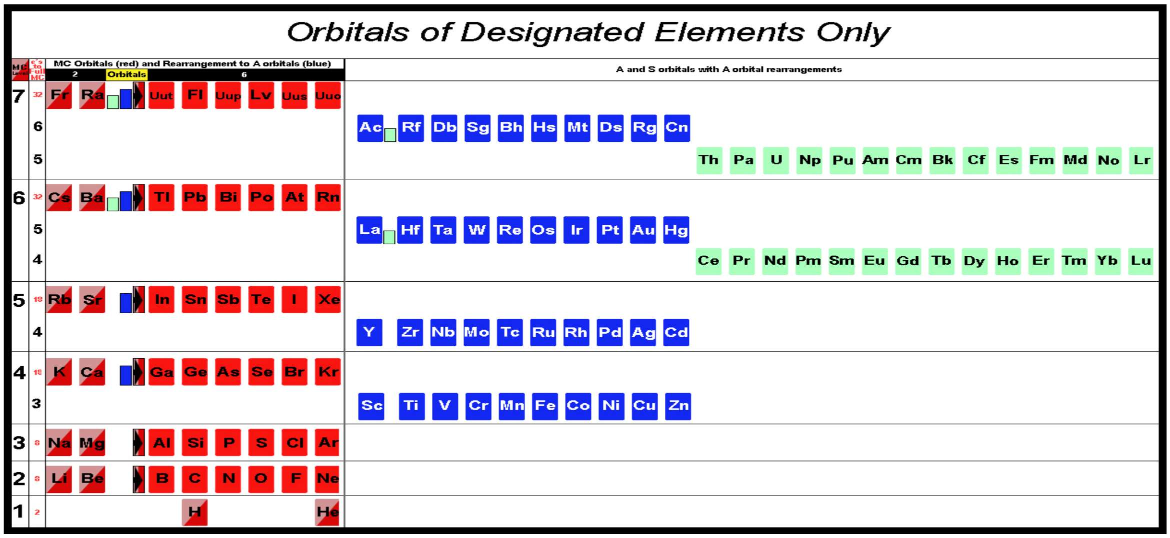
The familiar periodic table is very useful in its simplicity: periods with increasing proton mass in columns of similar chemical behavior. Implicit in its conveyance to newbies, however, is that all of the underlying electrons fit stoic “file cabinets”. This is emphasized by the use of [He], [Ne], [Ar], [Kr], [Xe], and [Rn] as the underlying cores. The foregoing section demonstrates that the packing of electrons around a nucleus is more dynamic and *at the same time* more uniform than the spdf model permits. The following set of images indicates what is lost in the compression of the **MCAS** orbital loadings to the familiar version of the periodic table. The starting image is given again for convenience.



First, the sub-orbitals that are below any element "labeled" level are removed.

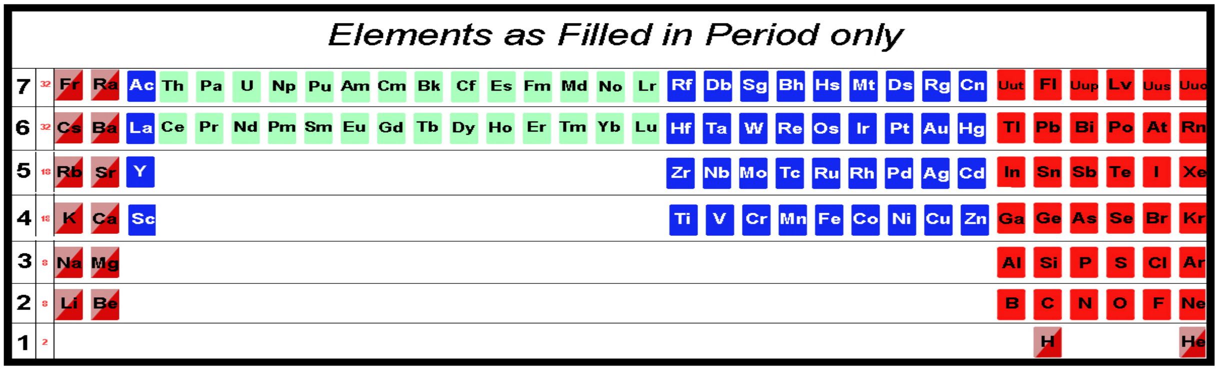


Next, all the "unlabeled" orbitals are removed.



Next, the elements are arranged as they are "filled" with the similar designations aligned over one another.

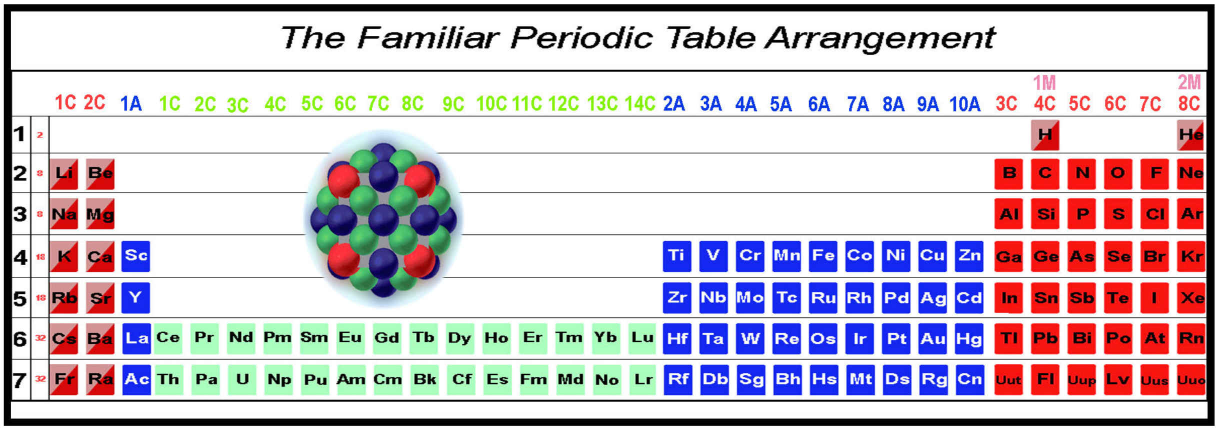
Now, all the individual levels are compressed to that of the outermost level (period) in the order of their filling – the inverse of the familiar periodic table which emphases the building upwards of the element mass.



Elements as Filled in Period only

7	32	Fr	Ra	Ac	Th	Pa	U	Np	Pu	Am	Cm	Bk	Cf	Es	Fm	Md	No	Lr	Rf	Db	Sg	Bh	Hs	Mt	Ds	Rg	Cn	Uut	Fl	Uup	Lv	Uus	Uuo
6	32	Cs	Ba	La	Ce	Pr	Nd	Pm	Sm	Eu	Gd	Tb	Dy	Ho	Er	Tm	Yb	Lu	Hf	Ta	W	Re	Os	Ir	Pt	Au	Hg	Tl	Pb	Bi	Po	At	Rn
5	18	Rb	Sr	Y															Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd	In	Sn	Sb	Te	I	Xe
4	18	K	Ca	Sc															Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As	Se	Br	Kr
3	8	Na	Mg																									Al	Si	P	S	Cl	Ar
2	8	Li	Be																									B	C	N	O	F	Ne
1	2																												H				He

The order is now reversed to reflect the lowest electron packing at the top as traditionally viewed.



The Familiar Periodic Table Arrangement

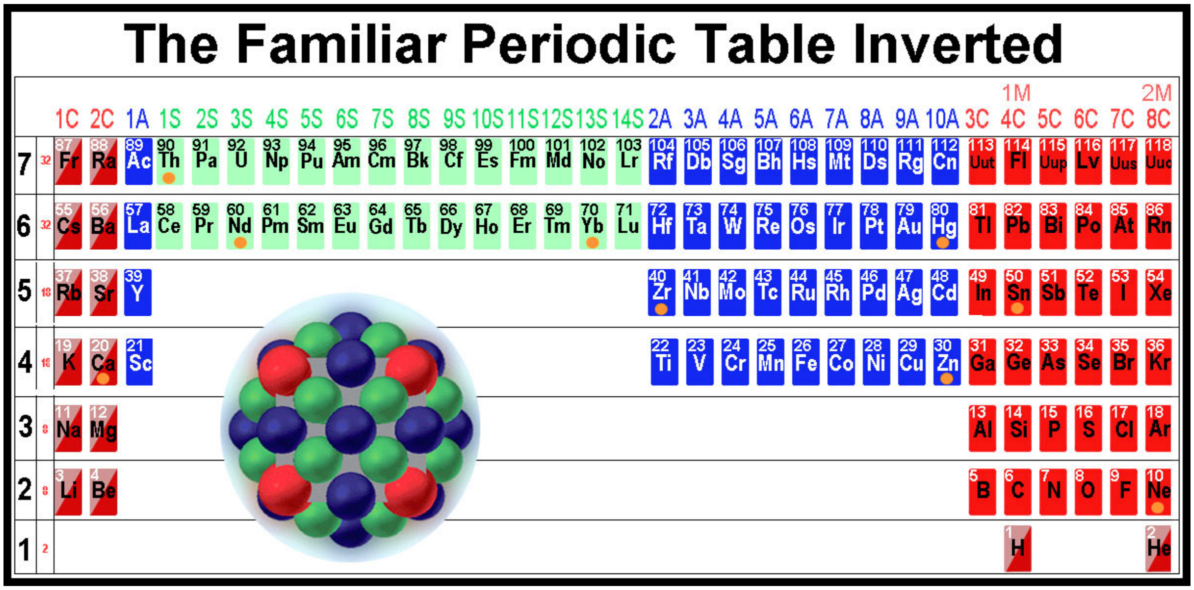
																													1M				2M
		1C	2C	1A	1C	2C	3C	4C	5C	6C	7C	8C	9C	10C	11C	12C	13C	14C	2A	3A	4A	5A	6A	7A	8A	9A	10A	3C	4C	5C	6C	7C	8C
1	2																												H				He
2	8	Li	Be																									B	C	N	O	F	Ne
3	8	Na	Mg																									Al	Si	P	S	Cl	Ar
4	18	K	Ca	Sc															Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As	Se	Br	Kr
5	18	Rb	Sr	Y															Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd	In	Sn	Sb	Te	I	Xe
6	32	Cs	Ba	La	Ce	Pr	Nd	Pm	Sm	Eu	Gd	Tb	Dy	Ho	Er	Tm	Yb	Lu	Hf	Ta	W	Re	Os	Ir	Pt	Au	Hg	Tl	Pb	Bi	Po	At	Rn
7	32	Fr	Ra	Ac	Th	Pa	U	Np	Pu	Am	Cm	Bk	Cf	Es	Fm	Md	No	Lr	Rf	Db	Sg	Bh	Hs	Mt	Ds	Rg	Cn	Uut	Fl	Uup	Lv	Uus	Uuo

While the periodic table arrangement is usefully interpreted in terms of “blocks” and columns of similar behavior, it is erroneous to indicate that the underlying orbitals are all the same for all the elements in that block. The sub-orbital information has been excluded! Labile electrons are those of uncompleted sets, thus the facile removal of electrons from the “interrupted set” orbitals indicated at the far left. Once completed, orbital sets are quite stable.

Each element is indicated by the unique orbitals it uses. Think in terms of each possessing all those in the period to its left. Thus, Chromium is characterized by MA, Uranium by MAS, but Tungsten by MSA. Their sub-orbitals may be quite different.

To summarize, the MCAS model yields the periodic table upon compression and does not require all the “hybridizing” that the highly touted spdf model needs to accommodate the chemical materials of our real world.

The Familiar Periodic Table in its inverted form is shown more annotated on the next page. The MCAS model is included for referencing.

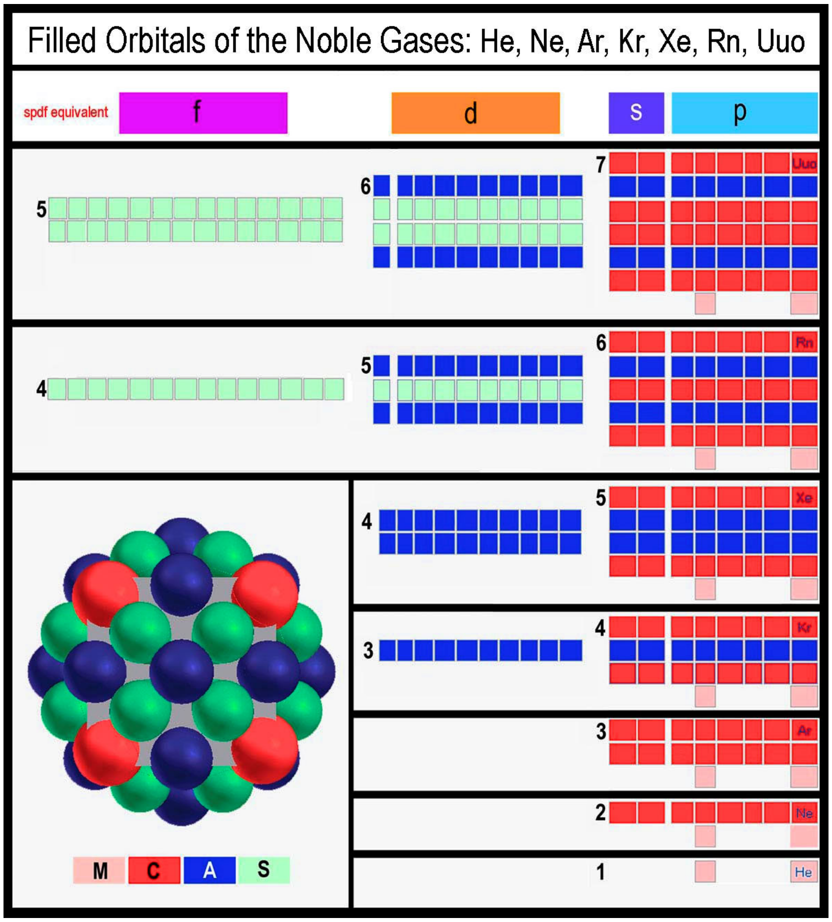


The Familiar Periodic Table Inverted

																												1M					2M
		1C	2C	1A	1S	2S	3S	4S	5S	6S	7S	8S	9S	10S	11S	12S	13S	14S	2A	3A	4A	5A	6A	7A	8A	9A	10A	3C	4C	5C	6C	7C	8C
7	32	87 Fr	88 Ra	89 Ac	90 Th	91 Pa	92 U	93 Np	94 Pu	95 Am	96 Cm	97 Bk	98 Cf	99 Es	100 Fm	101 Md	102 No	103 Lr	104 Rf	105 Db	106 Sg	107 Bh	108 Hs	109 Mt	110 Ds	111 Rg	112 Cn	113 Uut	114 Fl	115 Uup	116 Lv	117 Uus	118 Uuo
6	32	55 Cs	56 Ba	57 La	58 Ce	59 Pr	60 Nd	61 Pm	62 Sm	63 Eu	64 Gd	65 Tb	66 Dy	67 Ho	68 Er	69 Tm	70 Yb	71 Lu	72 Hf	73 Ta	74 W	75 Re	76 Os	77 Ir	78 Pt	79 Au	80 Hg	81 Tl	82 Pb	83 Bi	84 Po	85 At	86 Rn
5	18	37 Rb	38 Sr	39 Y															40 Zr	41 Nb	42 Mo	43 Tc	44 Ru	45 Rh	46 Pd	47 Ag	48 Cd	49 In	50 Sn	51 Sb	52 Te	53 I	54 Xe
4	18	19 K	20 Ca	21 Sc															22 Ti	23 V	24 Cr	25 Mn	26 Fe	27 Co	28 Ni	29 Cu	30 Zn	31 Ga	32 Ge	33 As	34 Se	35 Br	36 Kr
3	8	11 Na	12 Mg																									13 Al	14 Si	15 P	16 S	17 Cl	18 Ar
2	8	3 Li	4 Be																									5 B	6 C	7 N	8 O	9 F	10 Ne
1	2																												1 H				2 He

The Uniquely Different Symmetry of Each Noble Element's Underlying Orbital Filling

Unlike the constant, stoic, spdf "block-filling" of electrons around the nucleus, the MCAS model has the electrons flexibly filling space to minimize overlapping electron orbital density. The following image demonstrates the symmetry of each completely filled level terminating with a noble element. As seen, each noble element has a uniquely different, but highly symmetrical, distribution of electrons, as opposed to the currently taught "solid block filling" of the spdf model. In the MCAS model, an orbital is assigned to each and every individual electron and those orbital lobes are all the same shape. The spdf model has 2 electrons paired in orbitals of ever increasing complexity needed to generate them under the model's assumptions. Pairing in the MCAS model occurs with every orbital having a diametrically opposed orbital and thus requires no spin-reversal parameter.



The Periodic Table and the MCAS Electron Orbital Model Cusco

(The Third International Conference on the Periodic Table, Cusco, Peru 2012)
Special Topics Session: Relationship of the Periodic Table and quantum mechanics

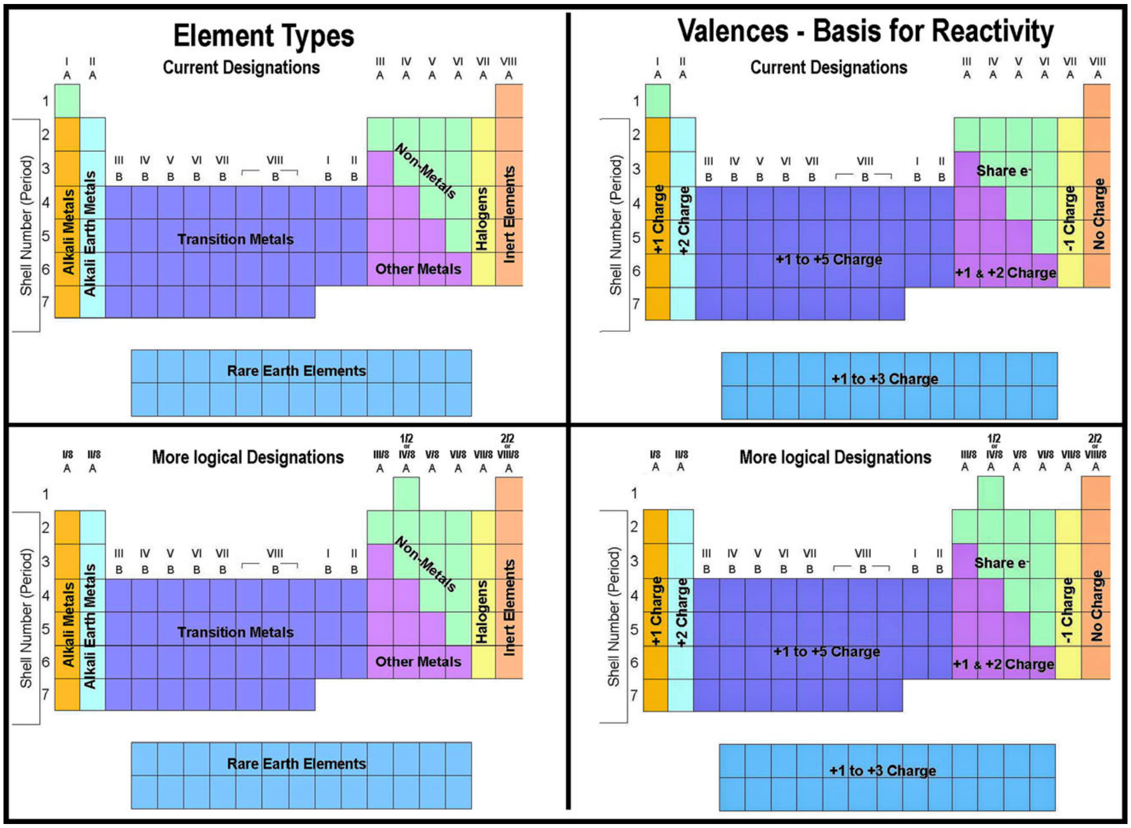
A handout by Joel M Williams

Abstract

A useful periodic table provides a number of important facts to its user. As a chemist, I found the implied chemical properties (valence, metallic vs non-metallic compound formation) and atomic weight to be the most valuable. Thus, I have always had a problem with the placement of Hydrogen. Of course, its placement in most periodic tables has been driven more by the acceptance of the spdf orbital model than by "element properties". The problem with Hydrogen and other concerns about hybridization of orbitals and chemical reactions led me to the MCAS electron orbital model.

Logical Place for Hydrogen in the Common Periodic Table

The periodic Table is useful to the chemist because it conveys a significant amount of information about the nature of the elements. The general construct of the most popular form provides this valuable information. Hydrogen's position does NOT conform to the chemistry and physical state classes, but bows to quantum physics and its spdf modeling. H is nowhere near like Li or F above which it is often placed! A more logical placement would be over C as both contain ½ (4/8=½) of the valence electrons that occur in its row. These ideas are presented in the figure below.



Original Table image is from http://www.homework-help-secrets.com/periodic-table.html

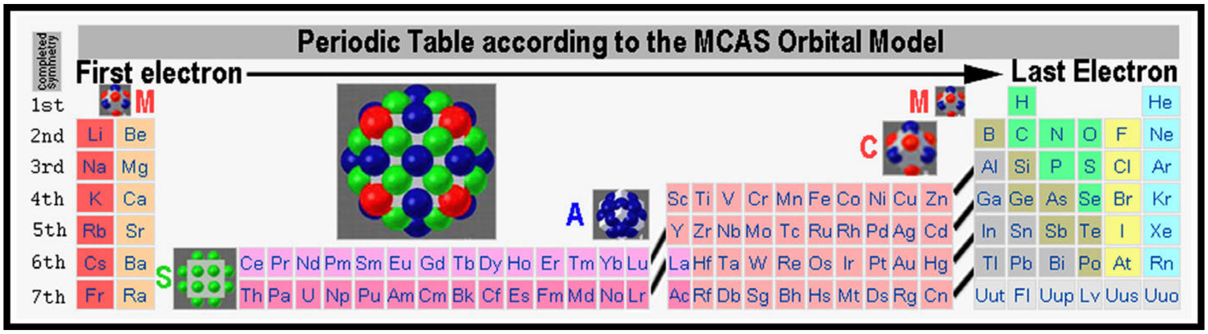
Expanded Periodic TableAccording to the MCAS Orbital Model

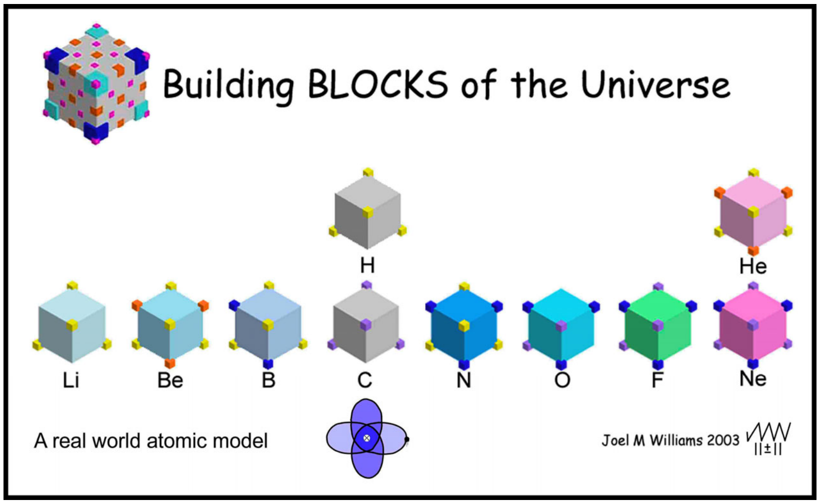
The MCAS electron orbital model[130] is based on the principles that electrons

- Are particulate in our 3D worldly concept with a negative “aura” that yields wave behavior, thus “AND duality”
- Repel one another; mathematical “spin-reversal” to allow then to cohabitate does not change the fact that electrons oppose one another
- Exhibit quantum energy level behavior because they interact with the nucleus. A simple, classical mechanic (Newtonian) machine demonstrates why electrons are modeled with the principal quantum numbers[131]. It is a timing phenomenon.
- Occupy very similar orbital space while filling 3D space. Thus, a particulate electron moving, even at random, in the d_z2 and f orbitals of the spdf model is illogical.
- Are not bound to fill underlying orbitals. Thus, underlying electrons can dynamically rearrange to provide optimal distribution and lower energy.

With the MCAS model itself presented elsewhere[1], its relationship to the periodic table is presented below. For those familiar with the extended form, it should be self-explanatory. Two notes, however:

- The first two elements in each row easily lose electrons to revert to the previous noble gas “completed symmetry”; only under extreme conditions would a hydrogen nucleus exist stripped of all electrons. Thus, Hydrogen forms covalent bonds rather than ionic ones.
- Underlying electrons order so that only two “layers” of the same type of orbitals are occupied (see diagonal connecting lines); contrasting with the stoic spdf model.





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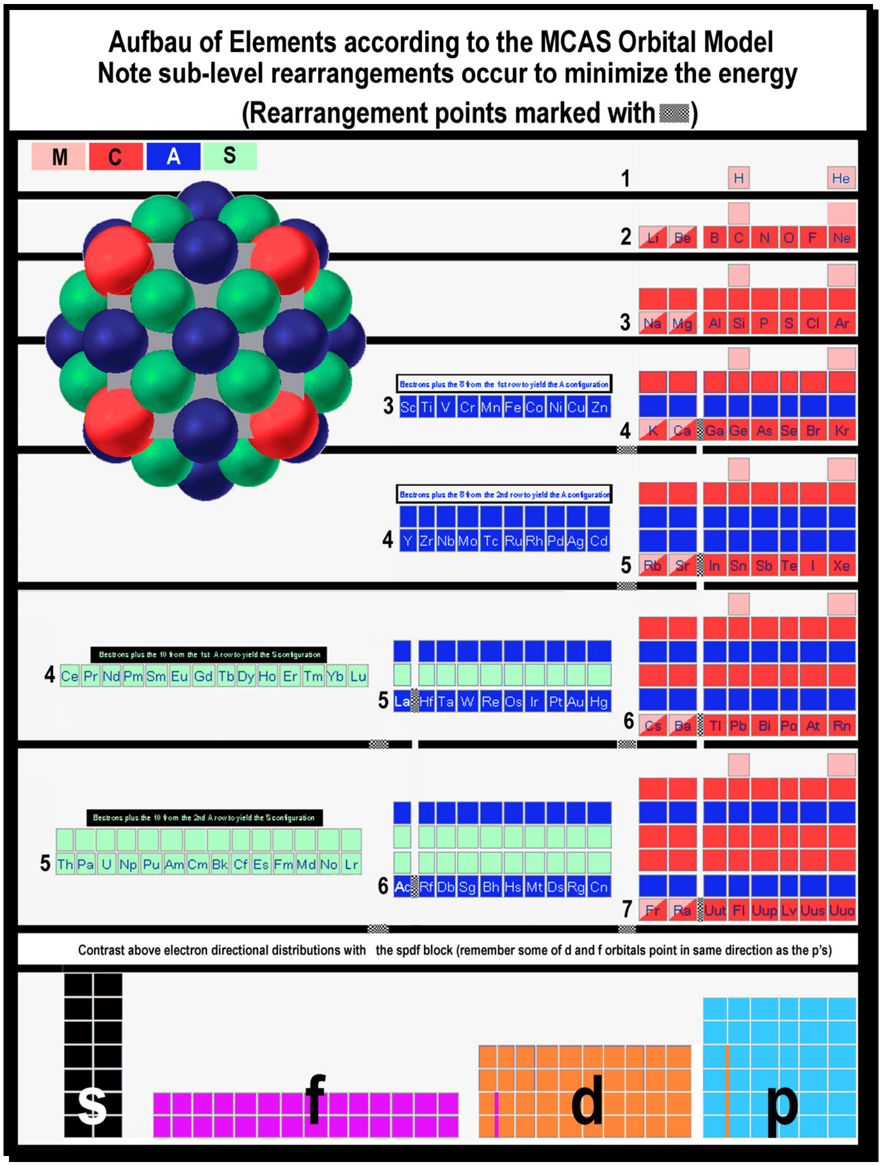
[130] Several citations: a)Challenging Science (2005) http://pages.swcp.com/~jmw-mcw/, Joel M Williams; b) the MCAS Electron Orbital Model, http://vixra.org/pdf/1205.0114v1.pdf, Joel M Williams

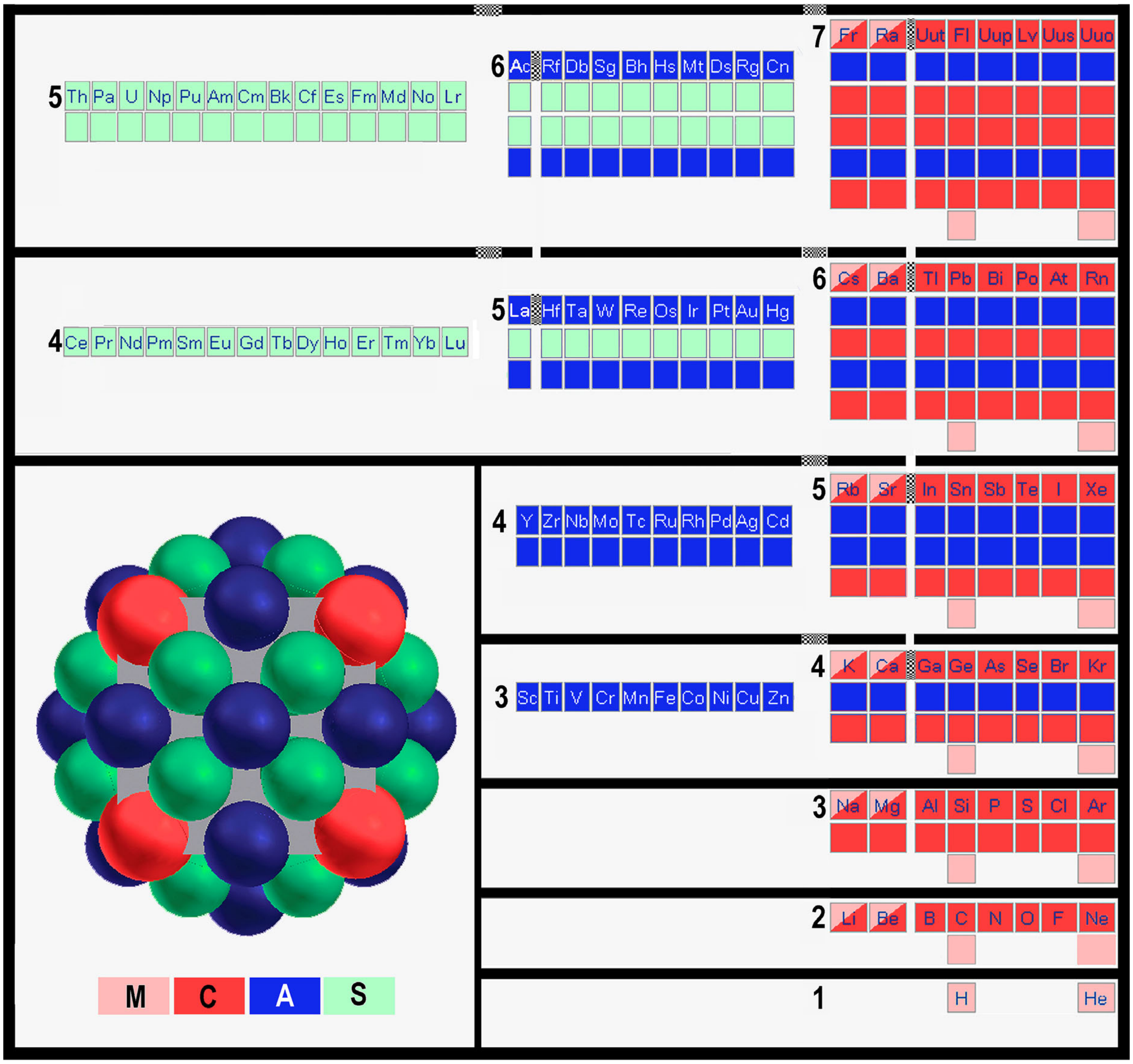
[131] Why do electron orbitals have discrete quantum numbers?, http://pages.swcp.com/~jmw-mcw/Quantum%20Numbers%20from%20a%20Simple%20Quantum%20Mechanics%20Machine.htm, Joel M Williams.

Aufbau of the Periodic Table Elements According to the MCAS Orbital Model

To better understand the aufbau of the periodic chart and why the transition element series and lanthanide and actinide series occur where they do, the following figure is presented. Before the 4-lobed M-orbitals can add more electrons and become C-orbitals at the 4th-7th levels, some underlying electron redistribution must take place. Thus, 8-electrons from a C-orbital series are moved to an A-orbital series which is then completely filled. After this, electron filling can convert the M-orbitals to C-orbitals. Likewise, when a third level of A-orbitals is started at La or Ac, an underlying A-orbital series must be redistributed to an S-series with 8 electrons returning to an M-series. Remember that the electron in the "La" or "Ac" orbital is there for the S-series elements that follow and accounts for the +3 behavior of those elements; esp, the lanthanides. The symmetry maintained and the more even distribution of electrons is readily apparent when viewed in this manner. In the spdf model, electron density is just piled on top of electron density, especially in the p's, without sub-level redistribution. How s-orbitals can be orthogonal to themselves (the last includes all those below in its space) and with other orbitals with whom they share space is a great contradiction to the spdf model. It is not clear what drives the d and f series elements to occur where they do in the spdf model. That such is modeled is a different matter.

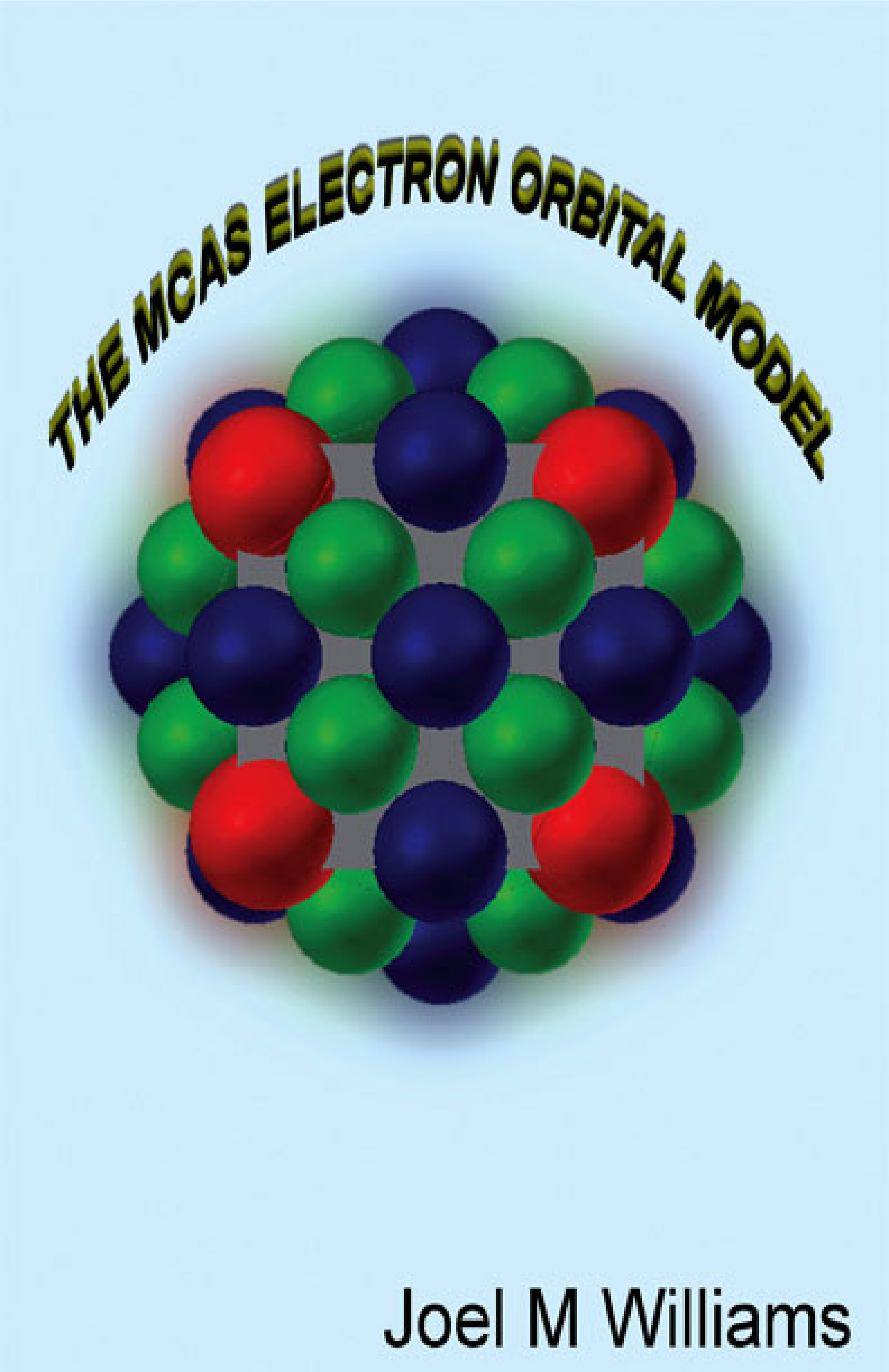


While the previous figure showed the electron distribution in-line with the conventional periodic table arrangement with the lowest-mass elements at the top, the following figure gives a different view. Here, the emphasis is on the electron loading as the number of electrons surrounding the nucleus increases. This reversal may help some see the sub-level reordering easier.



Aufbau of Elements according to the MCAS Orbital Model
Note sub-level rearrangements occur to minimize the energy
(Rearrangement points marked with ▨)
(arranged from lowest electron loading upward)

Chapter II



The MCAS Electron Orbital Model
plus Atomic Bonding and Newtonian Quantum Numbers

Abstract

This is a follow-up of my book entitled "Challenging Science".[132] *Here, I have created tear-shaped orbitals and placed them around a point, aka nucleus, to make them more in tune with conventional representations instead of the cubes I used earlier. The MCAS model clearly demonstrates how electrons can be spaced around the nucleus without resorting to the spin-reversal and oddly shaped orbitals of the spdf-model. Newtonian science is demonstrated to describe the physics of the Balmer-series whereas the Bohr model and subsequent treatment only applied the necessary mathematical formula without a physical explanation.*

Introduction

The Bohr spherical electron-orbit(al) ***still*** provides the base for current atomic model. Mathematical treatments that generate the spdf model have been rather stoic and even violate the orthogonality crutch they laud. There is no physical explanation about how the spectral emissions occur, only that they do and the models are massaged to produce them. In recognition of the shortcomings of the spdf model, the MCAS electron orbital model was developed In this update of its presentation in "Challenging Science"[1], I have shown the model in more conventional orbital forms. Also discussed are bonding images. Finally, but not least, the physical (Newtonian) reason that the Balmer series is generated by a single electron orbiting a nucleus is given.

A: The MCAS Electronic Structure of Atoms

In 1999, I described the MCAS model for the electronic structure of atoms.[133] This model recognized that, while *electrons* can *exhibit duality* (wave *and* particle properties; *not or*, in our physical reality), a proper model representing them about a nucleus could not ignore their repulsive nature as the spdf model does. I represented my model with cubes as that was the imaging software I had at the time and it was easier to make paper cubes[134] than other shapes. Some thought I was proposing angular orbitals, while I was just trying to depict spatial deployment of the electron orbitals in a different way than the spdf model did. For all its claims to orthogonality, the spdf model constantly violates this premise with all those spdf orbitals occupying some of same space as similar spdf orbitals do. I have now used blender 2.61 software[135] to create tear-shaped orbitals and place them around a point, ala nucleus.

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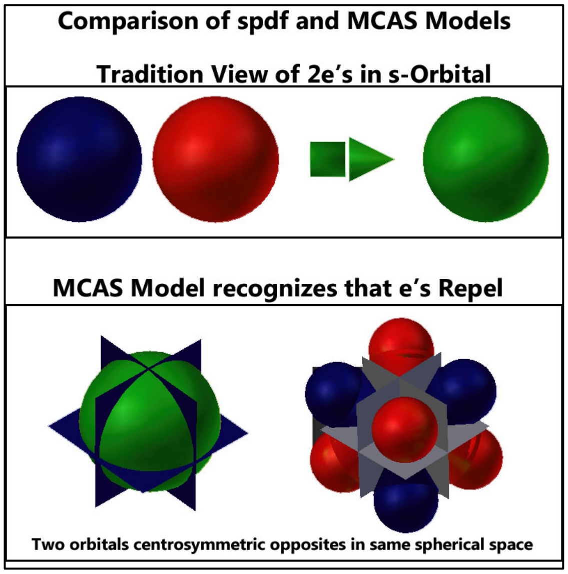
[132] "Challenging Science", Joel M Williams, 108 pages, AuthorHouse, English, ISBN-10: 1420842382, ISBN-13: 978-1420842388 (July 25, 2005)

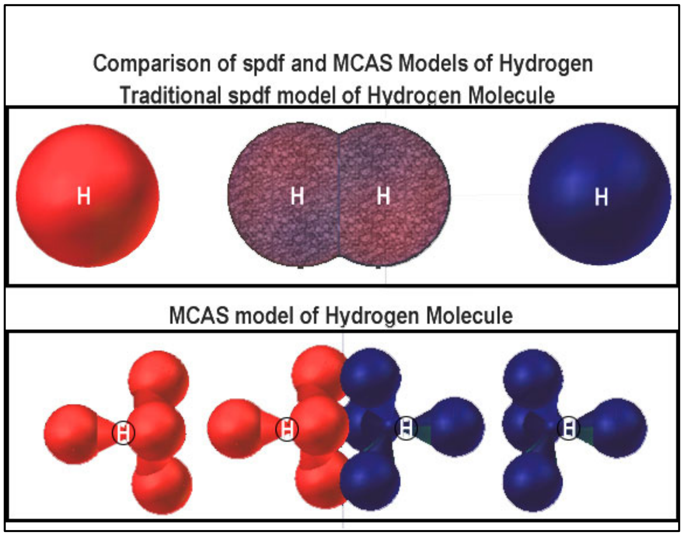
[133] http://arxiv.org/html/physics/9902046v1/Article.html and http://arxiv.org/html/physics/9909053v3. First submission of the concept for publication was in 1993. Also: *The Electronic Puzzle* 1994 (LIBCONG-TXu-632-452) [cited in *A BIT TOO FAR* http://arxiv.org/html/physics/9904031]

[134] Moles, bits, and cubes, LIBCONG-TXu000593728 (1996)

[135] www.blender.org



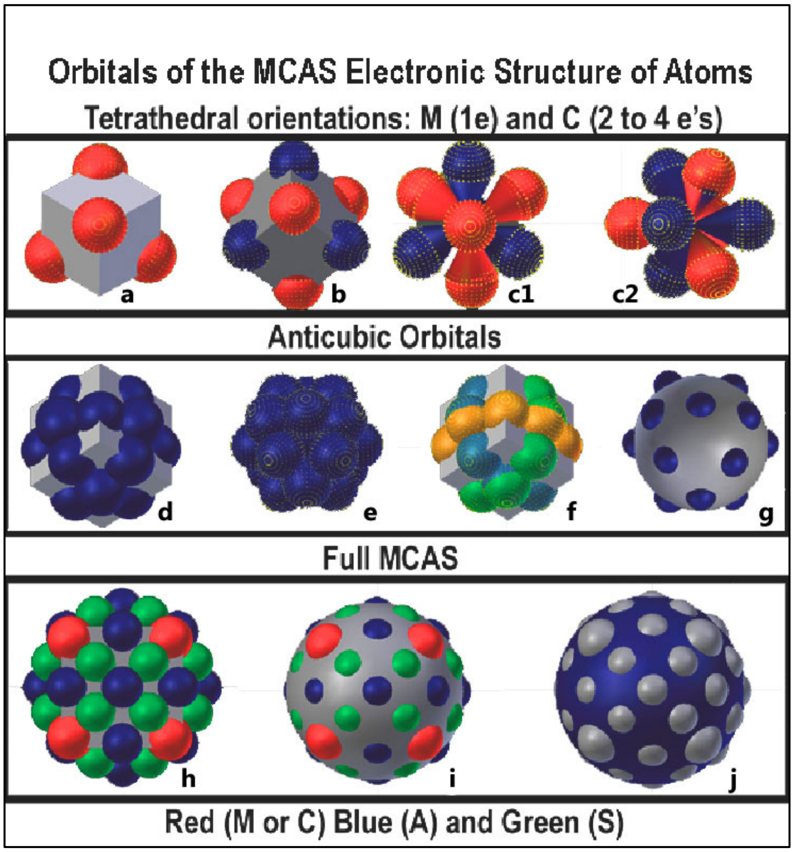
The simplest electronic orbital in the spdf model is a sphere. One electron was presumed to occupy it per the Bohr model. When a second electron was added, the two blended (paired by wave mechanics) to occupied the same spherical space – see the depiction on the right. Physics mathematicians made it happen and then created more elaborate arrangements. While a variety of shapes can rotate rapidly enough in our 3D space to appear as a uniform sphere, two repelling electrons would occupy "opposed positions" within that "sphere" - a point not addressed by the spdf model. A 3D xyz-grid divides the sphere into 8 equal parts (green sphere with x, y, and z planes below). These 8 can be combined into two identical, but opposing, orbital pairs having T_d-symmetry and a common center. This is the basis of the MCAS model. When each 4-lobed T_d-group contains a single electron, it is designated as an M-orbital. When the 4-lobed T_d-group contains more than one electron, it is designated as a C-orbital.



Before proceeding to the remaining MCAS orbitals, it is of value to see how the spdf and MCAS representations differ with regard to a simple molecule like hydrogen. In the spdf version, the spherical electron orbitals overlap with the electrons *again* blending and concentrating between the nuclei – see figure on the right. In the MCAS version, the electrons also concentrate between the nuclei, but are constrained to a single nucleus, in this case. The bond forms with each nucleus attracting the other's electron that "nest" trigonally and provide the rotational resistance observed in single bonds.

Now, for the remaining MCAS orbitals.

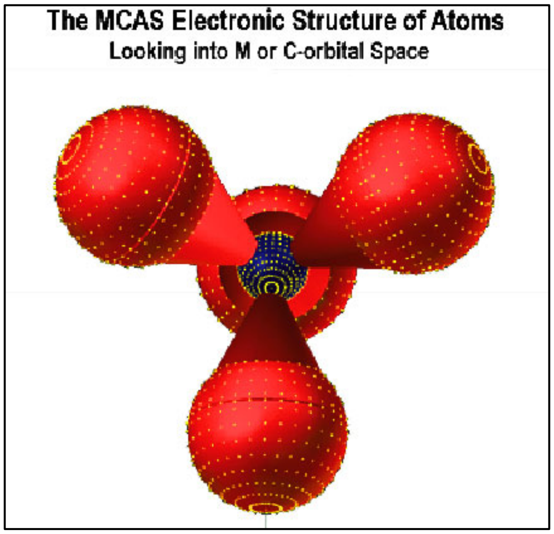
I originally represented the MCAS model with a cube because I find things are more easily viewed in the x,y,z-coordinates of our 3D world. The physics mathematicians apparently found this useful, too. Thus the images shown on the next page have the single M and paired M/C orbitals with a virtual cube (a/b). When the cube is removed (images c1 and c2), the projections into space are more difficult to evaluate with the distraction of the orbital portions that go towards the nucleus. The xyz alignment is even more difficult to visualize with more orbitals. The "trigonal" symmetry as one looks down one orbital lobe (b and c1) is seen either way.



When the number of electrons is greater than M or C-orbitals can handle (relate to the reason d-orbitals were created in the spdf model), then other orbitals are needed. The most open spaces are "anticubic". With a virtual cube present, the A (anticubic) orbitals are seen to band cubic space (d). This is less apparent in image (e) without the virtual cube. The bands in 3D are clearer when the orbitals are given different colors (f). Spatial orientation of the orbitals is more difficult to envision when the cube is replaced with a sphere (g), although the orbital outer limits are more clearly appreciated. The 18 A-orbitals match the requirement for reordering an entire level (row) in the periodic chart where 10 transition elements appear.

The next "open" symmetry after the Anticube can accommodate 24 orbitals. These are depicted as the green orbitals in the above image (h) with a virtual cube. The square-face alignment which gives this orbital group its S name in the MCAS model is clearly seen. The 8 orbitals needed to make 32 for the S group are in the C-orbital directions. With a virtual sphere (i), the xyz-visualization is more difficult. Without coloration (j), just the highly symmetrical, spherical arrangement of the MCAS orbitals is seen. There are no "weird" shaped orbitals, such as the d_z^2 orbital or the f-orbitals of the spdf model. All the electron orbital lobes of the MCAS model have the same basic shape, if not size/energy.

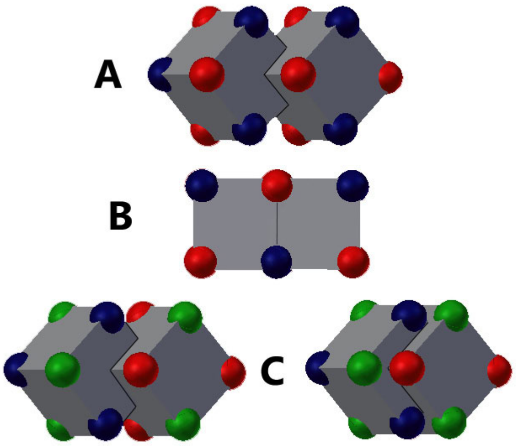
For more on the MCAS model and other scientific issues, see "Challenging Science" by Joel M Williams or www.swcp.com/~jmw-mcw. A number of web listings can be found by searching with "MCAS modeling Joel Williams".



B: Electronic Bonding of Atoms

Bonded atoms make up our physical world. The principal parts that provide this composition are positive nuclei and negative electrons. While these may be just "waves" in a highly dimensional, mathematical universe, they are "solid" entities with mass that can be shot, herded, assembled, etc and make up what we view in our 3D world. "Bonding" occurs through electrostatic attractions; "de-bonding" through repelling. Simple bonding can occur through electrostatic interactions between an atom's nucleus and another atom's electrons with each atom's electrons beholden only to its own nucleus. More complex bonding requires that each atom's electrons coordinate with those of other atoms so that the electrons move between the atoms in concert. In this essay, I have outlined how these interactions are manifested according to the MCAS electronic model of atoms.[136]

Figure 1
Orbital Overlap vs Electrostatics



In the MCAS electron model, the main orbitals involved in simple bond formation are 8-fold and point to cubic corner space. Bonding occurs when nuclei can approach one another on a line where there is an electron deficiency. The simple electrostatic meshing case is illustrated in Figure 1, image A. The bond length and strength are determined by the attracting and repelling electrostatic forces. For orbital overlap to occur, the electron orbiting network of each must be synchronized. A simple case is illustrated in Figure 1, image B. While it may be more aesthetically pleasing to some eyes, such a configuration may not necessarily produce an interaction with a lower energy state. The nuclei in images A and B are the same distance apart. The bond length in image B is set by the orbital overlap in addition to other electrostatics. The bond length for the simple electrostatic mesh (A) will be shortened when there are fewer negative non-bonding electrons (green colored orbitals in Figure 1, image C) present to repel the bonding electrons (mid-nuclei red and blue orbitals).

The simple electrostatic bonding model is sufficient to indicate the bonding in the diatomic molecules of the elements carbon to neon (see Figure 2, on the next page). While current MO bonding gives the diatomic molecules different "bond orders" (single, double, triple), the MCAS electrostatic model has them all the same (single) in the ground state. For oxygen, this gives the "triplet" state (C2-C4) with two unpaired electrons. Elevating an electron in each produces the "singlet" state (C3-C3). The molecule in this elevated state is best represented by the orbital overlap model (Figure 3, on the next page) wherein 6 electrons occupy each of the orbital networks, indicated as blue and red.

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[136] Williams, Joel M, http://www.wbabin.net/Science-Journals/Essays/View/4019 (in the General Science Journal)

The two models indicate how the difference in the oxygen atom ground-state [C2-C4, 2-unpaired electrons] and elevated-state [C3-C3, no unpaired electrons] pairings give the observed experimental electron pairing in the diatomic molecule: again, 2 unpaired in the ground-state and no unpaired in the elevated state. This was a driving force for the current MO modeling to explain why the reverse was not the case as indicated by the octet and electron spin-pairing rules.

Figure 2

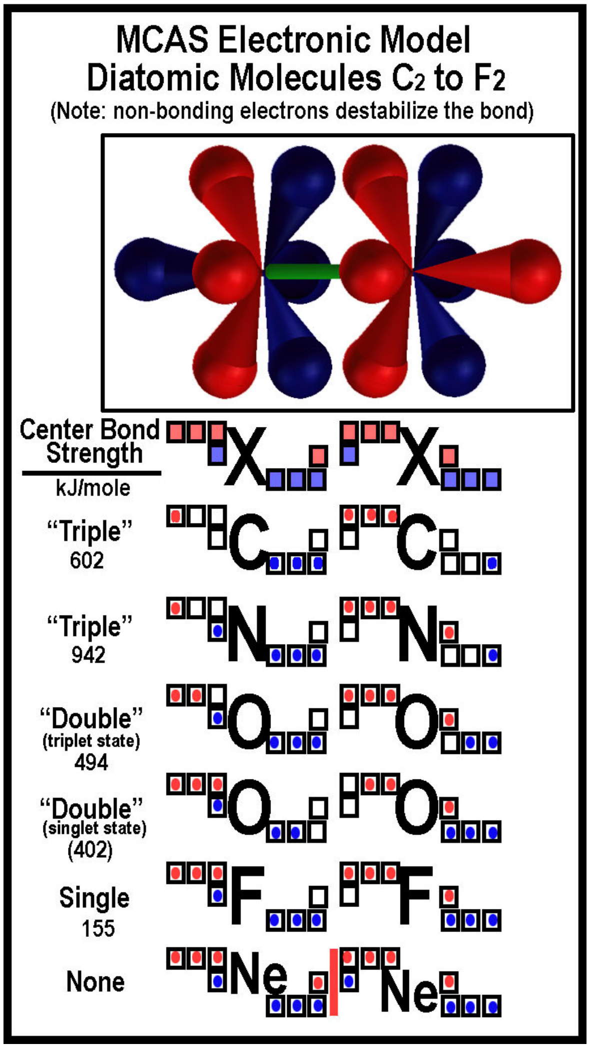


Figure 3

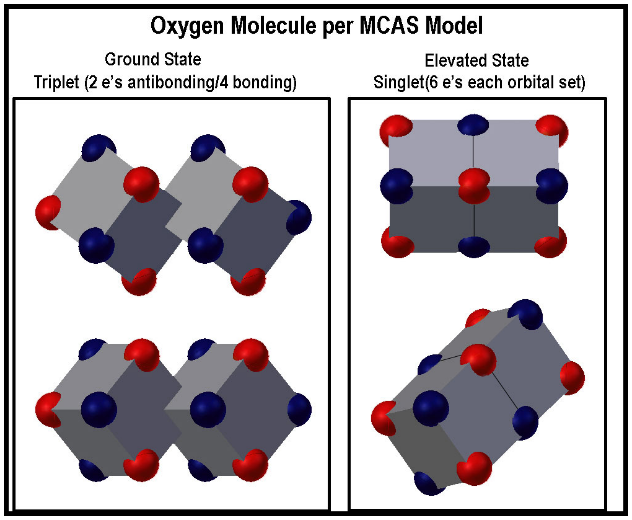
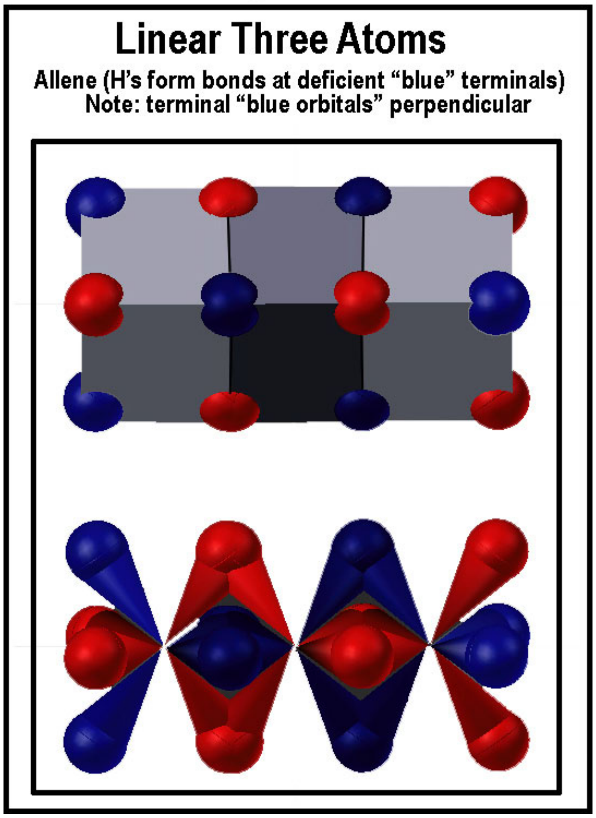


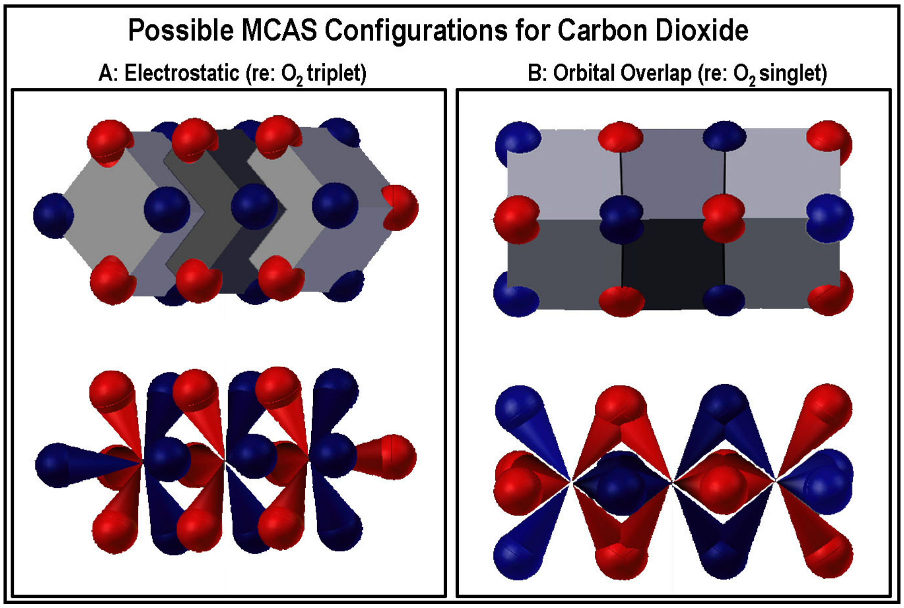
Figure 4



Allene (H_2CCCH_2) conforms to the orbital overlap model (see Figure 4). The 4 hydrogen atoms (not shown) attach at the e-deficient terminal blue positions. As observed experimentally the end pairs are perpendicular to one another. Bonding to the center atom forces them to be “perpendicular”. In the current MO model the orbitals have the center sp-hybridized with the unhybridized p-orbitals forming perpendicular pi-bonds. No such hybridizing is needed with the MCAS model, just orbital overlap.

This brings up an interesting question about the structure of carbon dioxide. The lowest energy of the oxygen molecule is the triplet state that has non-overlapped, electrostatic bonding. Does placing a carbon atom between them still follow the same form (Figure 5, image A)? Or, do the three overlap in the style above for allene (Figure 5, image B) in accord with the singlet form of O_2? Note that the “formal charges” on the two are -1+2-1 for A and 000 for B. What is the experimental evidence to favor B which is in conformity with the current MO, perpendicular double-bonded carbon?

Figure 5



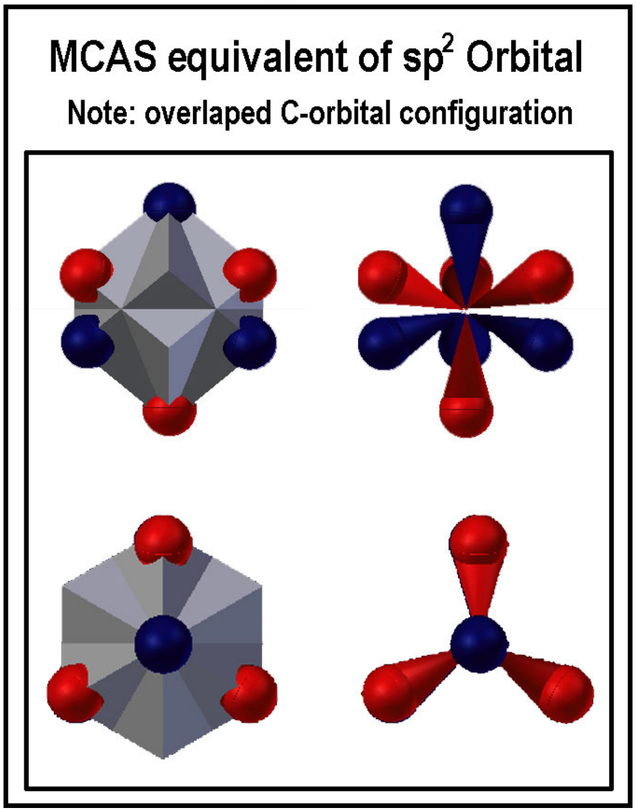
Possible MCAS Configurations for Carbon Dioxide

A: Electrostatic (re: O_2 triplet)

B: Orbital Overlap (re: O_2 singlet)

Resonance energy is the lowering of an electron’s travel energy by removing some of the “reversals” that occur when an electron normally returns towards the nucleus that it just passed. Maximum resonance energy is obtained when the electron returns to its “starting” point WITHOUT reversing its direction; i.e., it completes a closed, albeit circuitous, loop. Aromaticity is the epitome of this behavior. The current MO methodology uses the sp2 hybrid to provide the mechanism. The MCAS rendition of this hybrid is shown in Figure 6. Electrons in each C-orbital set enter or leave the atom in the same general direction, but divergently; i.e., the orbital sets are eclipsed instead of staggered. In accord with the general theory behind the MCAS model, electrons in the two orbital sets will be paired (moving opposite one another). An edge-edge distance is greater than a face-face distance.

Figure 6



MCAS equivalent of sp^2 Orbital

Note: overlaped C-orbital configuration

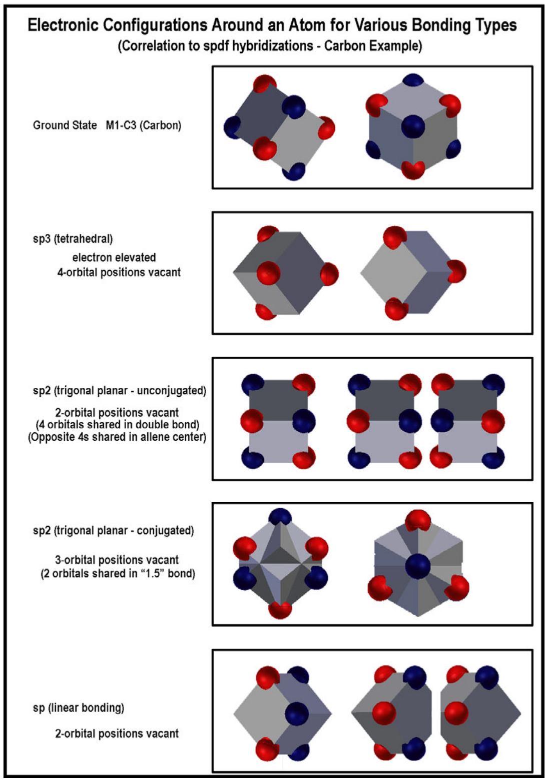
The basic bonding modes in the MCAS methodology have now been described. They are summarized in Figure 7.

1. C(orner) mode – "single" bond
   Meshing occurs electrostatically without orbital overlap.

2. Orbital overlap –"multiple" bonds
   a. **F**(ace)–non-conjugated double
   b. **E**(dge)– conjugated

3. The triple-bond of the current MO methodology is just a special case of the C(orner) mode where the "triple" bond between two carbon atoms, i.e., results from only a single electron in each of the anti-bonding orbital sets and thus destabilizes the bond much less. See C2 in Figure 2.

Figure 7

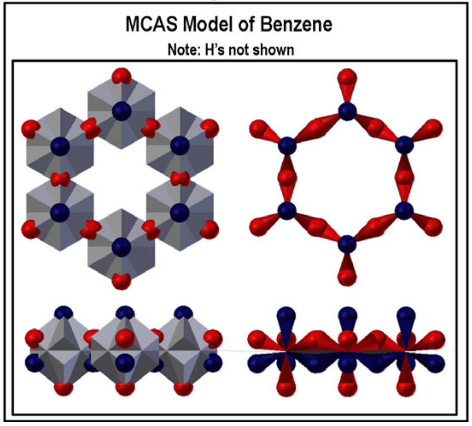


Electronic Configurations Around an Atom for Various Bonding Types
(Correlation to spdf hybridizations - Carbon Example)

Several examples of **E**(dge) bonding will now be given.

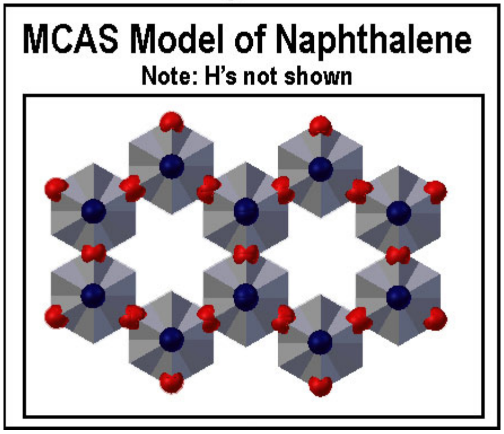
The most widely recognized molecule with this type bonding is benzene. The 6-membered carbon ring is shown without the hydrogen atoms, but with and without the reference objects in Figure 8. Note the two (red and blue) orbital groups. Also note that the electron orbitals between nuclei are not on a direct line between the nuclei, but are above and below the "bond-line". As the electrons are paired in opposing motion, the electrons in the two circuitous rings travel in opposite directions as required for pairing.

Figure 8



MCAS Model of Benzene
Note: H's not shown

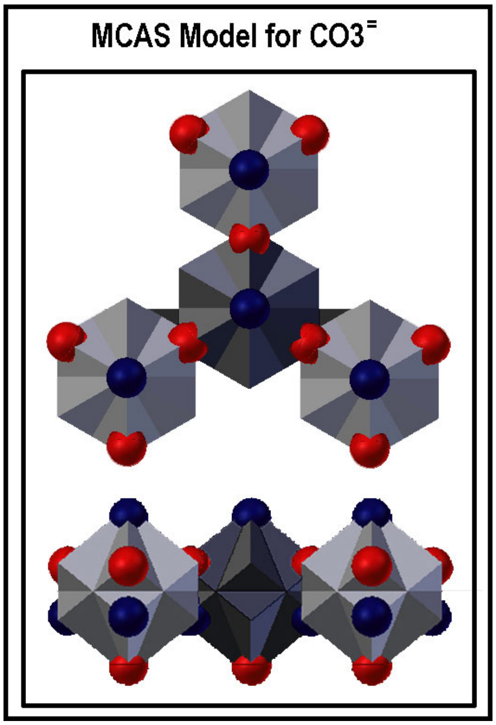
Figure 9



MCAS Model of Naphthalene
Note: H's not shown

The 10-carbon atoms of naphthalene are joined in the two rings structure shown in Figure 9 without the hydrogen atoms.

Figure 10

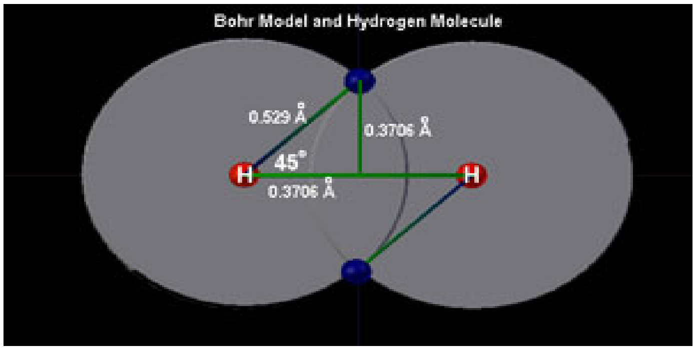

MCAS Model for $CO3^{=}$

The MCAS bonding in the carbonate ion is shown in Figure 10. The oxygen atoms are -1 each (6 unshared nodes and 2 shared nodes) with the central carbon +1 (6 shared nodes).

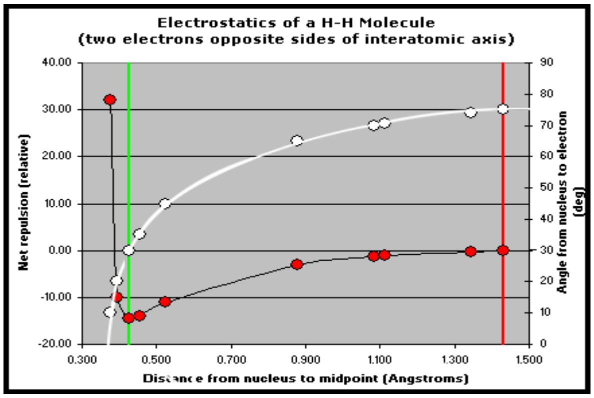
C: The Bohr Model and Electron

When first introduced to the Bohr model many decades ago, I was enamored like most students by its simplicity. I easily grasped the notion that an equation could be generated to model the simple case of an electron racing around a circular track. I had trouble, then and now, however, seeing what was causing the discrete “quantum jumps” that were thought to be needed to match the Balmer series. That i(***n***)teger factors would do the mathematical task was no great surprise as the subsequent, complex mathematical treatments clearly demonstrated that those steeped in that field could model just about anything. The physical world cause, however, never seemed to materialize for me.

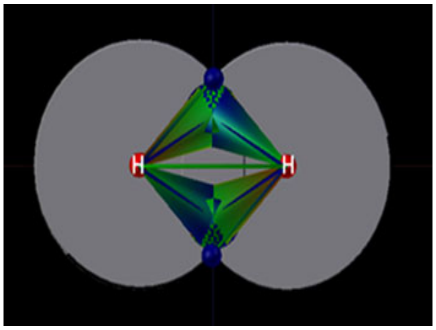
It is interesting to note a few things about Bohr’s model before proceeding. The Bohr radius for a hydrogen atom is just what would be expected for a 45-deg angle from the inter-nuclei axis (image on the right). Newton’s cannoneers would concur if the object was to reach the other nucleus with the optimum volley. This might have made sense if the electrons were simply “balls”. But it does raise the point about what Bohr had in mind beyond this fitting his equations to the observations.



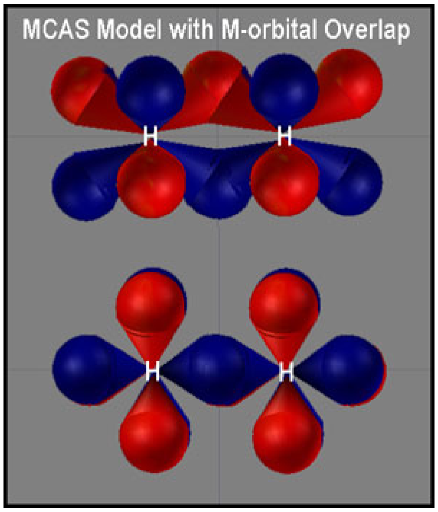
A 45-deg angle is not the optimum volley angle here, however! Unlike cannon-balls, electrons are ‘electrostatically attracted to each nucleus” and “repel one another”. Electrostatic energetics are minimized at the midpoint when the angle is 30-deg (see graph below).



If electrons are to be passed between hydrogen nuclei, then they should be passed at this angle. The image on the right shows how this is envisioned in the MCAS orbital model where the angle between adjacent M and M’ orbitals of the MCAS model is ~35-deg from the bisect.



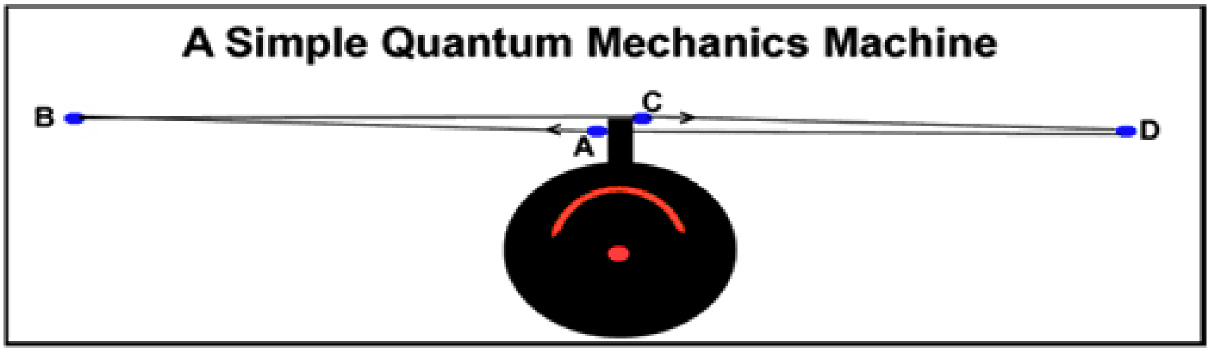
The full MCAS M-M’ orbital system of the hydrogen molecule *with e-transfer* is shown on the right. With orbitals meshed in this manner, the two electrons move in opposite, well-defined space between and around the nuclei. There is no need for “spin-reversal” (real or virtual) or cohabitation of orbitals. The bottom image could easily be mistaken for electron concentration on the inter-nuclear axis. Such is not the case, as the upper image indicates. Also, the electrons must interact with nuclei of the molecule in the same manner they do for separate atoms! This explains why the Balmer-series for the molecule translates to the atom. See the following section.



D: Newtonian-derived Quantum Numbers

So how does the Balmer series arise in all this? It does so because the nuclei and electrons have different motion parameters, but their interaction must coincide when the electron approaches the nucleus. It is not clear how a nucleus interacts with and directs the electron, but it must. Passing close to the nucleus allows the necessary intimacy, whereas the distant circular Bohr orbits never seemed to provide any such mechanism. None ever has been; just data fitting. Higher mathematical treatments have not provided a logical physical explanation either; just parameters to make it so. Retrofitting has met resistance even when the nucleus is being shown to be a highly structured assemblage of charges.

As a thought process about why energy character around a nucleus is “quantum” and not “continuum”, I present the following discussion of a simple quantum-mechanics machine. It consists of a robotic batter and a moving ball. Shortly, you will see how it generates a “ball-mer” (sic) series.



The ball, *moving with velocity V_o at point A*, receives positive, but discrete, energy input from the bat, if not perpetual motion, and continues on to max point B as governed by a constant decelerating force. Reversing, it accelerates to point C where it receives the same, discrete, positive energy input from the bat and continues on to max point D, again exposed to the same decelerating force. Returning to point A, the ball repeats the cycle. The robotic batter reverses rotation with each hit in this thought experiment (in order to “touch” the ball from behind in both directions), but comes back to point AC, as set by its constant rate of rotation, in integer time-quantities of t.

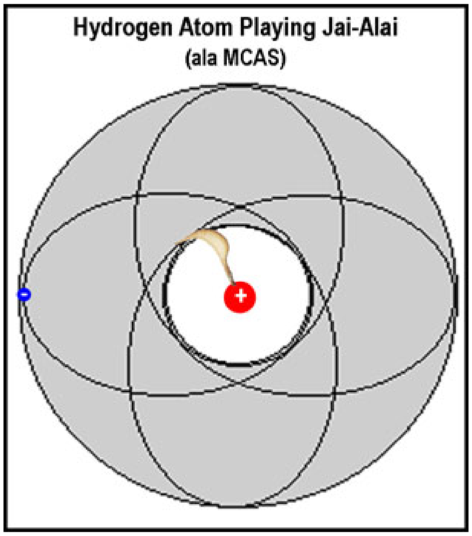
The bat and the ball operate under different parameters/forces, but must arrive at point AC at precisely the same moment.

$V = V_A = V_C = V_o + \text{energy from bat}$
$V_B = V_D = 0 = V - a(nt/2)$
$d_{A\text{-}B} = d_{C\text{-}D} = V^*(t/2) - 1/2a(nt/2)^2$
$d_{B\text{-}C} = d_{D\text{-}A} = 1/2a(nt/2)^2$
a = constant and t is set by the batter’s constant rate of rotation for the bat’s arrival at point AC

The “Ball-mer” series indicates what was needed to generate the Balmer Series with the Bohr model; adding “principal quantum numbers” (***n***) to produce discretely separated orbits rather than an infinite continuum of orbits. The energies differences are just that needed to achieve each timing-sequence of correlated interactions. Designating the “quantum” energy size does not indicate how it is applied or removed from the action; only that it is. Ball-mer behavior can occur in a multitude of similar situations as the accelerating-decelerating forces involved are not specified. The quantum-phenomenon is not size dependent as was used to justify why Newtonian physics did not work at the atomic level and, therefore, new physics was necessary. Quite clearly, Newtonian physics does apply in the electron-nuclear realm to define the parameters, ***if*** the physical model is appropriate.

# rotations to “hit” ball	V after “hit”	Ball-mer Series	H atom Bohr r	r ratio
n(t)	V	d_x	Å	
1	1 a(t/2)	1 $(a/2)(t/2)^2$	53	1
2	2 a(t/2)	4 $(a/2)(t/2)^2$	212	4
3	3 a(t/2)	9 $(a/2)(t/2)^2$	476	9
4	4 a(t/2)	16 $(a/2)(t/2)^2$	846	16
5	5 a(t/2)	25 $(a/2)(t/2)^2$	1322	25

The nucleus acts as if it is playing jai-alai with itself and other nuclei; just not with a cesta, of course, as the cartoon at the right indicates. Most likely there is a negative force-field that comes into play at close quarters that prevents the electron from crashing into the nucleus. This field sends the electron on its way pass the nucleus. In the MCAS model, the simplest “3D-way” is indicated by a group of tetrahedrally oriented orbitals.



E: Notes about some pioneers involved in the structure of the atom

23 of the 45 Solvay 1911/1927 conference attendees got Nobels; all by 1936, except Pauli (exclusion principle) in 1945 and Born (probability distribution) in 1954. Add Nobelist Rutherford’s mentor Nobelist JJ Thompson (in 1906 for discovering the electron; *not* for his “plum-pudding” atom model) and you have a tight, if not of singular mind, group.

Interestingly, Arnold Sommerfeld, who attended only the first of these two Solvay conferences, had these "Nobel" students [Werner Heisenberg (uncertainty), Wolfgang Pauli (exclusion), Peter Debye, Linus Pauling], but never got a Nobel himself. It was Sommerfeld who introduced "elliptical orbits" (quantum ℓ) in 1916 to replace Bohr's circular ones and then the quantum m in 1920 that led to the spin-factor (s). If Sommerfeld had connected his elliptical orbits to form a continuous 3-D spatial one, he surely would have come up with the MCAS model. BUT, the “Rutherford-Bohr” mold had “hardening”.

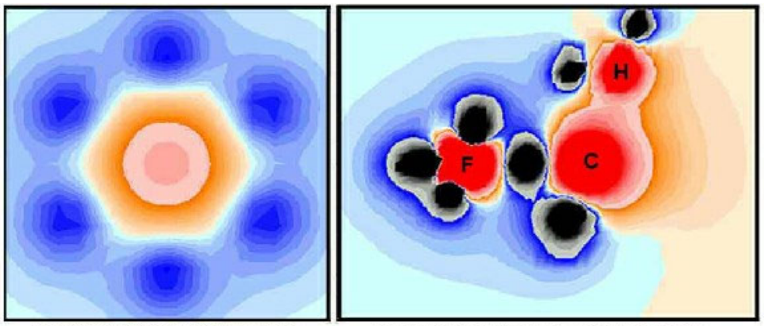
With the basic electron model seemingly agreed upon, though still debated in some quarters, the Solvay group with Bohr and Einstein moved on, in 1933, to tackle the nucleus. Atomic energy weaponry eventually fueled the efforts more than Nobel’s dynamite largesse ever could. Eighty years later, many (?) think ALMOST everything is known about the nucleus and how things were at the beginning of “time”; they just need a bigger “collider” to break that “nut” apart completely and get to the “God particle”. That the nucleus attracts electrons without capturing them is still a mystery, however. Maybe, the nucleus does play jai-alai – setting the electron’s color (spectral energy level) with each pass to specify the wave (return time). Schrödinger demonstrated that if you probe a box for a particle enough times you will get a wave pattern and maybe even touch upon the miracle of life. Scientists may eventually disassemble the nucleus into all of its components (glue, too?), but will they be able to reassemble them into anything worthwhile by playing God? Or will they have to finally sit back and just marvel at the current masterpiece and wonder how it came to be as opposed to what it is?

Chapter I

MODELING THE MCAS WAY

This has sharper images than the one in the arxiv database

A PARTICLE APPROACH TO THE ELECTRONIC BEHAVIOR OF ATOMS AND MOLECULES


ELECTROSTATIC FIELD - H_2 BOND
Plane perpendicular to axis mid bond

ELECTROSTATIC FIELD - ACTIVATED FCH_3
Electron between F and C - Plane through nuclei

ABSTRACT

The spdf-based atomic and molecular orbital theory is a sophism. Duality is based on the electrostatic property of an electron being substituted for the whole. The additivity of the property is used to justify the additive of the whole. In this way, electrons can statistically occupy the same space at the same time. The non-additivity of like-charged particles and the particles themselves vanish in directed logic. Reverent fostering perpetuates the stratagem. The homophilic electron gets praised as the creator of all things. Things are declared to be different at the electronic level and that classical physical laws do not apply. This paper shows that classical physics is still alive and well down at the electronic level! Electrons are particulate as long as they remain electrons; i.e., there is no mass-energy reversal on demand. Duality, as currently asserted, does not exist for an electron and is, thus, flawed logic.

*MCAS is an acronym for the orbitals [**M**ultilobed (tetrahedral), **C**ubic, **A**nticubic, and **S**quare-faced cubic] of a particulate orbital approach. The MCAS approach explains the behavior of an electron with classical physics that maintains the integrity of the particle. The electrostatic fields from electrons are additivity, but the probabilities of electrons occurring in the same space are mutually exclusive and, therefore not additive! That is, two electrons are not allowed to harmoniously share the same orbital space at the same time ¾ electrostatic particle orthogonality. Beyond this, the MCAS approach should yield to mathematical treatments in much the same way the spdf-based theory does. The MCAS approach demonstrates that atoms are indeed "the building blocks of nature".*

This treatise details the electrostatics of some simple molecules modeled the MCAS way. The orbital extent of an electron is finite! Its electrostatic presence, however, can be considered to stretch to infinity. An electron hardly ever occupies the region on the axis between two nuclei. Usually when this happens, the molecule is in an activated state. Excellent correspondence of NMR proton shift with the magnitude of the electrostatic field at the proton is found.

*Wholly integer quantum numbers are assignable to each orbital space of an atom. Electrons do not have quantum numbers! The acronym "**stogh**" (pronounced stow) stands for **s**hell (1-n), **t**ype (1-4), **o**rthogonality (1 or –1), **g**roup (1-k), and '**h**ome' (1-m). The electron of the hydrogen atom is assigned the **11111** orbital; those of helium are in the **11111** and **11-111** orbitals; and so on. Each electron is assigned to a separate 'home' orbital in a group, although they may alternately roam the orbitals within the group. Unlike the static spdf designation, an electron moves to a different **t**ype (**M**, **C**, **A**, or **S**) of orbital with sufficient electron loading of a shell!*

The MCAS way describes the behavior of electrons while preserving their wholeness, mutual orthogonality, and interactive adaptation. Inter-atom attractions and repulsions without spin-paired electrons on the direct line between nuclei properly explain bonding between atoms. Ionic and covalent bonding are explained by the same electrostatic rules. Classical physical laws continue down to at least the electronic level!

A description of S_N2 organic reactions based on the MCAS electronic structure of atoms and molecules is given. The concept of microscopic reversibility in the Transition State of S_N2 reactions is trashed.

PREFACE

This paper contains extensions and applications of the **MCAS** (an acronym for 3-D orbital types: **M**ultilobed (tetrahedral), **C**ubic, **A**nticubic, and **S**quare-faced cubic) approach to atomic and molecular orbitals. It is broken up into four parts, several of which have their own Introduction and Summary.

Part I: MCAS Models

This part provides a brief overview of the MCAS approach to atomic orbitals and molecular bonding.

INTRODUCTION; ORBITALS THE MCAS WAY; BULLIES, WIMPS, and the REST

SINGLE BONDS (HYDROGEN MOLECULE, CHLORINE MOLECULE, ETHANE)

TRIPLE BOND (ACETYLENE, NITROGEN MOLECULE); SUMMARY

Part II: Electrostatics for MCAS Models

This part provides electrostatic calculations for some MCAS-formulated molecules. Such electrostatic models would be impossible with current methodology because of electron-electron repulsion. Contour gradients are shown for a number of molecules. Correlations with NMR chemical shifts are made.

THE CUBE AND THE SPHERE; The SIMPLE SIGMA-Xi BOND

ELECTROSTATIC CALCULATIONS

ELECTROSTATIC PLOTS (HYDROGEN MOLECULE, CARBON DIATOM, NITROGEN MOLECULE,

OXYGEN MOLECULE, FLUORINE MOLECULE, NEON ATOM)

PNMR SHIFTS AND FIELD INTENSITY; SUMMARY

Part III: Quantum Aspects

This part discusses atomic orbital description, why the current methodology is faulty, and provides new quantum numbers for stowing electron around the nucleus.

ONE ELECTRON PER ORBITAL - Pauli

MCAS QUANTUM NUMBERS

NO NEED FOR PARTICLE THEORIES?

Part IV: Reactions the MCAS Way

This part provides a mechanism for S_N2 reactions based on MCAS modeling. The mechanism involves an electron-transfer in the Transition State. As a result, microscopic reversibility can not occur and the concept is trashed.

MODELS and REACTION PATHS, MCAS MODELS OF SEVERAL ATOMS

MCAS versus Currently-Accepted MODEL OF METHYL FLUORIDE

MICROSCOPIC REVERSIBILITY IS NOT

S_N2 REACTIONS THE MCAS WAY

PART I

MCAS MODELS

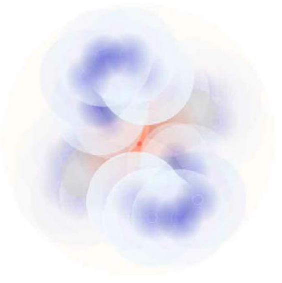
A. INTRODUCTION

The MCAS model of the electronic structure of atoms describes an orderly placement of the electrons around the nucleus without the need for electron spin reversal. This is achieved through opposing electron motion in nested orbitals that is equivalent to spin reversal. Major restructuring of a shell is part of the model when the electron load requires it. The energy to maintain an electron in an orbit/orbital is provided by its interaction with the nucleus — synchronization between electron and nucleus being required; attraction and repulsion implicit.

Before proceeding, it is appropriate to comment on two issues: electron spin-reversal and orbital character. In the beginning, the creator flipped the great coin of the universe: heads to the right; tails to the left. Its fate determined, the matter of the coin spiraled outward. The hand (spin) of the electron determined as well - a base descriptor. According to current atomic and MO treatments,[137] reversing spin does not negate electron charge, but it does negate negative-negative repulsion - a hallucinative tenet. Do you profess belief? Why?

Electrons form synchronous units with nuclei. Spectral data dictate that the motions of electrons be precisely repetitive, not fuzzy; hence, finite and closed. The physical volume of an electron is tiny, but its duality component (electrostatic charge) radiates outward at $1/r^2$ to yield an electrostatic cloud. Figure 1 simulates the planar (to the paper) radiation for a nucleus (red) and for temporal locations of an electron (blue) in a four-lobed (tetrahedral) distribution. The electrostatic presence of an electron extends to infinity in all directions with an ultimate intensity of $1/(\text{infinity})^2$ no matter where the electron might be. Spectral signature, on the other hand, defines a finite presence for an electron. The finite physical space occupied by an electron based on its spectral signature is more properly its orbital space. Electrostatic issuance is a boundless property, but electron presence (probability) is physically bounded.

Figure 1.
PLANAR ELECTROSTATIC PRESENCE
OF
ELECTRON AND NUCLEUS



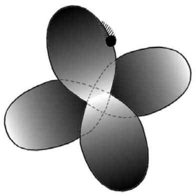
Two electrostatic clouds are always overlapped; be they positive-positive, negative-negative, or positive-negative. Everything in the universe is electrostatically connected to everything else this way. Thus, an electron is somewhere in its and every other electron's electrostatic cloud at all times. Electrostatic repulsion will minimize overlap intensity, however. Methodologies that maximize negative-negative overlap are, thus, invalid; be they probability or particulate based!

Pairing electrons by opposing their movement requires neither spin-reversal nor maximized negative-negative overlap and, thus, provides an electrostatically allowable methodology. This is "The MCAS Way".

B. ORBITALS THE MCAS WAY

Every electron in the MCAS electronic model has an instantaneously separate orbital space. The most basic electron orbital is the **M** (multi-lobed) orbital. The motion in this orbital is a 3-dimensional version of a hypotrochoid (Figure 2) that yields a tetrahedrally disposed electrostatic cloud (Figure 1). Note that the nucleus can be seen and hence provides routes of attraction of another atom's electrons. This is in sharp contrast to the commonly accepted spherical s-orbital that should present a uniform negative picture to another atom! The mathematician can model either the spherical or tetrahedral distribution. Indeed, the **M** orbital is just like a sp^3-hybrid orbital set, except that a single electron roams all four lobes. If you are squeamish about one electron traveling in more that one lobe, think about what happens in the p, d, and f orbitals of the current scheme.

Figure 2.
HYPOTROCHOID



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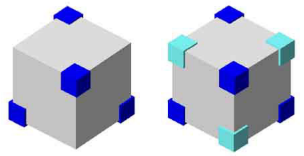
[137] Current basic concepts of molecular modeling and atomic structure are found in chemistry texts, such as: Chemistry, Raymond Chang, Random House, New York; Introduction to Organic Chemistry, A. Streitweiser Jr. and C.H. Heathcock, MacMillan, New York; Advanced Inorganic Chemistry, F.A. Cotton and G. Wilkinson, Interscience, New York; and Physical Chemistry, F. Daniels and R.A. Alberty, Wiley, New York; their progeny and similar ilk.

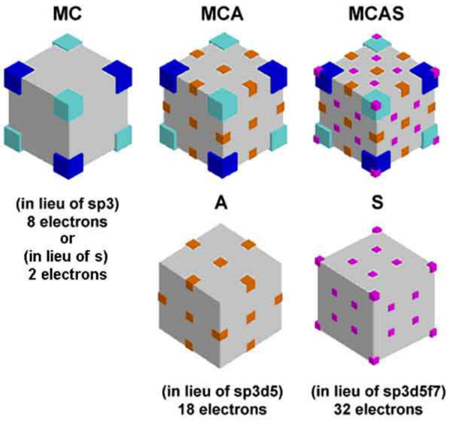
For ease of spatial comprehension, visualize[138] the **M** orbital as part of a cube (Figure 3a). Colored blocks (dark blue) located at the four diagonal corners of the cube indicate the orientation of the lobes. [Angular orbital shapes are not implied! The cubic depiction is a matter of graphic convenience.] Another **M** orbital (aquo blocks) nests with it to form the opposing electron motion (Figure 3b). When more electron density is required at a specified distance (energy level) from the nucleus, up to three more electrons can occupy the tetrahedral orbital space. This converts the **M** orbital (1 electron per tetrahedral orbital) to **C** orbitals (2 to 4 electrons per tetrahedral space, yet 1 electron per lobe). One **M** to **C** conversion completes before another begins; Hund's rule no longer needed. The electrons in the **C** orbitals interact synchronously with each other, with that (those) in the opposing **M** (or **C)** orbital(s), and with the nucleus. When even more electron density is required, the **C** (cube or corner) orbital configuration rearranges to the **A** (anticube) configuration wherein the lobes are aligned towards the center of the cube's edges (12) and faces (6). When even more electron density is needed, the **A** orbital configuration converts to the **S** (square-faced) configuration wherein the electrons' lobes are aligned towards the corners (8) and the faces (4*6=24) between those of the **A** configuration. Hence the electronic aufbau completed shell levels are 2 (**M**$_2$), 8 (**C**$_8$), 18 (**A**$_{18}$), and 32 (**S**$_{32}$) with every electron of a given energy level of a noble gas element being identical! The 3-dimensional spatial distribution of the lobes can be easily visualized with the help of cubes (Figure 4).

Figure 3.
CUBIC DISTRIBUTION OF M ORBITALS



(a) M (b) MM

Figure 4.
Spatial Distribution of the MCAS Atomic Orbitals



MC: (in lieu of sp3) 8 electrons or (in lieu of s) 2 electrons

MCA — A: (in lieu of sp3d5) 18 electrons

MCAS — S: (in lieu of sp3d5f7) 32 electrons

C. BULLIES, WIMPS, and the REST

The struggle for total electronic counterbalancing can be summed up this way: ***those that can take; those that can not cede or co-op***. Thus, are born ionic and covalent unions. In the first three periods, the rule of 2 (**M**$_2$) or 8 (**C**$_8$) prevails; just like Lewis wanted, but with a different e-pairing scheme! The business at hand is to negate all unopposed electronic motions. In the ionic case, the opposing motion will be achieved by centering the motion about each individual nucleus. In the covalent case, the opposing motion will be achieved by centering it between the two nuclei. Note that it is the **motion** of the electrons and not the electrons themselves that is **centered**! Electrostatics requires that the two opposing electrons remain as far from one another as possible. Thus, the probability that they will form an elevated electrostatic presence on a line between two nuclei is 0. Covalent bond formation is now little different than ionic bond formation - both controlled by electrostatics and motion counterbalancing. Cooperative (covalently bound) atoms are more like self-satisfied couples and small groups that can cluster in large arrays if so ordered. Atomic bullies (anions) and wimps (cations), on the other hand, loathe their own and love their opposite. Satisfaction (electrostatic bliss) comes in the crystalline or solvated state.

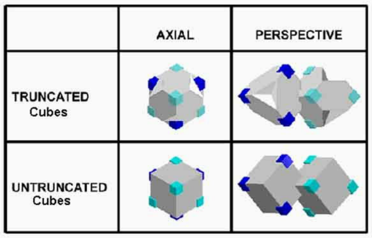
D. SINGLE BONDS

The MCAS modeling of single bonds will be illustrated with the following three molecules: H_2, Cl_2, and CH_3CH_3.

1. HYDROGEN MOLECULE

The hydrogen molecule provides the simplest covalent bond. In the spdf molecular bonding concept, this occurs with two spherical orbitals merging while one of the electrons changes spin. Electrostatic density piles up between the nuclei, especially on the axis between the two. At least that is the implication; even if mathematical "spin" (color, whatever) is not physical spin - a leap of faith! In the MCAS bonding concept, two tetrahedral **M**-orbitals mesh with their electrons paired by counter motion. Truncated and untruncated cube models are shown in Figure 5. One **M**-orbital is shown in aqua to emphasize its reversed placement. As in the current concept, electron density is mainly between the nuclei as would be expected, just not on the axis. Positive-negative electrostatics is clearly operating in the MCAS approach. The driving force in the spdf approach escapes me. Electrostatics is the only interaction of concern here. No electron spin reversal is necessary, just spin opposition.

Figure 5.
MCAS Structure for Hydrogen Molecule



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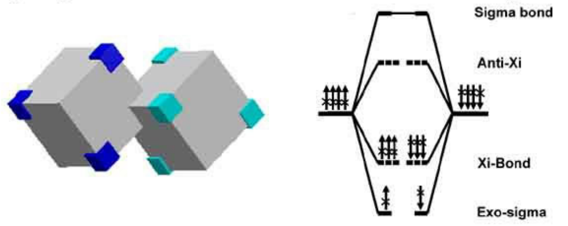
[138] 3-D modeling program: freeware downloaded from Artifice, Inc. at http://www.artifice.com

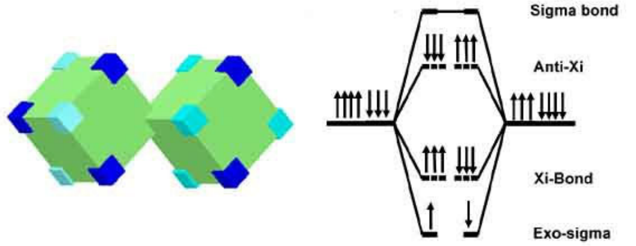
Figure 6.
Hydrogen Molecule MCAS Structure and MO Diagram



In the case of the hydrogen molecule, there are only two electrons and they will always be on opposite sides of the bond at any given time. Since the bond is actually formed by trigonal, epi-counterpoised orbitals, it should be called a Xi (Ξ) bond. To emphasize its conventional sigma bond relationship, I choose to call it a sigma-Xi (σΞ) bond. The MO diagram should be like that in Figure 6 with each of the " x"ed arrows indicating a 1/4 electron presence. Note that the molecule has stability because there are NO repelling electrons in the sigma bond!

2. CHLORINE MOLECULE

Figure 7.
Chlorine Molecule MCAS Structure and MO Diagram

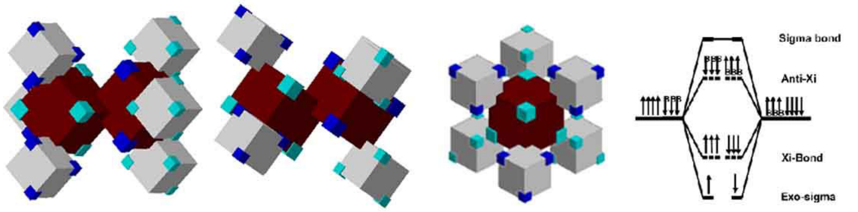


The MCAS structure of a chlorine atom's valence shell is $\mathbf{C^4C^3}$. A chlorine molecule occurs when two chlorine atoms minimize each other's single electron deficiency. The MCAS structure and MO diagram are given in Figure 7. The similarity between the current MO notation and the MCAS MO notation is easily seen. Like that for the hydrogen molecule, however, the designations of the various levels are different. Bond destabilization to that of a single bond is provided by e-e repulsion between the six anti-Xi and the six Xi-bond electrons; otherwise the Xi-bond would be stronger. (Hold that thought!) There is no reason to expect the anti-Xi destabilization to cancel the Xi-bond electron-for-electron. It is convenient to express it this way, however, and to put the difference in the exo-sigma level designation. Lewis' dots are paired as he would want, but they are on opposite sides of the bond, not in it.

3. ETHANE

The carbon valence-shell electrons in the ground state are $\mathbf{MC^3}$. For single bonding in the alkanes, the **M** electron is elevated to give the symmetrical $\mathbf{C^4}$ state. [Total electron distribution looks like that of hydrogen (**M**).] The staggered MCAS conformation of ethane is shown from several vantagepoints in Figure 8. Blue and aqua colored electrons are used to indicate opposing electron placements. Orbital symmetry and maximum distancing of electron density is readily apparent.

Figure 8.
MCAS STRUCTURES and MO of ETHANE



The C-C single (sigma-Xi) bond of ethane is like unto that for the chlorine molecule (compare Figures 8 and 7). Three electrons from each carbon are involved in the Xi-bond. The fourth electron of each carbon is exo-counterpoised to the bond — a feature seen in the hydrogen and chlorine molecules; the sigma bond is their opposite. Instead of the anti-Xi electrons that occur in the chlorine molecule, their CH Xi-bond replacements provide the e-e repulsion that reduces the strength of the C-C Xi-bond to that of a single bond. Thus, a **B-arrow** (bond) replaces the electron arrow in the MO. Of course, the B-arrow has a direction equivalent to the electron it replaces. The electrons involved here are the ones on the hydrogen atoms that form the CH-bonds Using the B-arrow notation indicates the situation more generally. Resistance to rotation about the C-C single bond is typically attributed to interactions of electrons in bonds on either side of the C-C bond. In the MCAS approach, the resistance is due to the Xi-orbital interactions between the carbons. This is more in harmony with data that shows that the resistance to rotation about the C-C bond of ethane is not significantly different from that for the center C-C bond of butane. All of the single bonds in saturated alkanes are sigma-Xi (σΞ) bonds.

E. THE TRIPLE BOND

Multiple bonds are bonds that are significantly stronger than comparable sigma-Xi bonds that have six anti-Xi electrons or bonds. Triple bonds, in fact, are just especially strong sigma-Xi bonds. A triple bond has no Π–type bonds!

1. ACETYLENE (ETHYNE)

The carbon valence-shell electrons in the ground state are **MC^{3}**. The **M** electron is not elevated to a **C** electron in the case of acetylene. Thus, the electronic structure of the acetylenic C-C bond is much like that of the chlorine-chlorine bond, except that in this case only two **M**-electrons counter the six **C^{3}** electrons that form the sigma-Xi bond. The MCAS structure and MO diagram are given in Figure 9 with the carbon **M** orbitals dark blue. From this smaller e-e repulsion results the strength of the triple bond. Thus, a triple bond is just a special case of a tri-lobed sigma-Xi bond where there are only two anti-Xi electrons instead of six. Extra strength may also result if the orbitals about each carbon were to wax and wane alternately. The **M** electrons may also pass from one atom to the other.

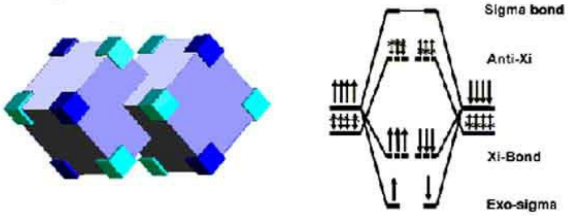
The **M**-orbital of acetylene is similar to its **C** counterpart that blooms out towards the hydrogen atom of ethane, except there is only one electron in the three lobes instead of three! This results in **1/3** the shielding that occurs in the saturated alkane case; hence acetylenic protons will look a lot like alkyl protons in NMR, but will be less shielded.[139] No fancy hand waving is needed and the hydrogen atoms at BOTH ends of acetylene look just alike!

2. Nitrogen Molecule

The nitrogen valence-shell electrons in the ground state are **MC^{4}**. The nitrogen molecule will look like the acetylene molecule with each carbon-hydrogen sigma-Xi bond replaced with an electron. See the MCAS structure and MO diagram in Figure 10. The lower energy **M**-orbitals have been left dark blue here to emphasize them. Again, only two anti-Xi electrons oppose the six Xi-bond electrons. There may be interatom transfer of the **M** electrons and alternate waxing and waning. Thus, N_2 is a very compact bundle with a minimally destabilized sigma-Xi bond that has triple bond strength.

Figure 10.

Nitrogen Molecule MCAS Structure and MO Diagram



F. SUMMARY

Covalent and ionic bonding should both be covered by the same rules. The difference should be degree, not kind. The MCAS Way shows that they can, indeed, be explained similarly! With the MCAS approach to atomic orbitals, electron spin-reversal and doubly occupied orbital overlap are eliminated! Both of these concepts should repulse; yet they opiate - so venerated.

The situation for double and conjugate bonding is a little more involved than the single and triple bond cases shown in this paper, but they are still governed by electrostatic interaction. For these, some inorganic groupings like $CO_3^=$, NO_3^-, SO_3, some involving phosphorous (P_4, P_4O_6, P_4O_{10}) and boron (B_2H_6, $B_6H_6^=$), and other single and tripled bonded molecules, the reader is referred "The MCAS Way" (1999) by the author. It can be inspected at http://arxiv.org/html/physics/9909053. Also, see "Challenging Science" by the author.

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[139] For a discussion of NMR, see Introduction to Organic Chemistry, A. Streitweiser Jr. and C.H. Heathcock, MacMillan, New York [especially the discussion on acetylene (p304 - 1976 version)]; similar general texts or specific NMR texts.

PART II

ELECTROSTATICS FOR MCAS MODELS

A. INTRODUCTION

The MCAS model of the electronic structure of atoms describes an orderly placement of the electrons around the nucleus without the need for electron spin reversal. This is achieved through opposing electron motion in nested orbitals that is equivalent to spin reversal. The outer shell of an element will normally have its period's noble gas maximum number (2 or 8) of electrons or less. Inner-shell packing is by uniform spatial allotment of orbital space between these orbitals. MCAS is an acronym for the orbital types that occupy 3-D space:

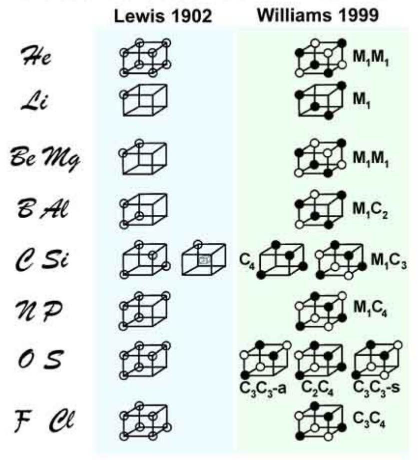
Multilobed (tetrahedral), **C**ubic, **A**nticubic, and **S**quare-faced cubic.

For more on the MCAS methodology and the interplay of these orbitals, the reader is referred "The MCAS Way" (1999) by the author. It can be inspected at http://arxiv.org/html/physics/9909053

This section was initiated to provide mathematical support for the MCAS methodology. Before embarking, however, G.N. Lewis deserves a bit more credit than he has been given in the past.

B. THE CUBE AND THE SPHERE

Figure 11.
Octet Structures of Atoms



G. N. Lewis made some of the earliest depictions of atoms. In doing so, he recognized the significance of the OCTET. The logical expression of an octet in 3-D space is a cube. Lewis[140] used one to represent his atomic structures in 1902 (Figure 11 - a rendition of Lewis' originals by this author). It is interesting that he depicted helium ("He") with "8" positions. However, since he also suggested that the indicated structure might be the "basis" for the "Na" row, it is more probable that he was thinking "Ne", not "He", when he wrote "Helium". It is not clear what he had in mind for the "kernel" in "C/Si". It is clear, however, that Lewis was not concerned about 3-D placement of electrons as he filled the "left" plane first and then the "right", with electrons placed next to one another. The exception, interestingly, is carbon/silicon! The significance of his depictions , however, is that when a shell is complete, all electrons will be alike! The author's MCAS model shows how electrons are placed orderly in this network to effect 3-D symmetry and spin-pairing. For Helium, the "black" and "white" tetrahedrally directed orbitals [designated M (multilobed) orbitals] contain one electron each. Hydrogen has just one M-orbital. With more than one electron, the tetrahedral M-orbital space becomes four **C** orbitals. MCAS orbital designations are given in Figure 11 for each atom. The C_4 states for Carbon and Silicon are elevated, as M_1C_3 is the ground state.

In 1913, Bohr[141] introduced his spherical model of the hydrogen atom. In 1916, Lewis[142], departing from his cube representation, proposed the familiar valence-bond octet structure wherein electrons pair to form a bond between atoms; so intent was he on surrounding atoms with 8 electrons. Schrödinger[143] and Pauli[144] sealed the fate of the spin-paired, overlapped, double-electron orbital and subsequent bond between atoms.

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[140] Lewis, G.N., "Valence", Dover Publications, New York (1966)

[141] Bohr, N, Phil. Mag., 26, 1, 476, 875 (1913)

[142] Lewis, G.N., J.Am.Chem.Soc., 38, 762 (1916); also Lewis, G.N., "Valence", ACS Monograph Series (1923)

[143] Schrödinger, E., Ann. Phys., 81, 109 (1926)

[144] Pauli Jr., W., Z. Physik, 43, 601 (1927); CA, 21, 3309f (1927); b) Pauli's Nobel Prize speech about the exclusion principle is in Science, 103, 213 (1946)

Scientists of the 20th century never looked back - too bad. Skillful mathematicians could/would have modeled anything. [The classical, mathematical modeling case involves the earth-centered versus sun-centered universe. Both were modeled. Neither, as it turns out, was correct concerning the universe! If righteous electrons can remain chaste in the presence of attractive protons, are they repelled by their sinister brethren down in the little nukey?] As it was/is, the homophilic couplet got sanctified. Humans have free choice, but I was not aware that electrons do.

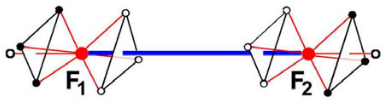
A significant feature of the original Lewis cubic representations was that no two electrons occupied the same space. Indeed, Pauli's exclusion principle should have been just that. (Actually, Pauli also had one electron per box — one oriented with the field and one against. He did not specify spin reversal, but spin opposition — the basic feature of the MCAS approach.) Instead of securing a model that would do this, the mathematicians simply modified their mathematics to allow two electrons to share the same space with different "spin" numbers. Pauli was happy and other reservations, if there were any, drown in the wake of the power(ful) surge.

Lewis' valence-bond octet followed the principle that an atom tries to surround itself with eight electrons. The octet rule should have been that "an atom tries to cover eight positions". Coverage does not require two electrons directly between the atoms! Indeed, the electrostatic repulsion of two electrons in the same space would preclude two electrons from occupying the same, or generally same, space at the same time! The MCAS Way covers positions without this whimsy.

C. THE SIMPLE SIGMA-Xi BOND

Fluorine is the least electron deficient atom (of those deficient) in the list of Figure 11. The MCAS method for alleviating this deficiency is for two fluorine atoms to combine as depicted in Figure 12. The bond between the two atoms is created by the attraction of the positively charged nucleus primarily on THREE of the other atom's electrons. For this reason, it is dubbed the "sigma-Xi" bond. This sigma-Xi bond is weakened by the repulsion between the electrons of one atom and those of the other and by the repulsion between the two nuclei. The eighth position of each atom is thus "covered". The axis (the traditional sigma bond) contains the non-bonding orbitals! Electrons are paired as "opposites" across the center of the bond.

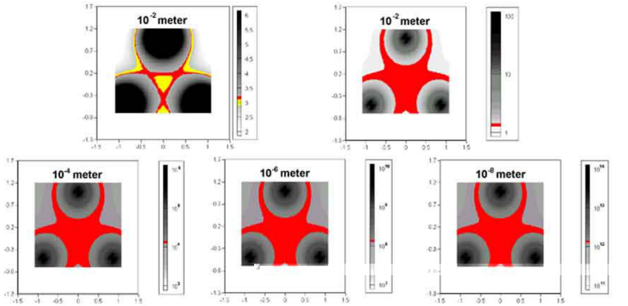
Figure 12.
Sigma-Xi Bonding of Fluorine



(Bond strength is the summation of all inter-atom attractions and repulsions; not intra-atom ones.)

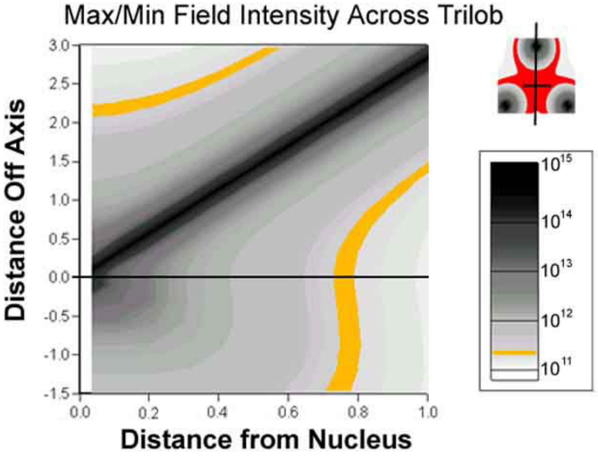
The same bonding depiction can be made for H2. In this case, no black positions are filled and a single electron occupies the four white positions of each atom. For O2, the three black positions of each atom are occupied by an electron 2/3rds of the time; hence the observed unpaired electron character of O2. For N2, the black positions of each atom are occupied by 1 electron (mirror-imaged). A similar situation occurs for the C2 portion of acetylene where the two electrons opposite the bond are replaced with sigma-Xi bonds to hydrogen atoms.

Figure 13.
Electrostatic Field from Three Point Sources



The three lobes of the sigma-Xi bond pose some interesting electronic effects around the bond axis. The electrostatic distribution of three lobes about the axis is the same regardless of their distance for the axis (Figure 13). The difference is in the magnitude. Because of the inverse square relationship, there is a minimum in the center. Surrounding the center is a crater-like rim that serves as a centering mechanism. The minimum and rim edge are more easily seen in Figure 14. The correct angle for the electron movement from a point for tetrahedral distribution is 70.52°. Because of differences in the x and y scales (y 1/2.8th that of x), the density in Figure 14 appears to fall off less rapidly along the axis than it actually does. Beware of graphic deception!

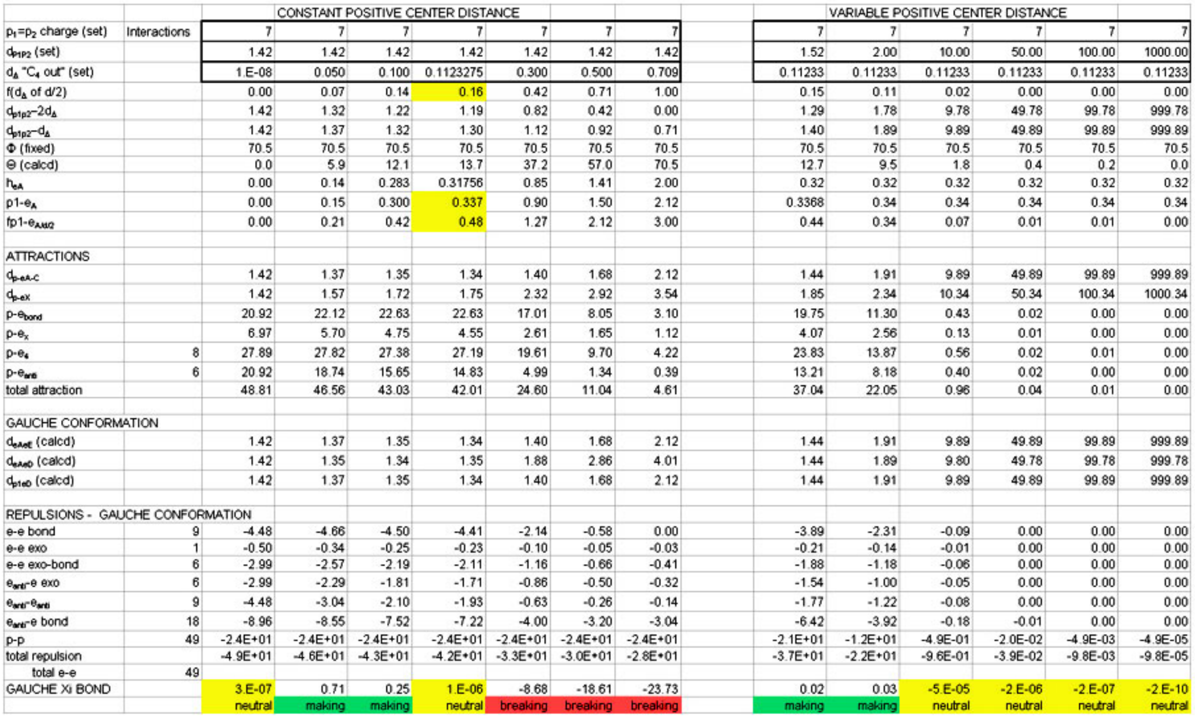
Figure 14.
Max/Min Field Intensity Across Trilob



D. ELECTROSTATIC CALCULATIONS

Electrostatic calculations for sigma-Xi bonds were determined for H_2, C_2 (triple bond), N_2, O_2, and F_2. Atomic distances were set to the published values. From this, the distance the electrons of the MCAS model could move outward at 70.52° before repulsion terms exceeded attraction terms was determined. Figure 15 illustrates the exercise for fluorine.

Figure 15.
Electrostatic Calculations for Fluorine Molecule

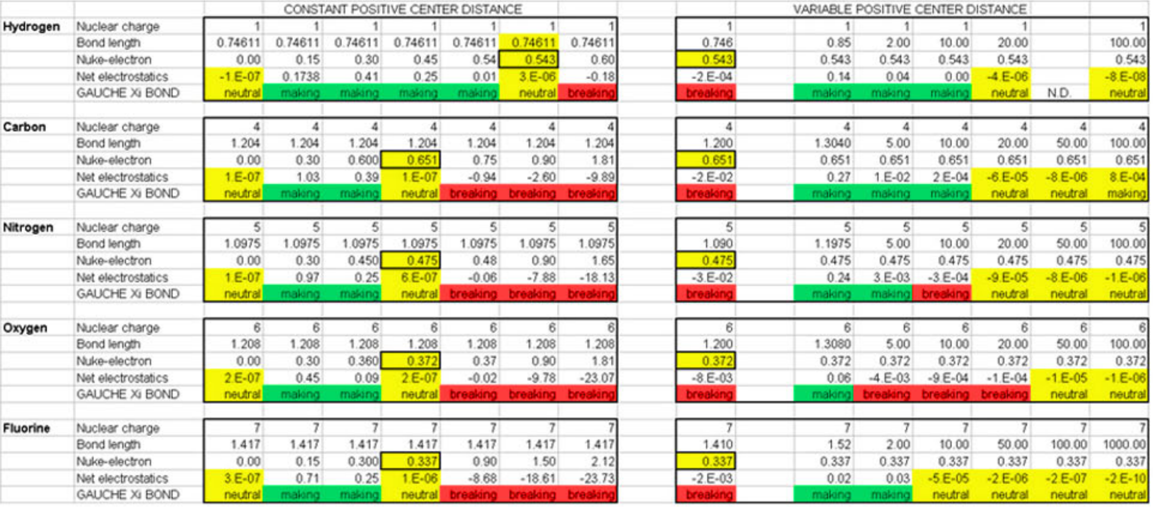


		CONSTANT POSITIVE CENTER DISTANCE							VARIABLE POSITIVE CENTER DISTANCE					
$p_1=p_2$ charge (set)	Interactions	7	7	7	7	7	7	7	7	7	7	7	7	7
d_{p1p2} (set)		1.42	1.42	1.42	1.42	1.42	1.42	1.42	1.52	2.00	10.00	50.00	100.00	1000.00
d_Δ "C_4 out" (set)		1.E-08	0.050	0.100	0.1123275	0.300	0.500	0.709	0.11233	0.11233	0.11233	0.11233	0.11233	0.11233
f(d_Δ of d/2)		0.00	0.07	0.14	0.16	0.42	0.71	1.00	0.15	0.11	0.02	0.00	0.00	0.00
$d_{p1p2}-2d_\Delta$		1.42	1.32	1.22	1.19	0.82	0.42	0.00	1.29	1.78	9.78	49.78	99.78	999.78
$d_{p1p2}-d_\Delta$		1.42	1.37	1.32	1.30	1.12	0.92	0.71	1.40	1.89	9.89	49.89	99.89	999.89
Φ (fixed)		70.5	70.5	70.5	70.5	70.5	70.5	70.5	70.5	70.5	70.5	70.5	70.5	70.5
Θ (calcd)		0.0	5.9	12.1	13.7	37.2	57.0	70.5	12.7	9.5	1.8	0.4	0.2	0.0
h_{eA}		0.00	0.14	0.283	0.31756	0.85	1.41	2.00	0.32	0.32	0.32	0.32	0.32	0.32
p1-e_A		0.00	0.15	0.300	0.337	0.90	1.50	2.12	0.3368	0.34	0.34	0.34	0.34	0.34
fp1-$e_{A,d/2}$		0.00	0.21	0.42	0.48	1.27	2.12	3.00	0.44	0.34	0.07	0.01	0.01	0.00
ATTRACTIONS														
$d_{p\text{-}eA\text{-}C}$		1.42	1.37	1.35	1.34	1.40	1.68	2.12	1.44	1.91	9.89	49.89	99.89	999.89
$d_{p\text{-}eX}$		1.42	1.57	1.72	1.75	2.32	2.92	3.54	1.85	2.34	10.34	50.34	100.34	1000.34
p-e_{bond}		20.92	22.12	22.63	22.63	17.01	8.05	3.10	19.75	11.30	0.43	0.02	0.00	0.00
p-e_X		6.97	5.70	4.75	4.55	2.61	1.65	1.12	4.07	2.56	0.13	0.01	0.00	0.00
p-e_4	8	27.89	27.82	27.38	27.19	19.61	9.70	4.22	23.83	13.87	0.56	0.02	0.01	0.00
p-e_{anti}	6	20.92	18.74	15.65	14.83	4.99	1.34	0.39	13.21	8.18	0.40	0.02	0.00	0.00
total attraction		48.81	46.56	43.03	42.01	24.60	11.04	4.61	37.04	22.05	0.96	0.04	0.01	0.00
GAUCHE CONFORMATION														
d_{eAeE} (calcd)		1.42	1.37	1.35	1.34	1.40	1.68	2.12	1.44	1.91	9.89	49.89	99.89	999.89
d_{eAeD} (calcd)		1.42	1.35	1.34	1.35	1.88	2.86	4.01	1.44	1.89	9.80	49.78	99.78	999.78
d_{p1eD} (calcd)		1.42	1.37	1.35	1.34	1.40	1.68	2.12	1.44	1.91	9.89	49.89	99.89	999.89
REPULSIONS - GAUCHE CONFORMATION														
e-e bond	9	-4.48	-4.66	-4.50	-4.41	-2.14	-0.58	0.00	-3.89	-2.31	-0.09	0.00	0.00	0.00
e-e exo	1	-0.50	-0.34	-0.25	-0.23	-0.10	-0.05	-0.03	-0.21	-0.14	-0.01	0.00	0.00	0.00
e-e exo-bond	6	-2.99	-2.57	-2.19	-2.11	-1.16	-0.66	-0.41	-1.88	-1.18	-0.06	0.00	0.00	0.00
e_{anti}-e exo	6	-2.99	-2.29	-1.81	-1.71	-0.86	-0.50	-0.32	-1.54	-1.00	-0.05	0.00	0.00	0.00
e_{anti}-e_{anti}	9	-4.48	-3.04	-2.10	-1.93	-0.63	-0.26	-0.14	-1.77	-1.22	-0.08	0.00	0.00	0.00
e_{anti}-e bond	18	-8.96	-8.55	-7.52	-7.22	-4.00	-3.20	-3.04	-6.42	-3.92	-0.18	-0.01	0.00	0.00
p-p	49	-2.4E+01	-2.4E+01	-2.4E+01	-2.4E+01	-2.4E+01	-2.4E+01	-2.4E+01	-2.1E+01	-1.2E+01	-4.9E-01	-2.0E-02	-4.9E-03	-4.9E-05
total repulsion		-4.9E+01	-4.6E+01	-4.3E+01	-4.2E+01	-3.3E+01	-3.0E+01	-2.8E+01	-3.7E+01	-2.2E+01	-9.6E-01	-3.9E-02	-9.8E-03	-9.8E-05
total e-e	49													
GAUCHE Xi BOND		3.E-07	0.71	0.25	1.E-06	-8.68	-18.61	-23.73	0.02	0.03	-5.E-05	-2.E-06	-2.E-07	-2.E-10
		neutral	making	making	neutral	breaking	breaking	breaking	making	making	neutral	neutral	neutral	neutral

For the purposes of the calculations, the two first-level electrons were always assumed to be near the nucleus and therefore neutralized two charge units. They are not always there, however, as all electrons move in and out in unison to form the electronic beat. To insure that the calculations would start correctly, little or no bond forming tendency was established when ALL electrons were very close to the nucleus - a null, hypothetical case. As the valence electrons moved outward, bond making was favored to an early maximum and then tapered off to a "neutral" point. This "neutral" point was established as the outmost extent of the electron movement (orbital). Bond length would be determined by the outmost extent of the electron movement, not the other way around! If the electrons moved further out, the bond would be destabilized. To determine whether bond formation was favored at a distance, the electron extension for "neutral" bond formation was held constant and the atoms moved apart. As seen for fluorine, bond formation is favored at short separations, but is essentially neutral (slightly repulsive) as greater distances. Figure 16 shows the essence of the activity for H_2 (M-M), C_2 (MC3-C3M), N_2 (MC4-C4M), O_2 (C2C4-C4C2), and F_2 (C3C4-C4C3), where the information in parentheses is the MCAS electron states of the atoms involved. Movement of the nuclei together at the outmost extension of the electrons destabilizes the bond (see the first column in the "Variable Positive Center Distance" portion). That the hydrogen orbital extent (0.543Å) is just half the typical C-H bond length is probably more than coincidental.

Figure 16.

Electrostatic Calculations for Several Molecules

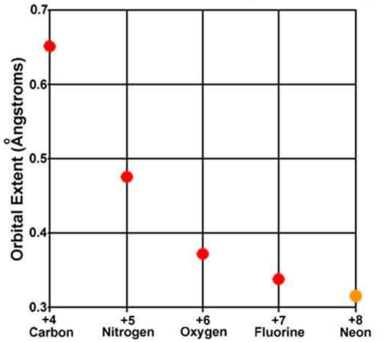


		CONSTANT POSITIVE CENTER DISTANCE							VARIABLE POSITIVE CENTER DISTANCE							
Hydrogen	Nuclear charge	1	1	1	1	1	1	1	1		1	1	1	1		1
	Bond length	0.74611	0.74611	0.74611	0.74611	0.74611	0.74611	0.74611	0.746		0.85	2.00	10.00	20.00		100.00
	Nuke-electron	0.00	0.15	0.30	0.45	0.54	0.543	0.60	0.543		0.543	0.543	0.543	0.543		0.543
	Net electrostatics	-1.E-07	0.1738	0.41	0.25	0.01	3.E-06	-0.18	-2.E-04		0.14	0.04	0.00	-4.E-06		-8.E-08
	GAUCHE Xi BOND	neutral	making	making	making	making	neutral	breaking	breaking		making	making	making	neutral	N.D.	neutral
Carbon	Nuclear charge	4	4	4	4	4	4	4	4		4	4	4	4	4	4
	Bond length	1.204	1.204	1.204	1.204	1.204	1.204	1.204	1.200		1.3040	5.00	10.00	20.00	50.00	100.00
	Nuke-electron	0.00	0.30	0.600	0.651	0.75	0.90	1.81	0.651		0.651	0.651	0.651	0.651	0.651	0.651
	Net electrostatics	1.E-07	1.03	0.39	1.E-07	-0.94	-2.60	-9.89	-2.E-02		0.27	1.E-02	2.E-04	-6.E-05	-8.E-06	8.E-04
	GAUCHE Xi BOND	neutral	making	making	neutral	breaking	breaking	breaking	breaking		making	making	making	neutral	neutral	making
Nitrogen	Nuclear charge	5	5	5	5	5	5	5	5		5	5	5	5	5	5
	Bond length	1.0975	1.0975	1.0975	1.0975	1.0975	1.0975	1.0975	1.090		1.1975	5.00	10.00	20.00	50.00	100.00
	Nuke-electron	0.00	0.30	0.450	0.475	0.48	0.90	1.65	0.475		0.475	0.475	0.475	0.475	0.475	0.475
	Net electrostatics	1.E-07	0.97	0.25	6.E-07	-0.06	-7.88	-18.13	-3.E-02		0.24	3.E-03	-3.E-04	-9.E-05	-8.E-06	-1.E-06
	GAUCHE Xi BOND	neutral	making	making	neutral	breaking	breaking	breaking	breaking		making	making	breaking	neutral	neutral	neutral
Oxygen	Nuclear charge	6	6	6	6	6	6	6	6		6	6	6	6	6	6
	Bond length	1.208	1.208	1.208	1.208	1.208	1.208	1.208	1.200		1.3080	5.00	10.00	20.00	50.00	100.00
	Nuke-electron	0.00	0.30	0.360	0.372	0.37	0.90	1.81	0.372		0.372	0.372	0.372	0.372	0.372	0.372
	Net electrostatics	2.E-07	0.45	0.09	2.E-07	-0.02	-9.78	-23.07	-8.E-03		0.06	-4.E-03	-9.E-04	-1.E-04	-1.E-05	-1.E-06
	GAUCHE Xi BOND	neutral	making	making	neutral	breaking	breaking	breaking	breaking		making	breaking	breaking	breaking	neutral	neutral
Fluorine	Nuclear charge	7	7	7	7	7	7	7	7		7	7	7	7	7	7
	Bond length	1.417	1.417	1.417	1.417	1.417	1.417	1.417	1.410		1.52	2.00	10.00	50.00	100.00	1000.00
	Nuke-electron	0.00	0.15	0.300	0.337	0.90	1.50	2.12	0.337		0.337	0.337	0.337	0.337	0.337	0.337
	Net electrostatics	3.E-07	0.71	0.25	1.E-06	-8.68	-18.61	-23.73	-2.E-03		0.02	0.03	-5.E-05	-2.E-06	-2.E-07	-2.E-10
	GAUCHE Xi BOND	neutral	making	making	neutral	breaking	breaking	breaking	breaking		making	making	neutral	neutral	neutral	neutral

The distance between the nucleus and the electron outward motion decreases as would be expected with increasing nuclear charge (Figure 17). Neon is estimated from the general trend.

Figure 17.

Extent of Valence Orbitals (MCAS Model)



E. ELECTROSTATIC PLOTS

The 3-D electrostatic fields of some simple molecules were determined. The methodology involved first setting the atomic components (nuclei and their electrons) staggered in 3-D space. Next, the electrostatic sum at various points on a plane, such as through the bond axis, across the bond axis mid-point between the nuclei, or through a nucleus perpendicular to the bond axis was determined. Electrons were assumed to extend without distortion at 70.52° to the distance determined in Figure 16. Non-valence electrons were assume to be near the nucleus and reduced the nuclear charge by their number. Once the electrostatic sum at each point on the plane was determined, a contour plot[145] was prepared. Planes were especially chosen to pass through the atomic components. Although 500-1200 points were usually used, some non-smoothness occurred where the contours were particularly steep. This should not detract from the understanding of the situation. Determinations were made for H_2, C_2, N_2, O_2, F_2, and Ne.

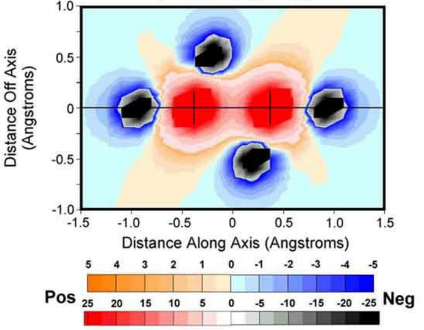
1. HYDROGEN MOLECULE

The hydrogen molecule is the simplest of molecules. In spite of this, the second electron has proven difficult to handle with current quantum theory methodology. With the MCAS model, the M-electron on each atom occupies tetrahedral spaces, which are placed with the tri-lobes staggered. Each lobe has an effective charge of -¼ — elementary probability. The electrostatic field through the bond and four of the lobes is shown in Figure 18. The electrons do not extend far enough to transfer to the other atom. Indeed, there may be too much emphasis on electron transfer. Neither do they cover all the space close to their own nucleus; ergo, positive zones ("handles" for reaction events) for the hydrogen molecule (and atom), if the interaction distance is not

Figure 18.

Electrostatic Field for Hydrogen Molecule

(Plane through axis)



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[145] Generated by SPSS DeltaGraph software during a 30-day review. The author found this program quite easy to use and the contour output nicely manipulable. The figures were made with Adobe Photoshop 4.0.

large. In general, the molecule is broadly bathed in negative charge and, therefore, has some innate stability towards other molecules. Unlike the current spdf-derived model, there are no electrons on the internuclear axis. There is a greatly diminished positive field at the mid-point of the bond, however. The bond is stable because positive-negative attractions match repulsive interactions.

Some other perspectives of the electrostatic field are provided in Figures 19-21. Figure 19 shows the field through two of the sigma-xi lobes parallel to, but offset from, the bond axis. The field between the two atoms is very negative at this point! Figure 20 shows the trigonal field through the cross-axis of one of the hydrogen atoms. Figure 21 shows the field cross-bond midway between the two nuclei. As would be expected, the meshing tri-lobes have formed a uniformly symmetrical, hexagonal distribution of charge. This is for the staggered configuration, of course. Rotating the fields to the eclipsed position would require energy; hence, the observed rotational resistance for ethane and butane.

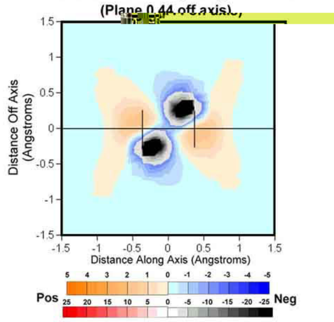


Figure 19.
Electrostatic Field for Hydrogen Molecule
(Plane 0.44 off axis)

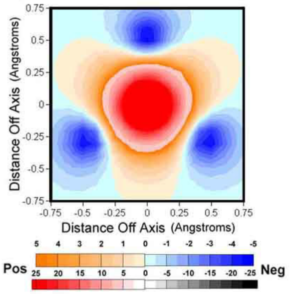


Figure 20.
Electrostatic Field for Hydrogen Molecule
(Cross axis at a nucleus center)

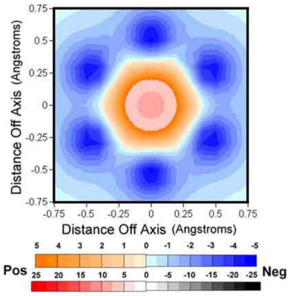


Figure 21.
Electrostatic Field for Hydrogen Molecule
[Cross axis at bond center (0)]

It can be argued that experimental evidence "proves" that electrons exist between the nuclei and, hence, on the internuclear axis. It is doubtful that electrons would stay there stationary for very long! In any case, <u>measured negative electrostatic density does not necessarily mean actual electron presence</u>! Figure 22 shows radial sums of the electrostatic field along the bond axis. The electrostatic sum was determined every 15° at the end of the specified radius and the sum of these values multiplied by the square of the radius to provide a cross-sectional value. The issue is "what is that 'experimental evidence' measuring?" If the experimental results show negative fields immediately over the nuclei, then the measurement is not close to the internuclear axis and the most intense negative field will be midway between the two hydrogen nuclei (see the **pink**, **blue**, and **black** curves where the radii are greater than 0.6Å). If the measurement is both for positive <u>and</u> negative fields, then the greatest negative field will again appear in the middle (the green "sum" curve). Only when the experiment is able to focus within 0.4Å of the internuclear axis (the **red** and **orange** curves) will the data not show a negative field concentration at the mid-point. All cross-sectional averages greater than this show a concentrated negative field at the mid-point of the H_2 molecule. All this occurs without the actual presence of even one electron, much less two!

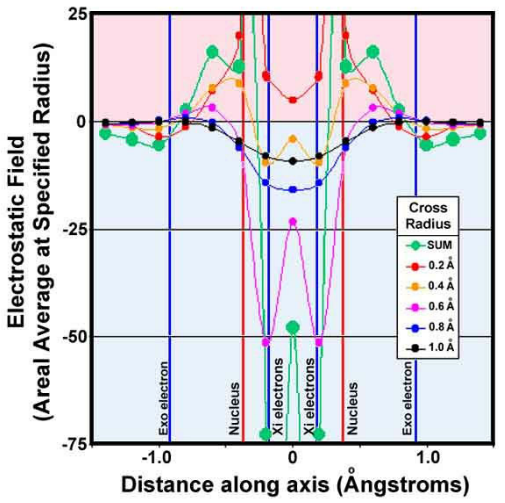


Figure 22.
Electrostatics of Hydrogen Molecule

<u>Actual electron presence in the sigma bond can occur</u> (surely, to the delight of those who must have it so!) when there is significant difference in the effective "nuclear" charges of the two nuclei forming a bond. This occurs, for example, between carbon and fluorine of fluoro-substituted methanes (see NMR discussion, Part II-F). It occurs <u>not</u> because <u>two</u> high e-density orbitals are <u>overlapped</u> by <u>spin-pairing</u>, <u>but</u>, rather, because <u>one electron</u> of the less electronegative nucleus is drawn into its anti-sigma orbital at the expense of filling Xi-orbital space elsewhere. Significant redistribution of electrons may occur several atoms away. Similar effects would be expected in crystal field splitting by group 7 and 6 elements; much smaller ones by group 5 and 4 elements. The overlapped bond in the current quantum theory (QT) represents the probability of electron density being present. Since only one electron can occupy the bond space at any given time, the current QT needs to find a place for the other electron to spend while it is not in the overlapped region. The MCAS method has such places.

2. CARBON DIATOM

Carbon atoms can join in several ways. In one, the atoms form a "triple" bond. This occurs when two carbon atoms join with M_1C_3-valence states. Figures 23-25 show the situation for the carbon diatom. The first thing that is obvious is the lack of "negative end-caps". One of the effects of electrons is to channel positive charge. Polymers are thus long, greatly sphinctered threads of positive charge surrounded by negative charge rather than alternating bits of positive and negative matter. Polyacetylene is a rigid "anaconda full of pacas". Because there are anti-Xi electrons, unlike the situation for hydrogen, the cross section through a carbon atom perpendicular to the bond axis has the nucleus well surrounded with negative field (Figure 24). Like the hydrogen molecule, the mid-point of the bond is symmetrical with a strong surrounding negative field (Figure 25).

Figure 23.
Electrostatic Field for Carbon Diatom (MC_3)
(Plane through axis)

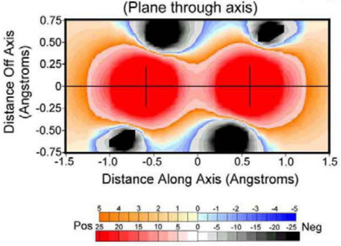


Figure 24.
Electrostatic Field for Carbon Diatom (MC_3)
(Cross axis at a nucleus center)

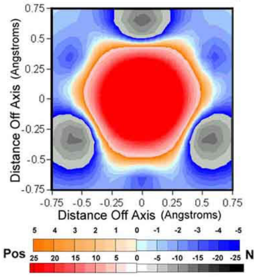
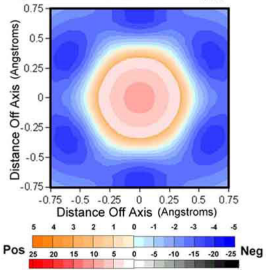


Figure 25.
Electrostatic Field for Carbon Diatom
[Cross axis at bond center (0)]



3. NITROGEN MOLECULE

The nitrogen molecule is similar to the carbon diatom except that it has electrons to cover its ends. The electrostatic field around the molecule is shown in Figures 26-28. As can be easily seen, the ends are very well covered and the nitrogen molecule presents a completely negative capsule. The difference of the M (1/4-time) and C (full-time) electrons is easily detected in the field sizes associated with them; especially in the atomic cross-section (Fig 27). As we move to the right in the periodic table, the negative field intensity at mid bond decreases while that around each atom increases.

Figure 26.
Electrostatic Field for Nitrogen Molecule
(Plane through axis)

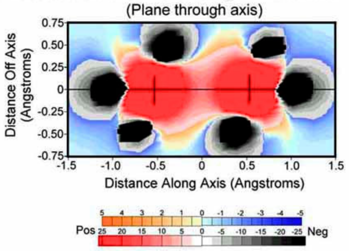


Figure 27.
Electrostatic Field of Nitrogen Molecule
(Cross axis at a nucleus center)

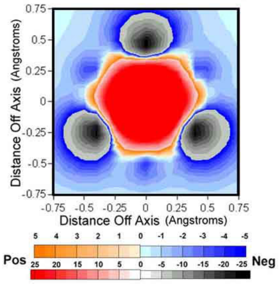
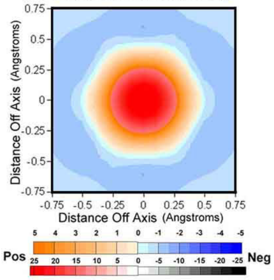


Figure 28.
Electrostatic Field of Nitrogen Molecule
[Cross axis at bond center (0)]



4. OXYGEN MOLECULE

Oxygen is deficient two electrons. In the molecule, 2 electrons fill the three anti-Xi positions of each oxygen atom to accommodate this. This results in a net of two unpaired electrons. The electrostatic field around the oxygen molecule is given in Figures 29-31. The strengthening of field at the nuclei and the weakening at mid-bond continue. The mid-bond is still covered weakly and so the molecule has modest stability among other molecules.

Figure 29.
Electrostatic Field for Oxygen Molecule
(Plane through axis)

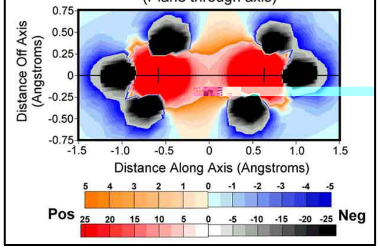


Figure 30.
Electrostatic Field of Oxygen Molecule
(Cross axis at a nucleus center)

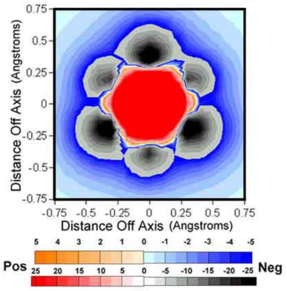
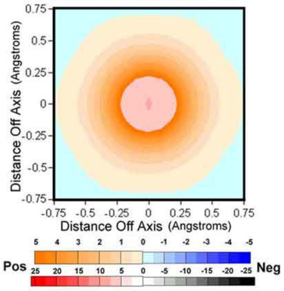


Figure 31.
Electrostatic Field of Oxygen Molecule
[Cross axis at bond center (0)]



5. FLUORINE MOLECULE

Fluorine is just deficient a single electron. The electrostatic field around the molecule is given in Figures 32-35. The trend of electron concentration around the nuclei and diminishing at mid-bond continues as indicated above. Indeed, while the positive-negative attractions suffice to provide a strong single bond, the mid-bond region is not covered! Thus, fluorine is a more reactive molecule than would be expected from its bond strength.

Figure 32.
Electrostatic Field for Fluorine Molecule
(Plane through axis)

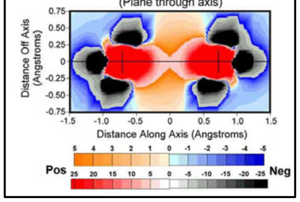


Figure 33.
Electrostatic Field for Fluorine Molecule
(Plane 0.3 above axis)

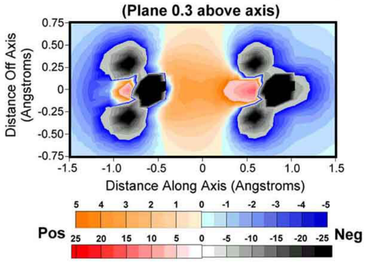


Figure 34.
Electrostatic Field of Fluorine Molecule
(Cross axis at a nucleus center)

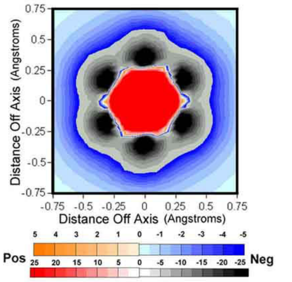
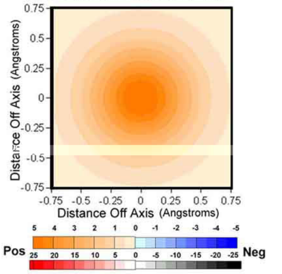


Figure 35.
Electrostatic Field of Fluorine Molecule
[Cross axis at bond center (0)]



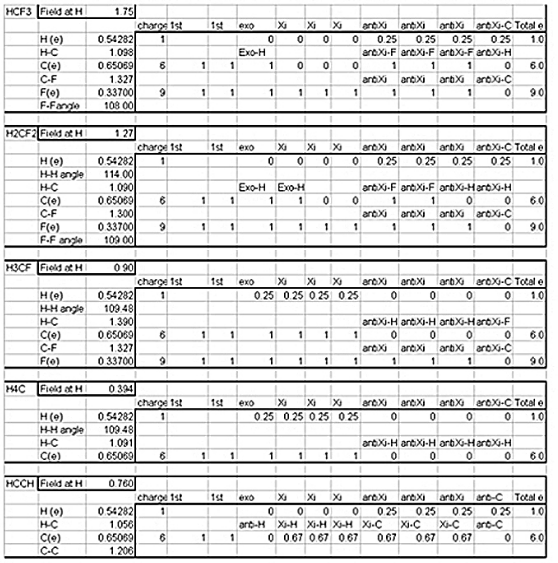
6. NEON ATOM

A cross-section through the neon nucleus would look much like that through the fluorine nucleus (Figure 34), only tighter. There would be no octet deficiency around the neon nucleus, however. Rather, it would be symmetrically well shielded cubically.

F. PNMR SHIFTS AND FIELD INTENSITY

Since the nucleus is essentially a point in the surrounding electrostatic field, the field intensity at its center is a good approximation of what the nucleus will be subjected to. The electrostatic fields of fluoro-substituted methane compounds have been determined and compared to their NMR chemical shifts. In the MCAS system, each hydrogen atom will have a single M-electron. The intensity of this electron and the proton at its center are omitted from the determination, as they are redundant. The MCAS electron distribution and the resulting electrostatic intensity at a proton center are given in Figure 36. Those who want electron density on the axis between two nuclei should find great joy in the difluoro-and trifluoromethane compounds. Note that the carbon electron that would be exo to the C-F bond occupies the "anti-sigma" position. In these, the hydrogen atoms must point one of their lobes towards the carbon nuclei as those "exo" electrons <u>were</u> their carbon Xi-electrons! Indeed, the two hydrogen nuclei in difluoromethane diverge because the two carbon Xi-electrons the two hydrogen nuclei would normally share and, hence, both be attracted to, are gone. Xi-bonding of the hydrogen atoms is favored in methane and fluoromethane. The electrostatic field for fluoromethane is shown as in Figure 37.

Figure 36.
MCAS Structures Used to Determine Electrostatic Field at Proton



HCF3	Field at H	1.75												
			charge	1st	1st	exo	Xi	Xi	Xi	antiXi	antiXi	antiXi	antiXi-C	Total e
	H (e)	0.54282	1			0	0	0	0	0.25	0.25	0.25	0.25	1.0
	H-C	1.098				Exo-H				antiXi-F	antiXi-F	antiXi-F	antiXi-H	
	C(e)	0.65069	6	1	1	1	0	0	0	1	1	1	0	6.0
	C-F	1.327								antiXi	antiXi	antiXi	antiXi-C	
	F(e)	0.33700	9	1	1	1	1	1	1	1	1	1	0	9.0
	F-F angle	108.00												
H2CF2	Field at H	1.27												
			charge	1st	1st	exo	Xi	Xi	Xi	antiXi	antiXi	antiXi	antiXi-C	Total e
	H (e)	0.54282	1			0	0	0	0	0.25	0.25	0.25	0.25	1.0
	H-H angle	114.00												
	H-C	1.090				Exo-H	Exo-H			antiXi-F	antiXi-F	antiXi-H	antiXi-H	
	C(e)	0.65069	6	1	1	1	1	0	0	1	1	0	0	6.0
	C-F	1.300								antiXi	antiXi	antiXi	antiXi-C	
	F(e)	0.33700	9	1	1	1	1	1	1	1	1	1	0	9.0
	F-F angle	109.00												
H3CF	Field at H	0.90												
			charge	1st	1st	exo	Xi	Xi	Xi	antiXi	antiXi	antiXi	antiXi-C	Total e
	H (e)	0.54282	1			0.25	0.25	0.25	0.25	0	0	0	0	1.0
	H-H angle	109.48												
	H-C	1.390								antiXi-H	antiXi-H	antiXi-H	antiXi-F	
	C(e)	0.65069	6	1	1	1	1	1	1	0	0	0	0	6.0
	C-F	1.327								antiXi	antiXi	antiXi	antiXi-C	
	F(e)	0.33700	9	1	1	1	1	1	1	1	1	1	0	9.0
H4C	Field at H	0.394												
			charge	1st	1st	exo	Xi	Xi	Xi	antiXi	antiXi	antiXi	antiXi-C	Total e
	H (e)	0.54282	1			0.25	0.25	0.25	0.25	0	0	0	0	1.0
	H-H angle	109.48												
	H-C	1.091								antiXi-H	antiXi-H	antiXi-H	antiXi-H	
	C(e)	0.65069	6	1	1	1	1	1	1	0	0	0	0	6.0
HCCH	Field at H	0.760												
			charge	1st	1st	exo	Xi	Xi	Xi	antiXi	antiXi	antiXi	anti-C	Total e
	H (e)	0.54282	1			0	0	0	0	0.25	0.25	0.25	0.25	1.0
	H-C	1.056				anti-H	Xi-H	Xi-H	Xi-H	Xi-C	Xi-C	Xi-C	anti-C	
	C(e)	0.65069	6	1	1	0	0.67	0.67	0.67	0.67	0.67	0.67	0	6.0
	C-C	1.206												

Figure 37.
Electrostatic Field of Methyl Fluoride
(Plane through FCH)

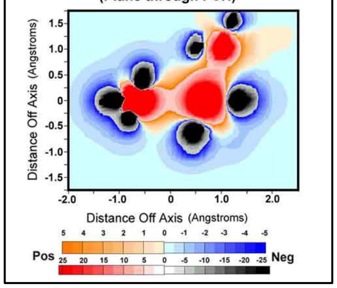
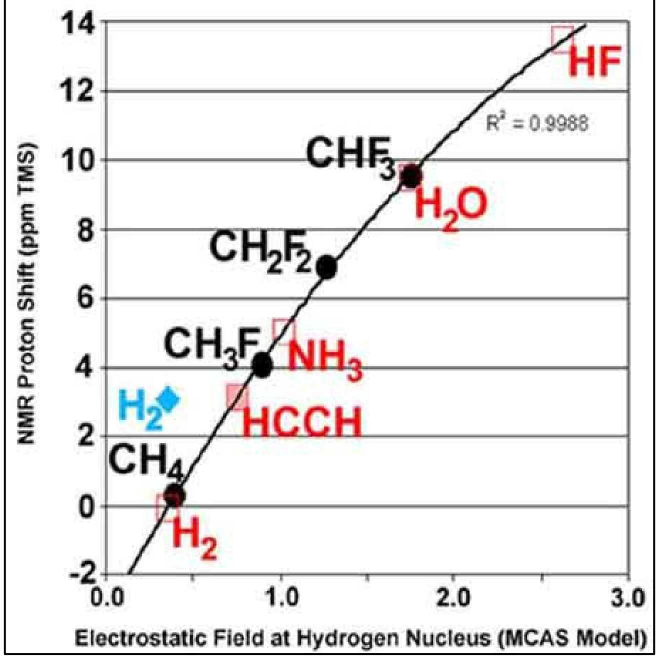


Figure 38.

NMR Shift and H Electrostatic Field



Proton chemical shifts of some molecules are compared to the calculated electrostatic fields at the hydrogen nucleus in Figure 38. The fluorinated methane series is shown in black. The NMR shift values are averages of available data

green[146], purple[147], blue[148]:
methane (0.0, 0.23, and 0.6 ppm relative to TMS), fluoromethane (3.70, 4.26, and 4.1 ppm), difluoromethane (6.86 ppm), and trifluoromethane (9.54 ppm).

The relationship appears very good. The red data in the plot for compounds whose location on the fluorinated methane curve is set by their electrostatic data. The data for acetylene corresponds to 3.1 ppm — data is reported[149] from 2 to 3.1 ppm. The data for NH_3, H_2O, and HF are what would be expected without hydrogen bonding. The HF value is consistent with, and higher than, those of acetic and sulfonic acids.[150] Hydrogen bonding brings a large, negative, electrostatic presence on the exposed side of the proton and can lower the shift value; to <1 for H_2O in benzene, for example. Pure water is at 4.63 ppm,[151] which is the midpoint between 9.63 and -0.37 ppm. The electrostatic level for the hydrogen molecule should correspond to a chemical shift just less than that of methane, **<u>if</u>** the electron around the adjacent hydrogen were always distributed -¼ per tetrahedral lobe. Experimental data[152,153] however, place the chemical shift of the hydrogen molecule proton near that of ethylene! The turquoise location for the hydrogen molecule represents the electrostatic field at the proton when the electron of the adjacent hydrogen is in the lobe exo to the bond. Momentary presence appears more important here than time-averaged probability.

G. SUMMARY

Single bonds between atoms do not need paired-electron couplets on the axis between the two atoms. Bonding can be satisfactorily explained by minimizing inter-atom electron-electron and proton-proton repulsions, while maximizing inter-atom proton-electron attractions of non-axial components. Opposing electron motion (alignment with or against the field) rather than spin-reversal provides spin-pairing. Triple bonds are just single bonds with less inter-atom electron repulsion. The anti-bonding orbital is in the axis of the bond, not opposite it. Under proper conditions, one electron can fill this anti-bonding orbital in a stable molecule. Classical electrostatic calculations and the MCAS approach provide a satisfactory explanation to atomic covalent bonding without the need for waiving the electron-electron repulsion necessary to generate high negative density in current approaches. The MCAS approach to the electronic structure of atoms and their interactions allows ionic and covalent bonding to be explained by the same set of rules.

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[146] From the gNMR freeware program. Information from Neil Glagovich, Central Connecticut State University

[147] From the Central Connecticut State web site: http://www.chemistry.ccsu.edu/glagovich/teaching/472/nmr/factors.html

[148] From the Colby College web site: http://www.colby.edu/chemistry/NMR/H1pred.html

[149] From the Cal State Stanislaus and U of South Maine web sites: http://wwwchem.csustan.edu/Tutorials/NMRTABLE.HTM, http://macweb.acs.usm.maine.edu/chemistry/newton/Chy251_253/Lectures/HNMR/ChemicalShifts.html

[150] Deroe, Andmrew E., "Modern NMR Techniques for Chemistry Research", Pergamon Press, Elsevier, Tarrytown, NY, pp32-35 (1987)

[151] Handbook of Chemistry and Physics, **<u>66</u>**, F-216 (1986)

[152] Expected chemical shift, W.T.Raynes, "Specialist Periodic Report NMR", 7, R.J.Abraham, ed (1978) is 26.26 (+/- 0.15) ppm ? courtesy of Nikolay M.Sergeyev, nser@nmr.chem.msu.su

[153] Experimental value of 26.2 ppm given at http://tiger.berkeley.edu/pfrommer/nmr/nmr.html with CH_4 (30.61), C_2H_6 (29.86), C_2H_2 (29.26), and C_2H_4 (25.43). These values have been converted by the current author to the TMS scale with a quadratic equation having R 2=1.0 for the carbon compounds: CH_4 (0.30 set), C_2H_6 (1.2 set), C_2H_2 (1.8), C_2H_4 (4.7 set), and H_2 (4.1)] ? this web site is no longer available

PART III

QUANTUM ASPECTS

A. INTRODUCTION

The overlap integral of molecular bond making is discussed first. Atomic orbital orthogonality is treated by the same approach. This discussion is followed by the designation of new quantum numbers for the orbitals of atoms described by the MCAS way. Electrons occupy these orbitals, but have no numbers themselves.

B. ONE ELECTRON PER ORBITAL - Pauli

Density functions are electrostatic field intensities associated with the probabilities of a particulate electron actually being present. No problem when only 1 electron is present. When two regions are overlapped to yield atomic or molecular orbitals, the resulting particulate probabilities in the overlap are determined in the current QT as cross-products and new field intensities related. The cross-product in the Schrödinger equation must be for an electron and it can not be an instantaneous sum of two electrons — probabilities may by fractional, but orthogonal particles are not. If c_Ac_A [read A OR A, not A AND A] and c_B^2 [read B OR B] correspond to 1 electron each, then so do c_Ac_B [read A OR B] and c_Bc_A [read B OR A]. Since the last two refer to the same region, the sum must be (A-NOT-B + B-NOT-A) or (A AND B). The last (used in the current QT) defies electrostatic law. One component or the other of such an overlap (if it could exist) would also repel the non-overlapped region at the interface. These are not bank mergers. The first summing can occur only when the regions oscillate reciprocally into the overlap.

Consider two single-point, atomic orbitals leading to a molecular orbital. This extreme case starts with two incompatible, electrons at two, separated, infinitesimally small points — each point, thus, has a probability of 1. Each electron has an identical, but separate nucleus. If the two points are combined, the combined point can also have a probability of 1 with respect to an electron. Thus, the overlap point can have an entity present; one, not two — electrostatic orthogonality (repulsion) forbids the combination of the two electrons into a single entity. The entity combination is OR not AND. That other entity must be put elsewhere. In other words, there must be a second location with a probability of 1 after overlapping. If neither electron occupies the overlap point, then there must be two other locations. The algebra goes

$$\Psi_{AB}^2 = (c_A\varphi_A + c_B\varphi_B)^2 = c_A^2\varphi_A^2 + 2c_Ac_B\varphi_A\varphi_B + c_B^2\varphi_B^2 \quad \ldots\ldots \quad \textbf{(1)}$$

For this point orbital case, $c_A = c_B$ and $\varphi_B = -\varphi_A$ (opposed orbitals equally placed between the two identical nuclei). Thus,

$$\Psi_{AB}^2 = p_A - 2p_{AB} + p_B = 0 \text{ (The overlap is a node!)} \quad \ldots\ldots \quad \textbf{(2)}$$

$$p_{AB} = 1. \quad \ldots\ldots \quad \textbf{(3)}$$

Taken further, as soon as one infinitesimal point is assigned the probability of an electron being present, points an infinitesimal distance away must also be assigned that same electron. Carrying this to the overlap boundary converts the OR-sum to an A-NOT-B or a B-NOT-A sum. Thus, an overlap region can possess only A-OR-B, but not both at the same time. In essence, renormalizing resets the total probability to unity for an electron. The result of this is that when two regions (orbitals) overlap, they must overlap completely, not partially, with respect to an electron being present. An electron, if present, may have a very low probability of being in the far parts of the overlap, but that finite probability precludes another electron from being in the overlap. If the total electrostatic field in the overlap is greater than the contribution from one electron within the overlapped region, the additional contribution must come from without. If the overlap field is less than that from one electron, there can be no full-time electron in the overlap. Indeed, there may never need to be an electron in the overlap. All electrostatic density might come from without. There must, however, be unoccupied orbital space (probability always able to be 1 as that is what defines orbital space) available elsewhere for any excess electrons that were in the orbitals that were overlapped!

Atomic orbitals conform to a similar treatment. φ_A is the $p_A \rightarrow e_A$ single point, orbital vector for electron A and its associated nucleus A. The complete atomic orbital for electron A is the vector space in which the p_A end of all the vectors is the same point. The reverse of the vector is $-\varphi_A$ $(e_A \rightarrow p_A)$! Molecular orbitals are formed by "noding" the negative (electron) end of proton-electron vectors. Atomic orbitals are formed by "noding" the positive (nucleus) end of these vectors. Equations 1-3 above hold for both. In the case of the atomic orbitals, protons A and B are overlapped between the two electrons. When the overlap demands A-OR-B, there is no problem as A and B are one and the same. The three nodes have a particle each — nothing extra. For the nucleus to remain a node, the two electrons must act as a synchronous, opposed couplet. The simplest (a guiding scientific truism) orbital structure that can be generated in spherical space without the two electrons occupying the other's space is one of diametrically opposed tetrahedra. Particle spatial probability may be random over time, but it is highly unlikely that this couplet moves randomly!

The "miracle" of the spdf-based quantum theory arises from allowing the renormalized probability summation of the overlapped and unlapped regions to represent 2 electrons and waiving the particle exclusion (repulsion) aspect of the exclusion principle. Pauli originally had no more than one electron per box — his requirement that each electron have a separate identity. [The exclusion principle simply reiterates the axiom that no two objects can occupy the same space at the same time!] Actually, it is the quantum box that has the number, not the electron which may or may not be present. When two boxes are overlapped, a single box with [A OR B OR neither] should result, not three pseudo-boxes with $\{[(1-f_A)A] + [(f_A A+f_B B)] + [(1-f_B)B]\}$ or one box with [A AND B]. Overlapping two boxes allows the system to reduce its electronic deficiencies, allows one electron to serve the purpose of two, and/or frees an electron for more constructive use elsewhere! The energy change can certainly be related to the hypothetical overlap integral that would result **if** electrons were combinable, but that does not verify that such an overlap actually occurs! Treating orthogonal electrons like money is what allows the current QT to subtly sell "two e's in a pod".

The single point orbital is the very center of the current Quantum Theory's overlap between two identical atoms. It should be the point with the highest probability of electron presence, yet $\Psi^2 = 0$ — even when an electron is present! Does $\int \Psi^2 dr = 1$ with two electrons present flow logically from this?

C. MCAS QUANTUM NUMBERS

Quantum electronic levels are energy levels that correspond to discrete synchronous actions and interactions of electrons among themselves and with their nucleus (or nuclei). Precise interactions (energies) are required to be "in-synch" while moving at nearly the speed of light. Orbitals define where the electrons of these synchronous actions and interactions physically reside. The probability description (negativeness contour) of the orbital will correspond to the time-averaged electrostatic radiance of an electron when present. Since orbitals form sets and subsets, discrete identities (quantum numbers) can be assigned to them. The electrons that occupy them do not have quantum numbers! An electron may enter an orbital as another is leaving, but two electrons can not harmoniously occupy the same orbital space at the same time — a requisite of orbital space (electrostatic particle orthogonality). Since several orbitals may form a group, electrons can synchronously visit separate orbitals of the group. Taking a time interval from mid-occupancy to mid-occupancy to indicate that two electrons can share the same orbital at the same time would be statistical quackery. Electrostatic field additivity cloaks electrostatic particle orthogonality. Probability might not know the difference, but electrons do.

The Pauli exclusion principle is about energy "boxes" (orbitals, levels). Orbitals exist from a quantum number aspect whether they have an electron in them or not. That is, they represent allowable synchronous interactions. The orbital "spin" factor corresponds to an orthogonal set of diametrically opposed, non-coincident orbitals. This factor should have been called the "ort" factor instead of the "spin" factor. An electron does not set the orthogonality of an orbital. Rather, electron spin allows the electron to shape the orbital terrain. E.g., 100(+½) H Street and 100(-½) H Street are contoured as mirror images. The combined lot relinquishes the orthogonality component to become 100(0) H Street. It still must obey the single occupancy zoning law (electrostatic particle orthogonality), however. Since an electron need not be present at all, ever-present orbital "spin" ("ort") is unrelated to the spin of an occasionally present electron!

Each atomic orbital has a unique quantum number (currently specified by nlms, although nlmo would have been better as it would have severed the implied connection to electron spin) that permits instantaneous, harmonious, space assignment to an electron. For the MCAS approach, "**stogh**" (pronounced "stow", where s = shell, t = type, o = ort, g = group, and h = 'home' orbital) is used in place of nlms. Shell has a value 1-n; type is 1-4 (M=1, C=2, A=3, S=4); and ort is +1 or –1 (mirror-image type sets). The number of groups in each orbital type is: 1 for M; 2 for C; 3 for the transition (A orbitals) series; and 4 for the rare earth or actinide (S orbitals) series. The 'home' orbital value specifies the group lob. The M-orbital type has a single group that has 4 orbitals. For the M-type, the same electron occupies all four orbitals and h can only be 1. For the C-orbital set, h is 1-2. For the A-orbitals, h = 1-3, while h = 1-4 for the S-orbitals (see below).

For the **H** atom, the ground state electron is in the **11111** orbital [as opposed to the nlms 100(+½)].

The first electron in **He** is the same, while the second is in the reciprocal set. Thus, **11±11** is the quantum designation for helium; it's a gas!

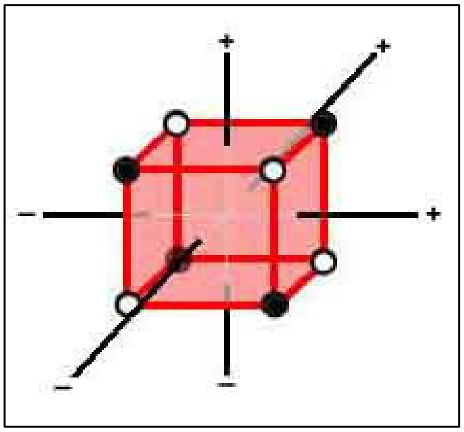
	1st e	**2nd e**
H	**11111**	
He	**11111**	**11-111**

The orbitals for the 3rd to **last** Aufbau **electrons** in the ground states of the second row elements are

	3rd e	**4th e**	**5th e**	**6th e**	**7th e**	**8th e**	**9th e**	**10th e**
Li	**21111**							
Be	**21111**	**21-111**						
B	**21111**	**22-111**	**22-112**					
C	**21111**	**22-111**	**22-112**	**22-121**				
N	**21111**	**22-111**	**22-112**	**22-121**	**22-122**			
O	**21111**	**22-111**	**22-112**	**22-121**	**22-122**	**22112**		
F	**21111**	**22-111**	**22-112**	**22-121**	**22-122**	**22112**	**22121**	
Ne	**21111**	**22-111**	**22-112**	**22-121**	**22-122**	**22112**	**22121**	**22122**

"stogh" designations allow each orbital space to be specified. Whether electrons move into and out of orbital groups or not, they must have a unique 'home' orbital. Changes in the underlying electronic structure may occur as additional electrons are added. These changes are accompanied by the appropriate change in the "stogh" designation. The changes in the type designation of the 3rd and 4th electrons above, for example, reflect additional electron loading in the M-orbitals to convert them to C-orbitals. Converting the –1 "ort" set to higher loading first is a matter of convention as the third and fourth electrons are identical. When there is no external field, **22-112** and **22-121** are equivalent and filling of either can occur before the other. In the presence of a field, however, the lowest energy state fills first. Quantum numbers are easily related to the field by placing the x-y-z axes through the MCAS cube faces. Note the primary alignment to the field running - - - to +++ and secondary ones along the axes.

For A-orbitals, there are two opposing sets of nine subdivided into three sets of three (coplanar) — g = 1-3 and h = 1-3 (one orbital is face-centered and the other two are edge-centered in the MCAS approach). For S-orbitals, there are two opposing sets of sixteen subdivided into four sets of four [a "C" set rotated 60º (relative to the standard C-orbital) about the "corner" orbital] — g = 1-4 and h = 1-4 (one orbital is corner-directed and the other three are squared-faced in the MCAS approach). The theorist can add, subtract, multiply, or do whatever (even change) these numbers to allow him/her to "integer-ize" his/her mathematics. (+½ and -½ must be integer quotients in the nlms scheme!) Indeed, the theorist might find it convenient to consider the C orbital as just a more heavily loaded M-orbital (or vice versa) since there are no new orbital spaces defined. From a pragmatic point it seems desirable to separate them to emphasize the uniqueness of the single loading of multiple orbitals. The numerical symmetry, as demonstrated in the next table with the inert gases, is quite suggestive, too! $2s^2$ gives the maximum number of electrons (2, 8, 18, 32) in the s-shell!



Shell	Element	e's	MCAS Structure	stogh of last electron in shell					
				1st	2nd	3rd	4th	5th	6th
1	**He**	**2**	M2	**11-111**					
2	**Ne**	**10**	M2C8	**11-111**	**22122**				
3	**Ar**	**18**	M2C8C8	**11-111**	**22122**	**32-122**			
4	**Kr**	**36**	M2C8A18C8	**11-111**	**22122**	**32-122**	**42122**		
5	**Xe**	**54**	M2C8A18A18C8	**11-111**	**22122**	**32-122**	**43133**	**52-122**	
6	**Rn**	**86**	M2C8A18S32A18C8	**11-111**	**22122**	**32-122**	**44144**	**53-133**	**62122**

The "**ort**" values will be determined by the field relationship chosen to define the orbitals. The sequence is alternated here, although the "last" electron in each shell should be against the field. The conversion of the 5th shell C-orbital system to an A-orbital set with one electron to allow the conversion of the 4th shell A-orbital set to an S-orbital set is the main factor why the primary valence of the lanthanide series is +3.[154]

No electron has a quantum (plat) number — only an orbital! Every electron must have a 'home' address, however. The "miracle" of the current Quantum Theory occurred when two opposing orbitals were allowed to merge into a sphere (Bohr's orb — Pauli's mentor) and their "spin" ("ort") numbers, which defined immobile physical space (as diffuse and probable as required), transferred to two electrostatically antagonistic, mobile electrons. Mathematical magic.

D. NO NEED FOR PARTICLE THEORIES?

The challenge for any QT is to include particulate solutions that satisfy electrostatic requirements, if they are to claim completeness and robustness and, of course, to be correct. The MCAS particulate model gives electrostatic solutions with all e-e repulsions "orthogonalized"; i.e., e-e overlaps are minimized. These solutions are excluded from the currently accepted QT, however, where maximized e-e overlap is the rule!

The reason MCAS solutions are excluded from the current QT is the special attribute given to electron spin-reversal in this QT. Spin-reversal is a form of orthogonality. Unlike orthogonality practiced elsewhere in the current QT, however, spin-reversal orthogonality negates e-e repulsion rather than "orthogonalize" it!

The MCAS approach will raise the ire of those who have bought spin-reversal bonds. The ultimate QT must be reconciled to ALL aspects (probability, wave, AND particulate). As the particle component apparently sets a stricter bound than probability, the appropriate response is,

> *"If you want a theory that is correct, you need to address particulates, too"*.

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[154] J.M. Williams, "The Electronic Puzzle, US LibCong ©1994

PART IV

REACTIONS THE MCAS WAY

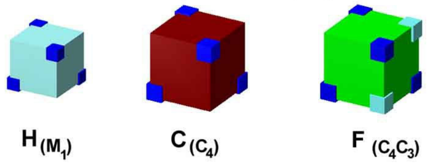
A. MODELS and REACTION PATHS

Before proceeding, it is appropriate to comment on: some MCAS structures (hydrogen, carbon, and the halogens) and microscopic reversibility.

1. MCAS MODELS OF SEVERAL ATOMS

The MCAS structures for hydrogen, carbon, and fluorine are shown in Figure 39. The blue and aquo corners indicate the directions of orbital lobes. Note the two sets. Hydrogen is in its M_1M_0 base state wherein one electron roams a mono orbital occupying tetrahedral space. Carbon is in its C_4C_0 (four orbitals tetrahedrally oriented in cubic space) elevated state needed for four singles bonds, rather than its M_1C_3 (M and C's counterpoised) base state. Fluorine is in its C_4C_3 (two C units counterpoised) base state. The MCAS structures are nicely understood with the use of cubes. Every electron in the MCAS methodology has its own instantaneous orbital space. Electron pairing occurs through diametrically opposing motion rather than through spin-pairing and negative-negative repulsion negation required for dual orbital occupation.

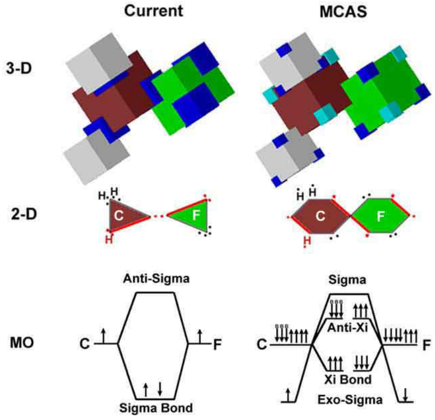
FIGURE 39.
MCAS Structures for H, C, and F



2. MCAS versus Currently-Accepted MODEL OF METHYL FLUORIDE

Models for methyl fluoride are shown in Figure 40. Like the MCAS cube model for carbon, a cube representation for carbon in the currently accepted vernacular nicely depicts the spatial orientation of the orbitals (sp^3) - larger dark blue corners indicate 2 electrons per lob instead of 1. Think spheres for the cubic hydrogen atoms in the currently accepted model, however. Like carbon, the cube represents fluorine well whether it is the currently accepted (sp^3) or MCAS model. Other halogens will be larger than fluorine. The important feature is their common C_4C_3 outer shell, however. Cubes are use for the currently accepted model to help with spatial effects and because spheres and tetrahedral shapes are not available with the modeling program used.

FIGURE 40.
Models of Methyl Fluoride



The 2-D models shown in Figure 40 give a touch of 3-D character to the planar. The dense red lines indicate point-to-point lines in the plane of the paper. Two H's or two electrons at any point in the MCAS representation should be interpreted as one above and one below the plane. Wedges would give even more 3-D character. In the currently accepted representation, one H and two electrons are above and one H and two electrons are below, while four electrons should be read two up and two down. The similarity between this 2-D representation of the currently accepted model and the Lewis octet structures should be apparent. The more dispersed electron nature of the MCAS structures should also be obvious. Every electron in the MCAS methodology has its own instantaneous orbital space. Electron pairing in the MCAS models occurs with opposing motion rather than orbital overlap, however! Negation of negative-negative repulsion (required for two electrons to be in the same orbital) is not needed in the MCAS methodology as it is in the currently accepted methodology. Thus, in the MCAS models, the sigma bonds have no electrons in them. The bond between the carbon and the fluorine is called a sigma-Xi ($\sigma\Xi$) bond; as are those between carbon and hydrogen.

The MO for the currently accepted methodology is straightforward, IF spin-paired negation of negative-negative repulsion is accepted. The MCAS MO depicts the bond between the carbon and fluorine as a 6-electron Xi bond (see the 3-D view for the electron placements). The three electrons on the opposite side of the fluorine and the three CH bonds (**B-arrows**) oppose the Xi bond. The Xi/anti-Xi levels are shown with no net change in energy, although this is not the case. The net gain in energy in forming the bond is allotted to the exo-sigma electrons that are now paired by opposing action. They are placed on opposite sides of the atoms from the bond to give them spatial meaning. As noted before there are no electrons in the sigma bond — only overlapped negative fields. Placing electrons in the bond negates the reason for forming the sigma bond.

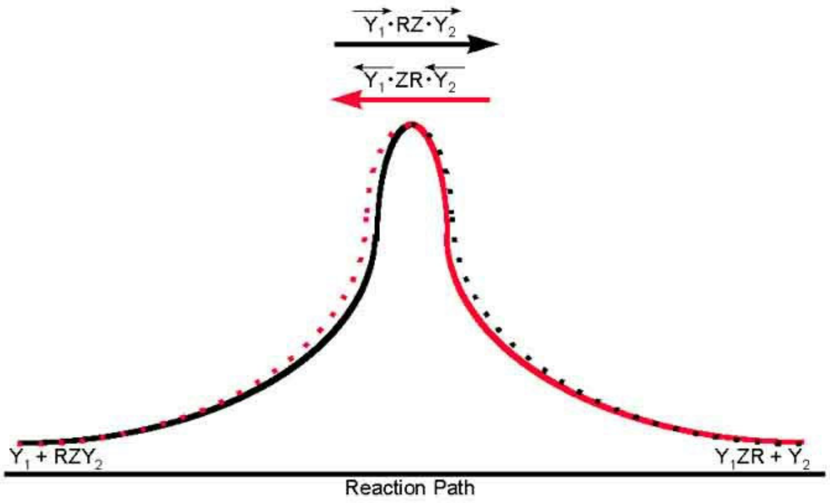
3. MICROSCOPIC REVERSABILITY IS NOT

Microscopic reversibility has been invoked to justify that S_N2 racemization reactions have a single Transition State regardless of direction. The rationale being that momentum (and every other action!) is instantaneously reversible at every moment. This seems a rather unlikely situation for this type reaction! Indeed, the situation is much like pole vaulting. The vaulter starts down the runway and vaults up but not over. Eventually, he vaults over the wall feet first. After falling down on the other side, the vaulter goes to the head of the runway and reverses the event - again feet first over the wall. In the macrosense, the forward and reverse actions are identical, although the attempts might not be the same! At the instance of going over the wall, "the Transition States" of the two are mirror images! The fall after the max is the same for the forward and reverse; neither the same as the rise - to imply otherwise, as is commonly done, over simplifies and misleads. In the more correct and, I believe, original interpretation of microscopic reversibility with Y_1 and Y_2 identical (!),

$$Y_1 + RY_2 \rightarrow Y_1R + Y_2 \text{ and } Y_1R + Y_2 \rightarrow Y_1 + RY_2$$

proceed through identical paths. Since, in this case, the forward and reverse reaction paths are mirror images, the Transition States will be mirror images. Having the two Transition States be independent of path direction (centrosymmetric here) would be most unusual, but still highly touted! The pre-transition and post-transition routes might, however, be similar as in the graphical presentation of Figure 41.

FIGURE 41.
Nucleophilic Racemization



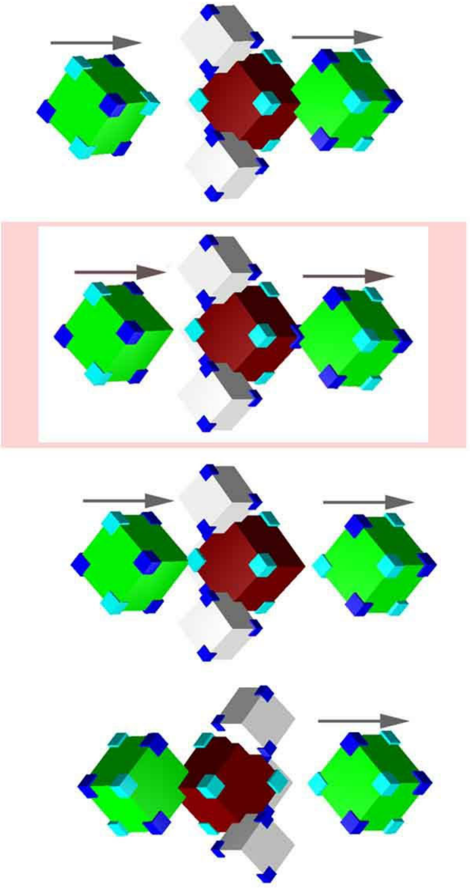
The Transition State is said to be the highest energy level to which reactants can go, reverse momentum, and return to base. In this sense, an infinite summation of momentum reversals equates to microscopic reversibility. No single trip up the energy curve, however, is reversible at every point - only at its energy maximum! Only the maximum-maximum Transition State can reverse in either direction and then only if it is path-independently identical. More generally, the Transition State is that assemblage on the reaction energy path at which the assemblage components can NO LONGER reverse to base.

B. S_N2 REACTIONS THE MCAS WAY

The C—Y_2 bond is constantly stretching and contracting. When the bond stretches extensively, the exo-sigma electron (low-energy state -carbon in C_4C_0 state) moves to the sigma bond (high-energy state - carbon now in a C_3C_1 state) to minimize charge separation (see the MO in Figure 40). [Note that when •CF• becomes C•F•, it becomes naturally highly polarized (+ − + −)!] Stretching becomes more difficult as bond energy increases - thus, a strong dependence of leaving group propensity on bond energy. If the stretch is violent enough, the Y_2 group will leave with the electron in spite of the separation of charge — S_N1 type. Usually, however, the C —Y_2 bond returns to normalcy and the electron returns to the exo-sigma orbital (C_3C_1 returns to C_4C_0 — MCAS vernacular). If there is an e-donor (Y_1) nearby when the exo-electron is transferred to the sigma bond, this e-donor can supply an electron to the now vacant exo-sigma orbital, IF the electrostatics (electrode potential) is satisfactory. When this occurs, the electron in the sigma bond can no longer return to the exo-sigma orbital as the carbon is in the C_4C_1 state. The destabilized sigma bond now dissociates with the Y_2 group leaving with the sigma bond electron. This allows the bond to dissociate at significantly lower Transition State energy as charge separation is minimized. The e-donor, now electron deficient, follows its electron and, thus, "attacks" the carbon. At this point, the C_3C_1 carbon reorders to C_0C_4, the non-dissociating bonds on the carbon move to their new location (Walden inversion), the leaving group is further repelled, and the "attacking" group forms a sigma-Xi bond with the carbon. The sequence is depicted in Figure 42, where the e-transfer step (the Transition State) is highlighted.

FIGURE 42.

S_N2 THE MCAS WAY

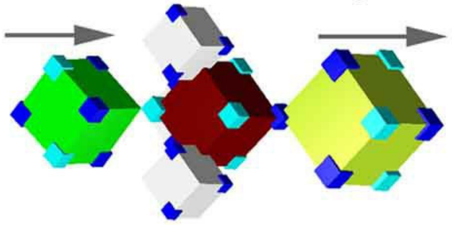


Carbon will become more positive in the Transition State as the leaving group stretches away. Therefore, electron-withdrawing groups on benzyl halide should retard the reaction by making carbon C_4C_0 to C_3C_1 more difficult. The reaction of pyridine with substituted benzyl bromides in acetone shows just an effect.[155]

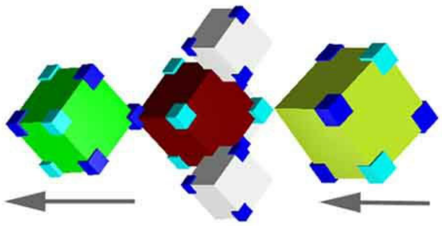
The Transition States of F^- + H_3CCl and FCH_3 + Cl^- are shown in Figure 43. Note that the two do not have the same Transition State (hence, identical energy levels are not required). At the time of electron transfer ("the kicker"), the two are neither superimposable nor mirror images! The same Transition State exists only IF all the atoms (and electrons for that matter) are in identical positions; i.e., they must be superimposable. In the currently accepted explanation of S_N2 reactions, the amount of bond formation and bond breaking are said to differ (polarization invoked to explain the halogen behavior, see below). A superimposable Transition State exists only if attacking and leaving groups are identical; maybe not then — just mirror images! Microscopic reversibility, in this sense, is trashed.

FIGURE 43.

F^- Nucleophile on CH_3Cl



Cl^- Nucleophile on CH_3F



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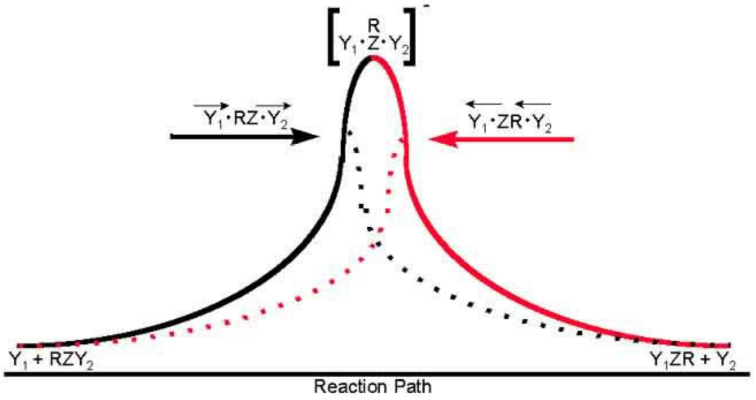
[155] Sudgen, S. and Willis, J.B, J. Chem. Soc., 1460 (1951); cited in Physical Organic Chemistry, J. Hine, McGraw-Hill, New York, p172 (1962) with an earlier reference to Baker, J.W. and Nathan, W.S., J. Chem. Soc., 236 (1936)

One way to think about the S_N2 reaction is to consider the barrier as a moveable incline. The lowest energy path available without help is the top of the incline (actually a saddle in energy space) at its highest level. When this occurs, the Transition State is path-independent (centrosymmetric when Y_1=Y_2) and should be governed by bond strengths. The nucleophilic center and its associated groups (all those R's) will be in their maximum energy (planar) state, however - maximum-maximum! At the moment this transition forms, all components are stationary. Indeed, microscopic reversibility is possible (see Figure 44). If the height of the incline is suddenly lowered while the species are racing up it, however, they will careen over the brink and down to the base on the other side. In the MCAS version of the S_N2 reaction, electron transfer suddenly lowers the height of the incline. The lowering need not be, and is very unlikely to be, the same in both directions. Note that when Y_1=Y_2, Figure 44 becomes Figure 41 if the upper portion between the two Transition States is eliminated. The Transition State is direction dependent and not reversible, however! A microscopic reversal in atomic positions is hardly sufficient to allow the electron to overcome the energy barrier required for its return. Thus, a microscopically reversible Transition State becomes a very rare event — the most energetic way to go.

FIGURE 44.

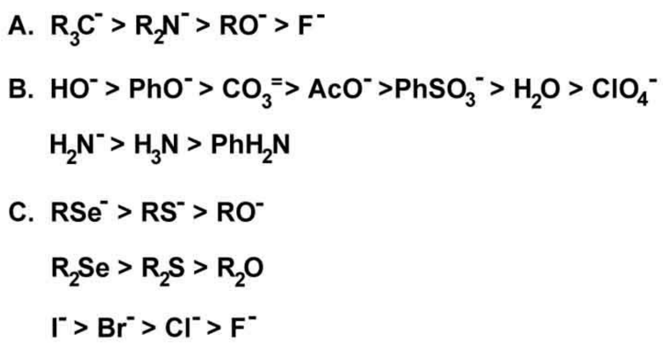
S_N2 Reaction Path the MCAS Way



e-Transfer is "the kicker" that destabilizes the bond of the leaving group (Y_2) at a time when Y_2 has moved away (stationary or no) from the carbon atom and, thus, facilitates S_N2 substitution. It is called "the kicker" because, even if the leaving group has stopped moving away (the situation when the molecule has just enough energy to reach this point), it gives it a "kick". The nucleophilicity of some species are given in Figure 45.[156] Those in series A and B have the same nucleophilicity order as their basicity or bond strength. In the currently accepted scheme, strong bonds make for strong initiation. Those in series C have the reverse relationship — polarization invoked to explain the turn-about. Of course, polarization is mainly the ability to "depart" with one's electrons. All three series should, however, correlate with the following, 1-electron transfer, half-reaction: $\mathbf{RZ\bullet^{-} \rightarrow RZ + e^{-}}$

FIGURE 45.

S_N2 Nucleophilicity


A. $R_3C^- > R_2N^- > RO^- > F^-$

B. $HO^- > PhO^- > CO_3^{=} > AcO^- > PhSO_3^- > H_2O > ClO_4^-$

$H_2N^- > H_3N > PhH_2N$

C. $RSe^- > RS^- > RO^-$

$R_2Se > R_2S > R_2O$

$I^- > Br^- > Cl^- > F^-$

In 1954, Edwards demonstrated mathematically[157] that the oxidation potential of nucleophiles was the dominant factor in their nucleophilicity. The exact reason unclear until now.

---

[156] Gould, E.S., Mechanism and Structure in Organic Chemistry, Holt, New York, 259, (1959)

[157] Edwards, J.O., J. Am. Chem. Soc., 76, 1540 (1954); O. Foss, cited therein, is credited in 1947-1949 with observing that nucleophilicity followed electrode potential!]

Those familiar with leaving group effects will recognize the series I^- >Br^- >Cl^- >F^- for S_N2 reactions. The table below (not in the arxiv version) provides some relative leaving rates for them as found in several study cases.

Substrate	Base	Product	Solvent	T°C	F^-	Cl^-	Br^-	I^-	Ref
CH_2 / \\ HO CH_2-X	HO^-	CH_2 / \\ O—CH_2	H_2O	0	0.002	10	59	52	158
CH_3-X	Cl^-	CH_3Cl	$(CH_3)_2CO$	25		1	425 1	3400 8.0	159
O O \\ / S / \\ ΦH$_2$C CHXΦ	CH_3O^-	O O \\ / S / \\ ΦHC—CHΦ ↓ ΦHC═CHΦ +SO_2	CH_3OH	40		1	190 1	640 3.4	160
				0		1	620		

C. ELECTROSTATICS OF METHYL FLUORIDE

Electrostatic models of methyl fluoride support the S_N2 reaction model given above. Fluoromethane is a simple molecule with an electronegative leaving group. Fluorine is not a particularly good leaving group, because of its strong bond with carbon, but it provides the necessary ingredients for illustrating a S_N2 reaction. Figures 46-48 show the permanent polarization afforded by the fluorine atom attached to methane and the extreme polarization effected by the transfer of the exo electron to the C-F sigma bond. Note the repulsive interactions in Fig 48 created when there is an electron in the sigma bond! The strength of the F-C bond counters the destabilizing movement of the electron into the region on the axis between the two nuclei to a greater extent than occurs with the other halogens, thus making fluoride a poorer leaving group even if it holds it 8 valence electrons more tightly than do the other halogens!

FIGURE 46.

Electrostatic Field of Methane
(Plane through HCH)

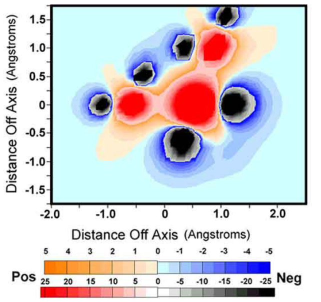


FIGURE 47.

Electrostatic Field of Methyl Fluoride
(Plane through FCH)

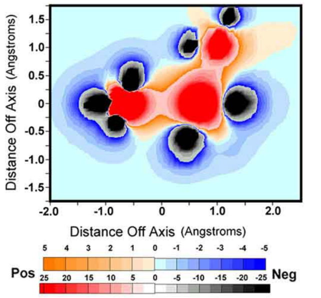
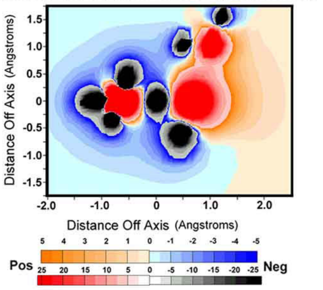


FIGURE 48.

Electrostatic Field of Methyl Fluoride
(Plane through FCH)
[Carbon exo electron in anti-sigma position]



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[158] CL McCabe and JC Warner, "The Kinetics of the Reaction between the Ethylene Halohydrins and Hydroxyl Ion in Water and Mixed Solvents", JACS, **70**, 4031 (1948)

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Figure 49 (not in the arxiv paper) illustrates the changes in electrostatics that occur for a SN2 reaction. Note the negative repulsions that result when an electron is transferred to the bond region so it can be transferred to the leaving nucleus.

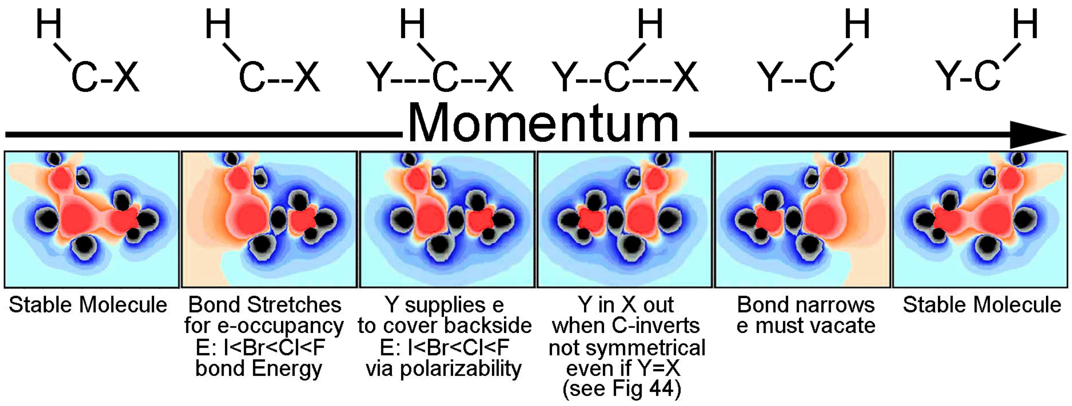

Figure 49

S_N2 reaction illustrated with CH_3F electrostatics

Figures 50 and 51 show the electrostatics opposite the sigma bond before and after the exo electron is transferred to the sigma bond. As seen, the exo electron protects the carbon from attack opposite the bond.

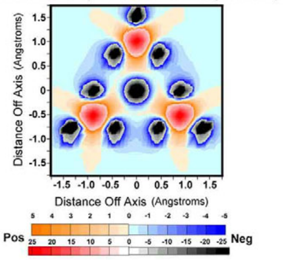

FIGURE 50.

Electrostatic Field of Methyl Fluoride
(Cross axis at 9 equivalent H electron positions)

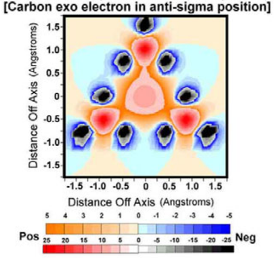

FIGURE 51.

Electrostatic Field of Methyl Fluoride
(Cross axis at 9 equivalent H electron positions)
[Carbon exo electron in anti-sigma position]

The previously protected posterior of the carbon now provides a rather strong "attraction" for "loosely attached" electrons (Figure 51). If none is around, the electron will shift back to the exo-position, as the carbon-end of the bond is now more electronegative (positive) than the fluorine-end. Actually, the electron is still part of the carbon's orbital system. If, however, an electron jumps from the protruding lobe of a nearby donor (irreversible REDOX lightning!), the fluoromethane molecule becomes an anion and the anti-bonding electron can no longer return to the exo-position, but departs with the fluorine atom (Figures 42 and 49). "Push" is provided by the repulsion between the anti-bonding electron and the three carbon electrons that formed the C-F sigma-Xi bond. As the leaving group departs, the nucleophile that lost the electron follows that electron to form a new, sigma-Xi bond with the carbon atom. The carbon electron structure and the accompanying substituents undergo Walden inversion.

D. SUMMARY

There are no persistent electrons in the sigma bond in the MCAS methodology. Those corresponding to the bond are exo (on the other side of the atoms) to the bond. When the exo-electron is transferred to the sigma bond, the bond is destabilized. If an electron donor (nucleophile) is near enough, it supplies one electron to the now vacant exo-sigma orbital, **IF** the redox potential is sufficient to allow such a transfer. When this occurs, the electron in the sigma bond can no longer return to the exo-sigma orbital. The destabilized sigma bond now dissociates with the leaving group taking the electron. The electronic structure of the nucleophilic center now reorders with Walden inversion of the attached atoms as the nucleophile continues forward to form the new bond. The S_N2 reaction path is direction dependent and not microscopically reversible after electron transfer! Even if the atoms could take a microscopic step backwards, such a move would be insufficient for the electron to overcome the electrode potential required for its transfer back to the nucleophile. Thus, microscopic reversibility and path-independence as pertains to the Transition State is a highly improbable event is S_N2 reactions.

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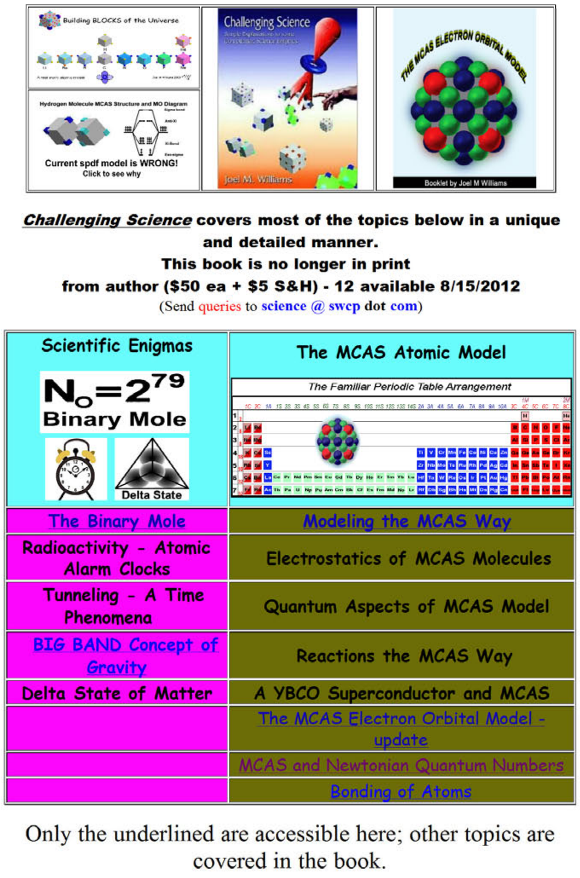

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Career Vitae

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1940 - ____

BS Chemistry 1962 (William and Mary, Williamsburg, VA)
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staff member1972-93 (Los Alamos National Laboratory, Los Alamos, NM)
Contractor to LANL 1995-7 (Ray Raskin Associates)
Consultings: 1986-91 (GV Medical, Minneapolis); 1991-93 (Shell, Houston); 1993-present (JMC Williams Consultants)

Fellow NIH, 1963-66, NSF, 1966-67
Life member Sigma Xi
Listed in Marquis Who's Who and American Men and Women in Science
Federal Laboratory Consortium Technology Transfer Award 1988
Distinguished Performance Award (Los Alamos National Lab) 1989

Publications

80+ pre-2005 citable publications (author or coauthor) are listed from most recent to earliest. They are also separated into fields of endeavor. Those in this book, except for "Modeling the MCAS Way" arxiv listing, are not included in this listing.

Website Listings

- GeneralScienceJournal: http://www.gsjournal.net/Science-Journals-Papers/Author/952/Joel,%20Williams
- vixra: http://vixra.org/author/joel_m_williams
- Website: www.swcp.com/~jmw-mcw
- Natural Philosophy Alliance; Dr. Joel M. Williams Los Alamos, NM 87544, United States; http://www.worldsci.org/php/index.php?tab0=Scientists&tab1=Display&id=1602

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[161] Excerpts from the article:

"Not until early January 1987, during a visit with Joe(l) Williams, our super performer polystyrene foam fabricator at the Los Alamos National Laboratory, was silica aerogel casually shown to be one of the many microcellular foam materials they had made. One sight of that small piece of aerogel generated such tremendous hope of actually having found an even better capture medium.

"Thus far, the highest intact mass recovery in the 6 km/s range has been obtained using foams made from polystyrene with extremely fine mesostructure.

"We are indebted to Joel Williams for the inspiration he provided by showing us his aerogel as well as for his production of high performance polystyrene foam."

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- 1973 Research on Carbon and Graphite, R.J Imprescia, R.D Reiswig, J.M Williams, Los Alamos Scientific Laboratory Progress Report, LA-5413-PR
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- 1968 Developments in the Study of A-S_E2 Reactions in Aqueous Solution, J.M. Williams, Jr. and M.M. Kreevoy, In Advances in Physical Organic Chemistry; Gold, V., Ed.; Academic Press: London, 1968; Vol. 6, p 63
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- 1967 Structure and Infrared Spectrum of the Solvated Proton in Dimethyl Sulfoxide, J M Williams, M Kreevoy J. Am. Chem. Soc. 89 481 (1967)

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- 1968 Reaction of sodium methoxide with α-bromobenzyl sulfone and with 2,3-diphenylthiirene 1,1-dioxide, Frederick G. Bordwell, Joel M. Williams Jr., Bruce B. Jarvis, J. Org. Chem., 1968, 33 (5), pp 2026–2030
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About the Author

Joel M Williams received a BS in Chemistry from William and Mary and a PhD in Chemistry from Northwestern University. He was a postdoctoral fellow at the University of Minnesota before teaching a year of first year chemistry there. After four years as a research chemist at DuPont, he spent the next 21 years as a staff member at the Los Alamos National Laboratory, received a Distinguished Performance Award in 1989 and retired in 1993. He is a life member of Sigma Xi and is listed in Marquis Who's Who and American Men and Women in Science.

Dr. Williams has spent over 50 years in the application and study of Chemistry. By 2005, he had generated over 80 citable publications, as author or coauthor, which covered a very broad scope of scientific research and materials creation. Dr. Williams has studied the interaction of atoms and molecules at the atomic level upwards to the creation of bulk materials. He has studied the occurrence and association of elements in minerals. During his study of the interaction of fluids at various temperatures and pressures, he determined that the physicists' and chemists' "*standard state of matter*" is actually a well-defined arrangement and not just a point on a phase diagram. He dubbed it the "Delta State - the 4th state of matter" because of the way the atoms or molecules collected together. In a materials' sense, a plasma is not a state of matter at all since assemblages are irreversibly destroyed during its formation; the Delta State, on the other hand, is a classical 4th state of matter wherein assemblages are conserved so that they can still return to their other states.

It is Dr. Williams' very broad range of scientific studies that has led him to rethink how atoms are viewed. With his broad background, he has had a chance to gauge how well the current atomic quantum model explains what is happening. He finds that it has basic deficiencies; in spite of being proffered in texts and journals as beyond reproach - the reader is reminded that it is still called quantum *theory*. Dr. Williams has therefore set forth a new model of the atom. His model does not have to declare that macro-physical laws cease at the atomic level; nor does it need to be "hybridized", as does the current model does, in an awkward effort to fit the physicists' model to the observations of the chemists; nor does it place hydrogen in a conspicuously awkward location in the periodic table.