Comparing the Logic behind the spdf and MCAS Models

By Joel M Williams (text and images © 2013)

Click here for the html version

Abstract

This essay provides a side-by-side comparison of the currently accepted, quantum mechanical, spdf model and the author's MCAS electron orbital model of atoms. spdf and MCAS refer to the orbital shapes in the two models. The orbital image renditions have been generated with 3D software.

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[1]

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[2], however, what often is required:

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

Max Planck indicates[3] 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.

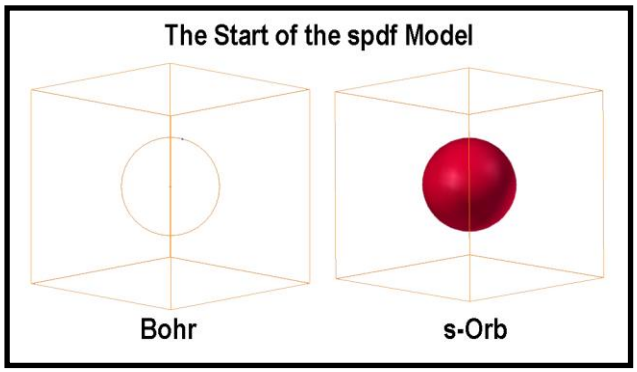
Occam's razor states that **among competing hypotheses, the hypothesis with the fewest assumptions should be selected. In other words, the simplest explanation is usually the correct one[4].**

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 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.

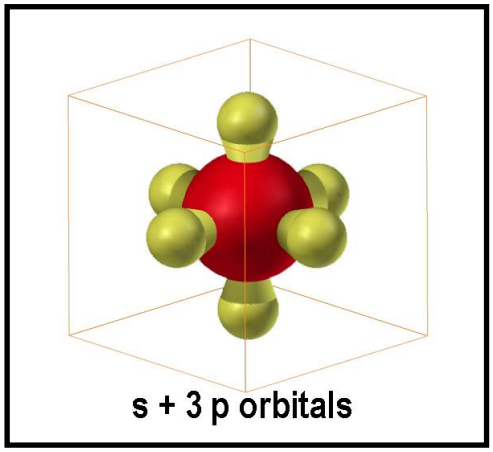


It is at this point that the spdf model was "cast in concrete", as the saying goes. Here, the definition of orbitals was decreed: an orbital contains only 1 or 2 electrons (therein the constant requirement of spin-pairing) regardless of the number of lobes or tori. Orbitals are fixed. That is, there 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.

The MCAS Model

The spdf 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.

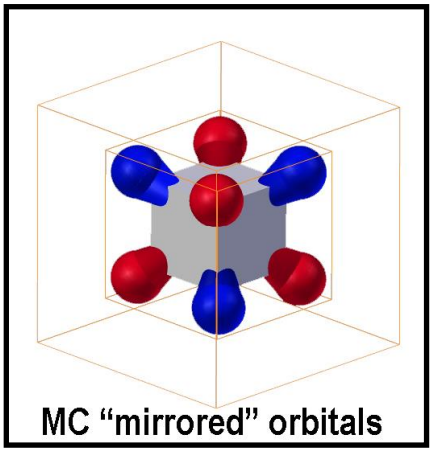


An interesting point here is that, while 2 electrons shared the same spherical, single-lobed space and thus had to be spin-paired[5], two electrons in a p-orbital could occupy opposing orbital lobes and thus be paired without spin-reversal. Reciprocal behavior would serve to "pair" them. Rigid adherence 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 MCAS Model

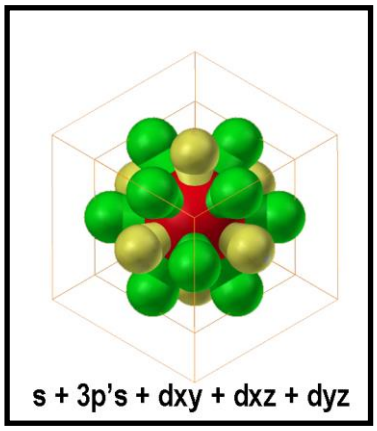
It is now time to introduce an alternative particulate model: the "mirrored orbital" MCAS model.



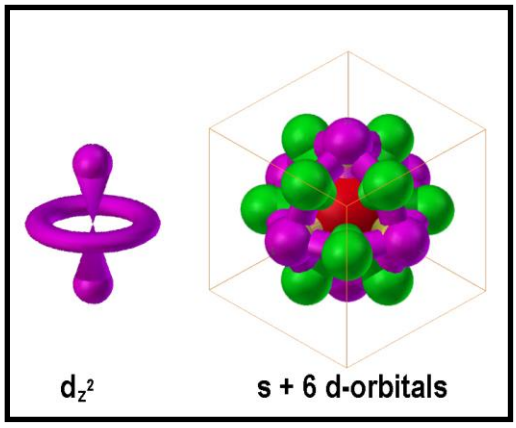
The MC "mirrored" orbital sets provide 8 lobes for the 8 electrons that the s+3p orbitals do. An electron in each of the red and blue sets is equivalent to the s orbital without requiring spin-reversal and cohabitation in a single lobe. When there is only a single electron in a set, it is referred to 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

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.

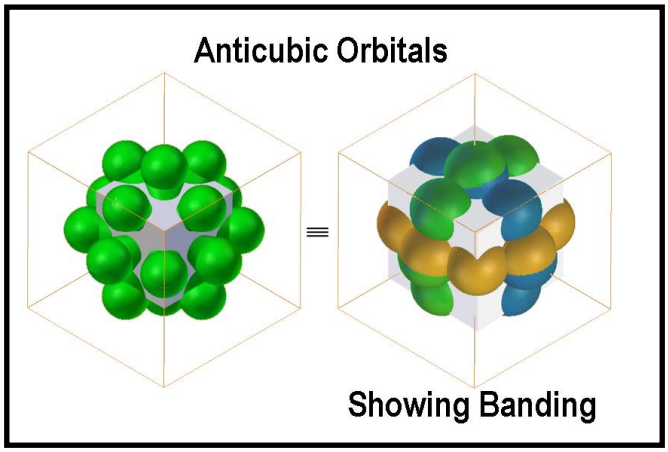


But, alas, the model is not flexible. Thus, the s and p-orbitals must be filled. And, by definition, a d-orbital can only house 2 electrons even with 4 lobes; so 4 electrons still need space The extra orbitals needed are provided with a new orbital shape. Enter d_{x^2}, d_{y^2} and d_{z^2} orbitals with torus belts. These orbitals smother the p-orbitals, placing 4 electrons in the same general space. But the orbital distribution is nicely symmetrical.



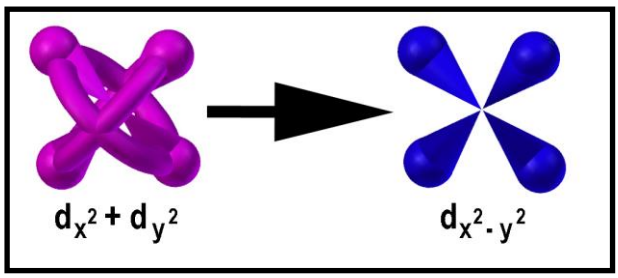
The MCAS Model

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.

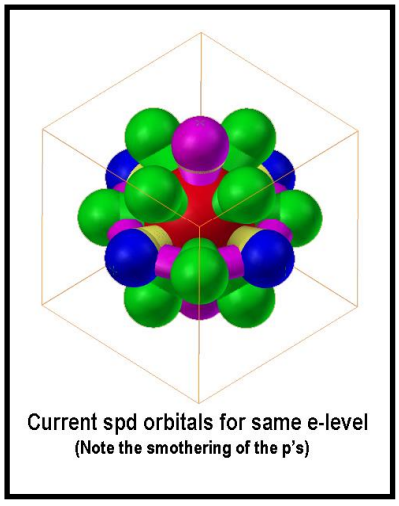


The spdf Model

Of course, only 2 more orbitals are needed. Thus, 2 are declared "mathematically



equivalent" and combined.
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.

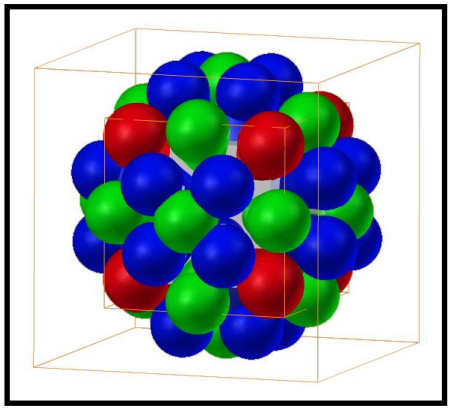

Current spd orbitals for same e-level
(Note the smothering of the p's)

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 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.

REFERENCES

[1] Sigma Xi SmartBrief, July 3, 2013
[2] John Dewey, The Quest for Certainty: A Study of the Relation of Knowledge and Action, 1929, republished April 30th 2005 by Kessinger Publishing
[3] Max Planck, Scientific Autobiography and Other Papers, 1950
[4] http://en.wikipedia.org/wiki/Occam's_razor
[5] 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