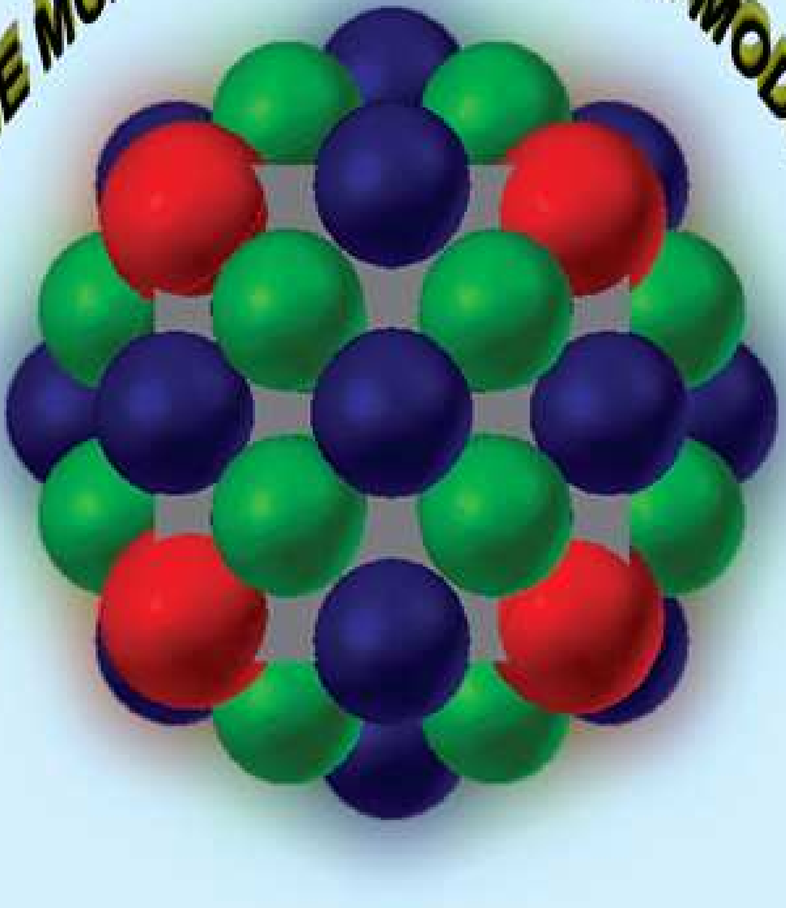
THE MCAS ELECTRON ORBITAL MODEL



Joel M Williams

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

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Abstract

This is a follow-up of my book entitled "Challenging Science".[1] *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 The MCAS model recognizes that electron packing around a nucleus is dynamic and spatially uniform. 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.

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

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A: The MCAS Electronic Structure of Atoms

In 1999, I described the MCAS model for the electronic structure of atoms.[2] 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[3] 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[4] to create tear-shaped orbitals and place them around a point, ala nucleus.

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 below. 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

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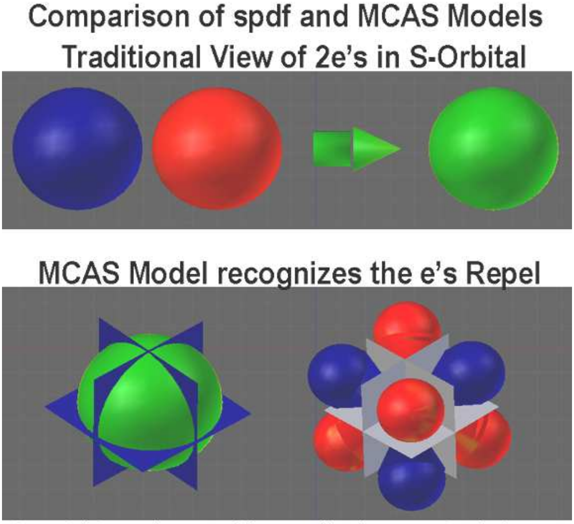
[2] http://arxiv.org/html/physics/9902046v1/Article.html and http://arxiv.org/html/physics/9909053v3. First submission of the concept for publication was in 1993. Also: *The Electronic Puzzle* 1994 (LIBCONG-TXu-632-452) [cited in *A BIT TOO FAR* http://arxiv.org/html/physics/9904031]

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

[4] www.blender.org

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.


Comparison of spdf and MCAS Models
Traditional View of 2e's in S-Orbital

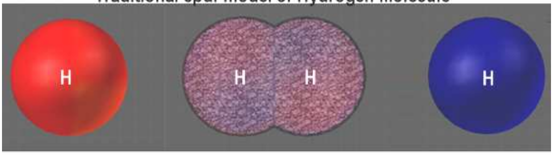
MCAS Model recognizes the e's Repel

Two orbitals centrosymmetric opposites in same spherical space

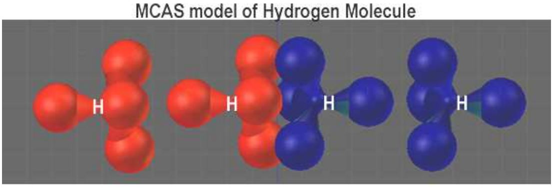
Before proceeding to the remaining MCAS orbitals, it is of value to see how the spdf and MCAS representations differ with regard to a simple molecule like hydrogen. In the spdf version, the spherical electron orbitals overlap with the electrons *again* blending and concentrating between the nuclei – see below. 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.

Comparison of spdf and MCAS Models of Hydrogen

Traditional spdf model of Hydrogen Molecule



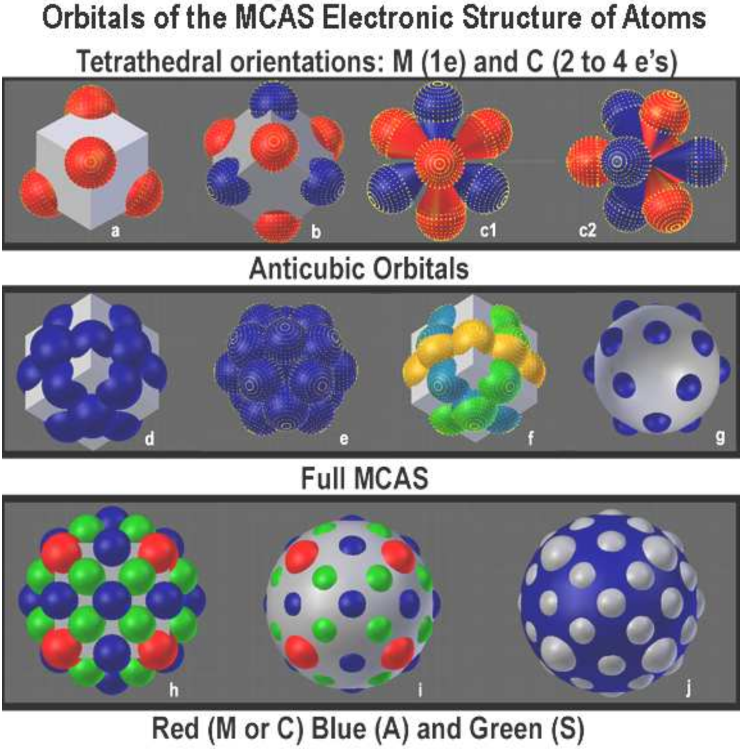
MCAS model of Hydrogen Molecule



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 below 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.


Orbitals of the MCAS Electronic Structure of Atoms

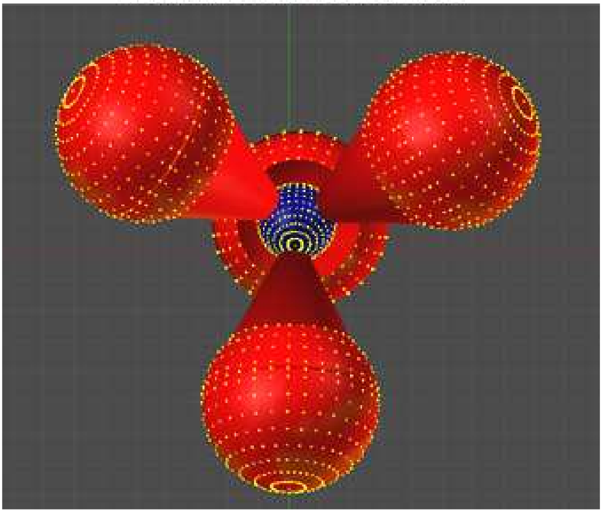
Tetrathedral orientations: M (1e) and C (2 to 4 e's)

Anticubic Orbitals

Full MCAS

Red (M or C) Blue (A) and Green (S)

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.



The MCAS Electronic Structure of Atoms

Looking into M or C-orbital Space

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.

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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.[5]

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

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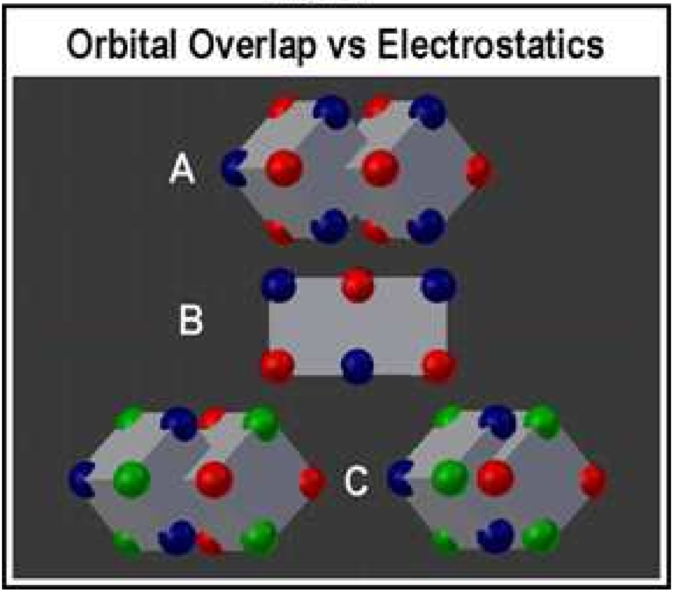
[5] Williams, Joel M, http://www.wbabin.net/Science-Journals/Essays/View/4019 (in the General Science Journal)

electrons (green colored orbitals in figure 1, image C) present to repel the bonding electrons (mid-nuclei red and blue orbitals).

Figure 1

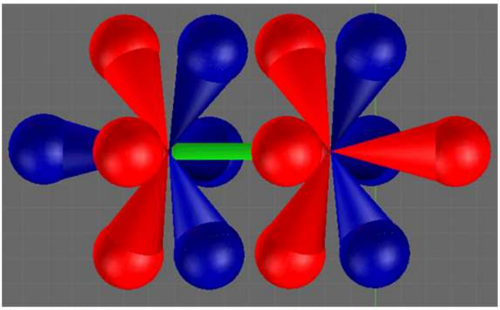


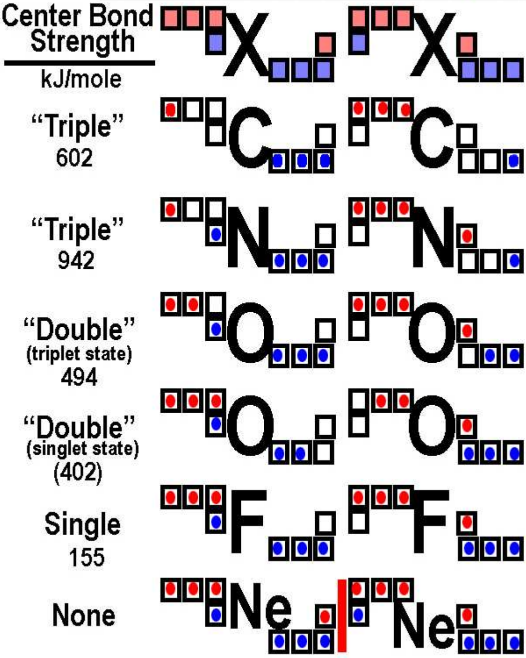
The simple electrostatic bonding model is sufficient to indicate the bonding in the diatomic molecules of the elements carbon to neon (see figure 2). While current MO bonding gives the diatomic molecules different “bond orders” (single, double, triple), the MCAS electrostatic model has them all the same (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) wherein 6 electrons occupy each of the orbital networks, indicated as blue and red.

Figure 2

MCAS Electronic Model
Diatomic Molecules C_2 to F_2

(Note: non-bonding electrons destabilize the bond)





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.

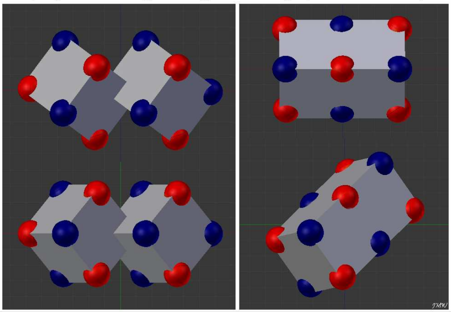


Figure 3

Oxygen Molecule per MCAS Model

Ground State
Triplet (2 e's antibonding/4 bonding)

Elevated State
Singlet(6 e's each orbital set)

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.

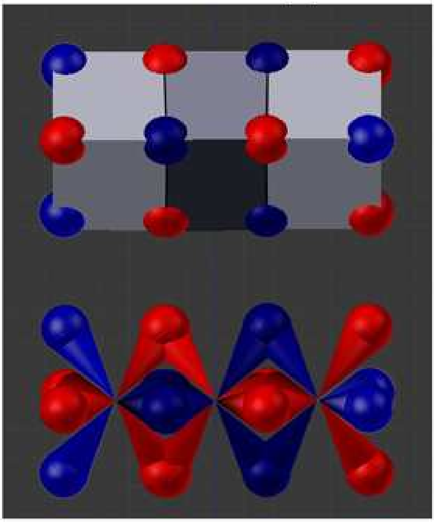


Figure 4

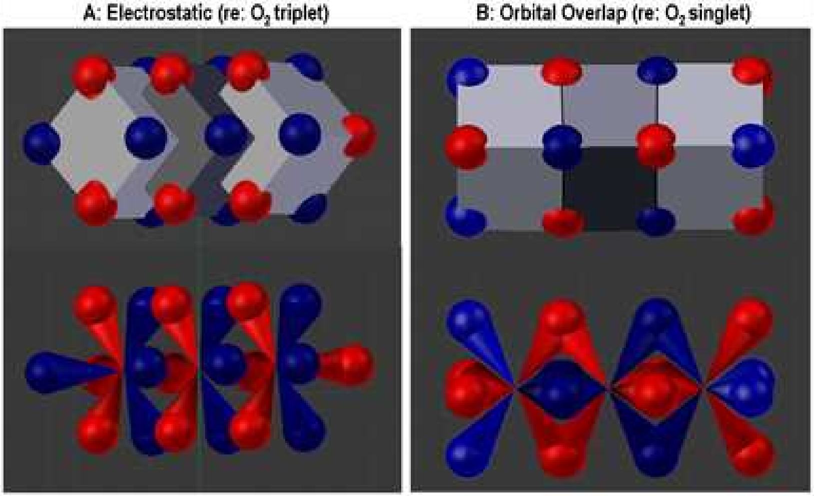
Linear Three Atoms

Allene (H's form bonds at deficient "blue" terminals)
Note: terminal "blue orbitals" perpendicular

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)

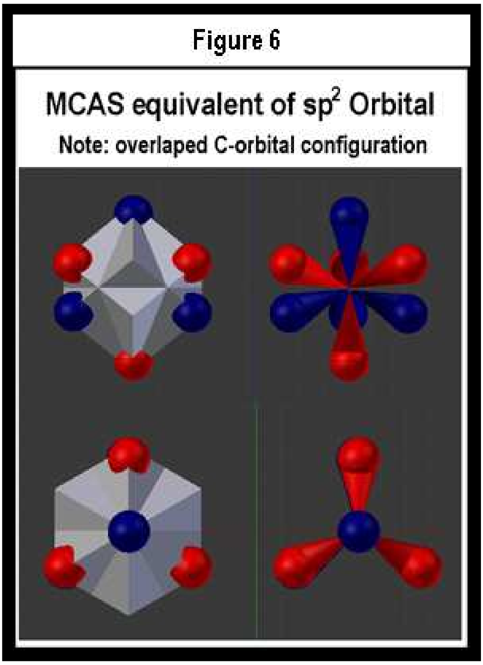


Figure 6

MCAS equivalent of sp^2 Orbital

Note: overlaped C-orbital configuration

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.

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
   - **F**(ace)– non-conjugated double
   - **E**(dge)– conjugated

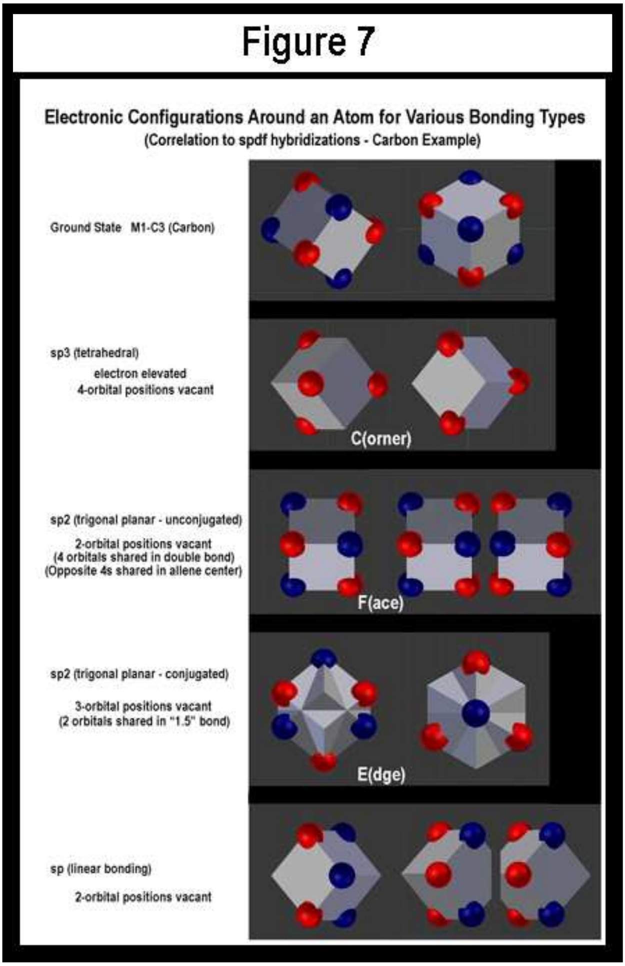


Figure 7

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

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 C_2 in figure 2.

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

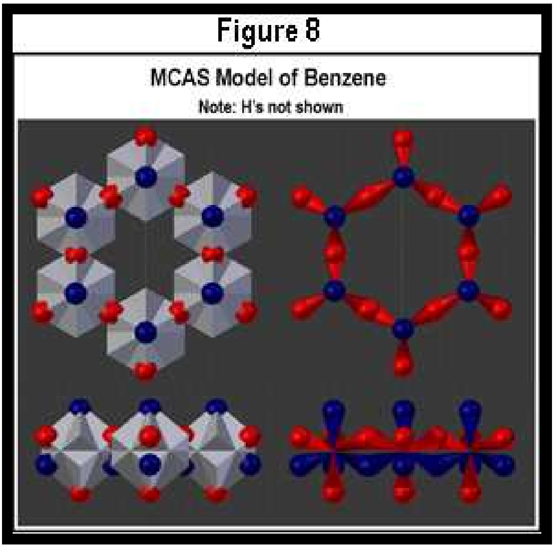


Figure 8

MCAS Model of Benzene

Note: H's not shown

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.

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

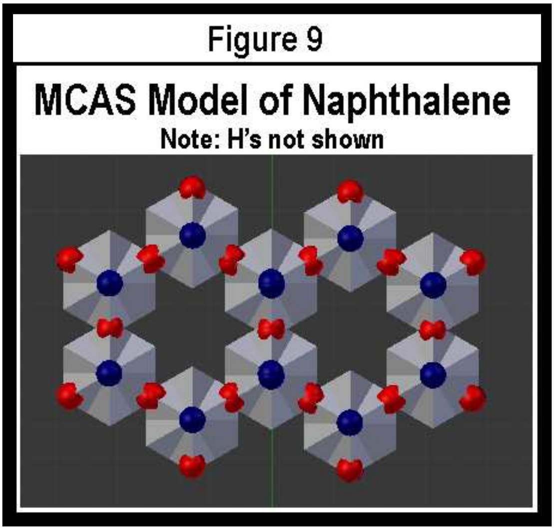


Figure 9

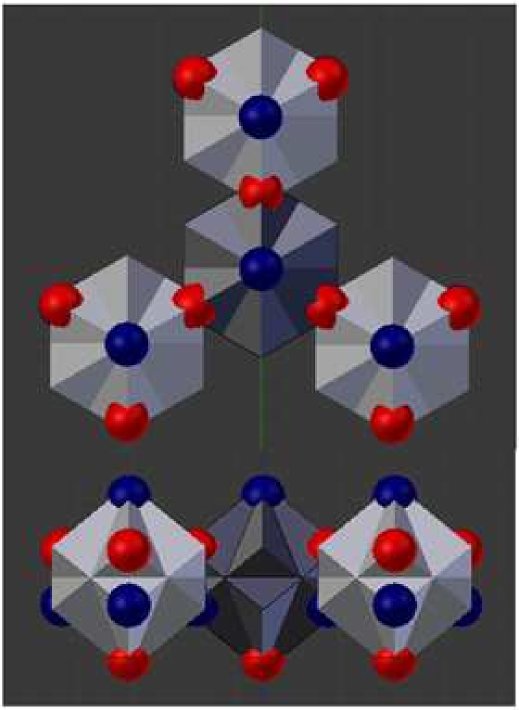
MCAS Model of Naphthalene

Note: H's not shown

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).

Figure 10

MCAS Model for $CO3^{=}$



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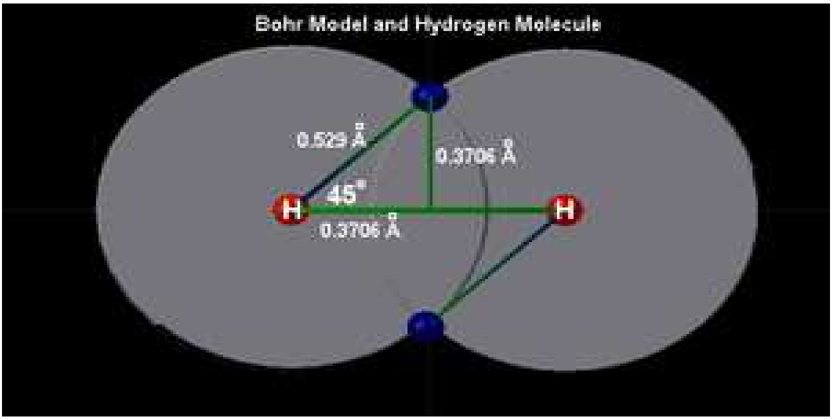
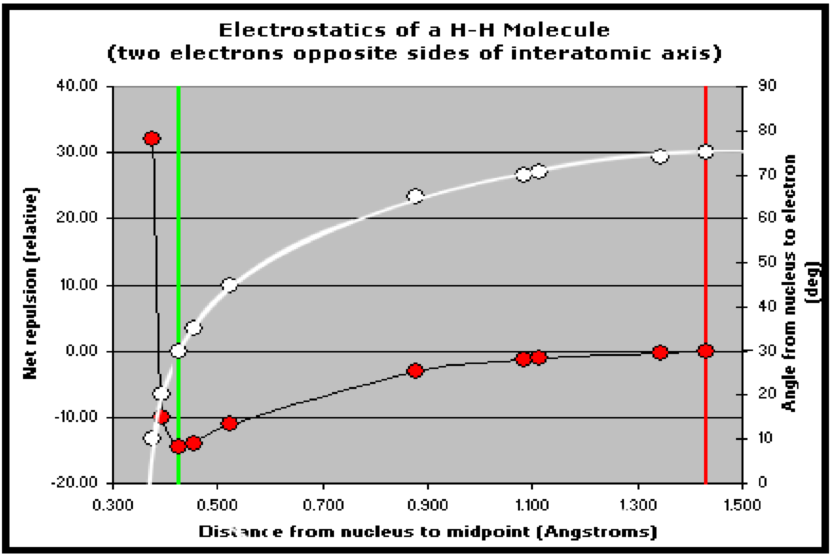
C: The Bohr Model and Electron

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.

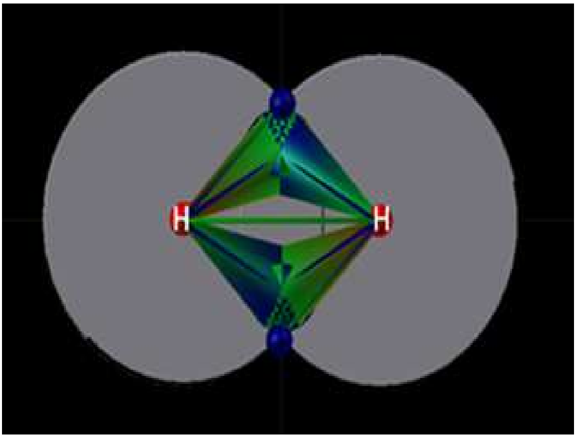
It is interesting to note a few things about Bohr's model before proceeding. The Bohr radius for a hydrogen atom is just what would be expected for a 45-deg angle from the inter-nuclei axis (image below). Newton's cannoneers would concur if the object was to reach the other nucleus with the optimum volley. 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.



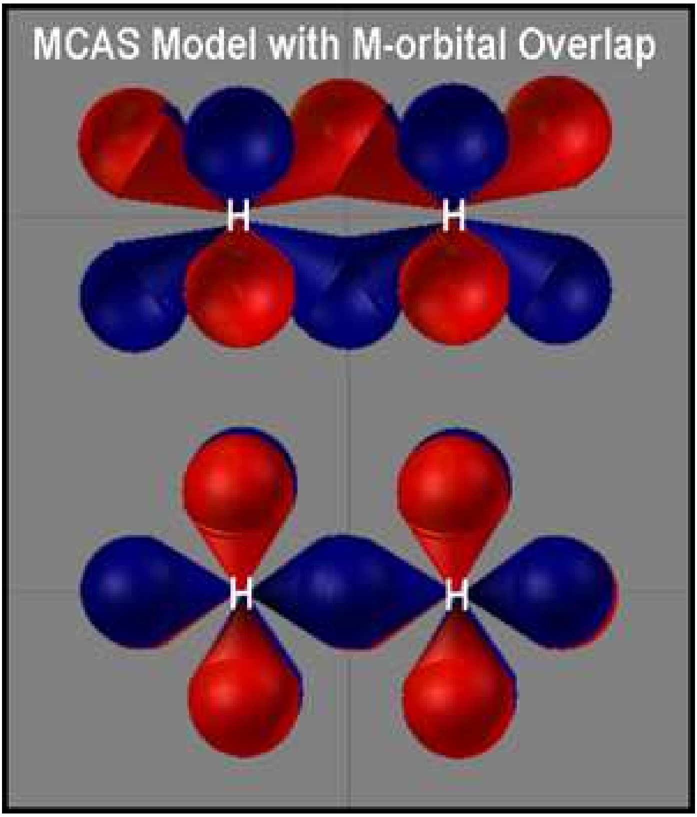
A 45-deg angle is not the optimum volley angle here, however! Unlike cannon-balls, electrons are ‘electrostatically attracted to each nucleus” and “repel one another”. Electrostatic energetics are minimized at the midpoint when the angle is 30-deg (see graph below).



If electrons are to be passed between hydrogen nuclei, then they should be passed at this angle. The image below 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 below. 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.



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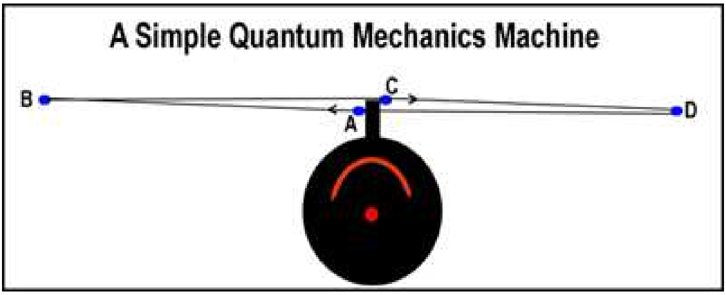
D: Newtonian-derived Quantum Numbers

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.

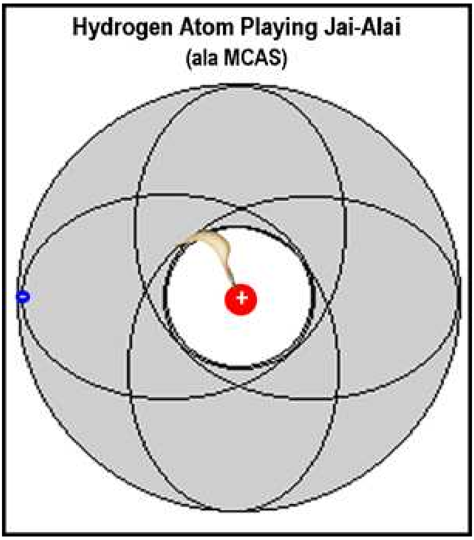
The bat and the ball operate under different parameters/forces, but must arrive at point AC at precisely the same moment.

$V = V_A = V_C = V_o$ + 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

# 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 “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.

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.



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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 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?