

Creating the Familiar Periodic Table via Electron Orbital Filling

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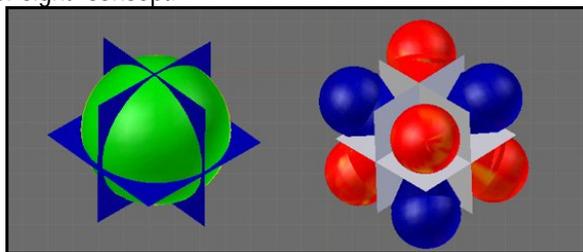
Abstract

While the periodic table arrangement is usefully interpreted in columns of similar behavior, it is erroneous to imply that the underlying orbitals are the same for all the elements in each column of a block. It is important to understand that much of the 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 configurations of the elements. Octahedral, square-planar, and pyramidal coordination complexes of the transition elements follow logically without the need of hybridizing. This brief paper describes a rational packing of electrons around an atomic nucleus that ends up mimicking the familiar extended periodic table when compressed to similar behavior.

Electron Orbitals and the Aufbau of the Elements

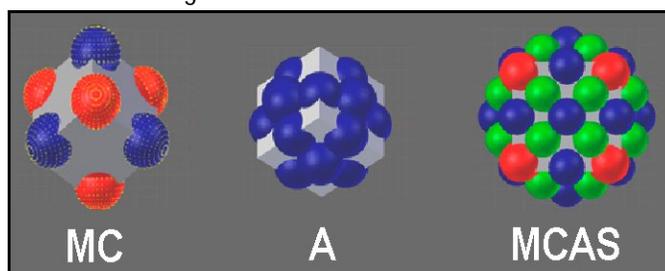
The currently accepted electron orbital structure of atoms is a concession to Bohr's circular orb. To this orb-turned-sphere, the modelers added 3 more orbitals, then 5 more, and then 7 more of various shapes. Explanations of everything related to the electron behavior of atoms have been forced to fit 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 , sp^3 , etc. etc. There was no looking back for models that needed less massaging to explain reality. Embellished for a century, it is too engrained to be considered challengeable; too much theory would need to be rethought.

From the viewpoint of chemistry, G.N. Lewis' "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 below shows how non-intersecting orbital spaces can arise by utilizing the "rule of eight" concept.



As seen in the image to the right, there can be two symmetrical and opposed 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) or "hybridizing". Unlike Bohr's orbs which are scaled to fit observed spectral data, but have no other rationale, an electron in a 4-lobed-orbital scales according to simple classical physics motion and electrostatics to produce the observed spectral data.¹

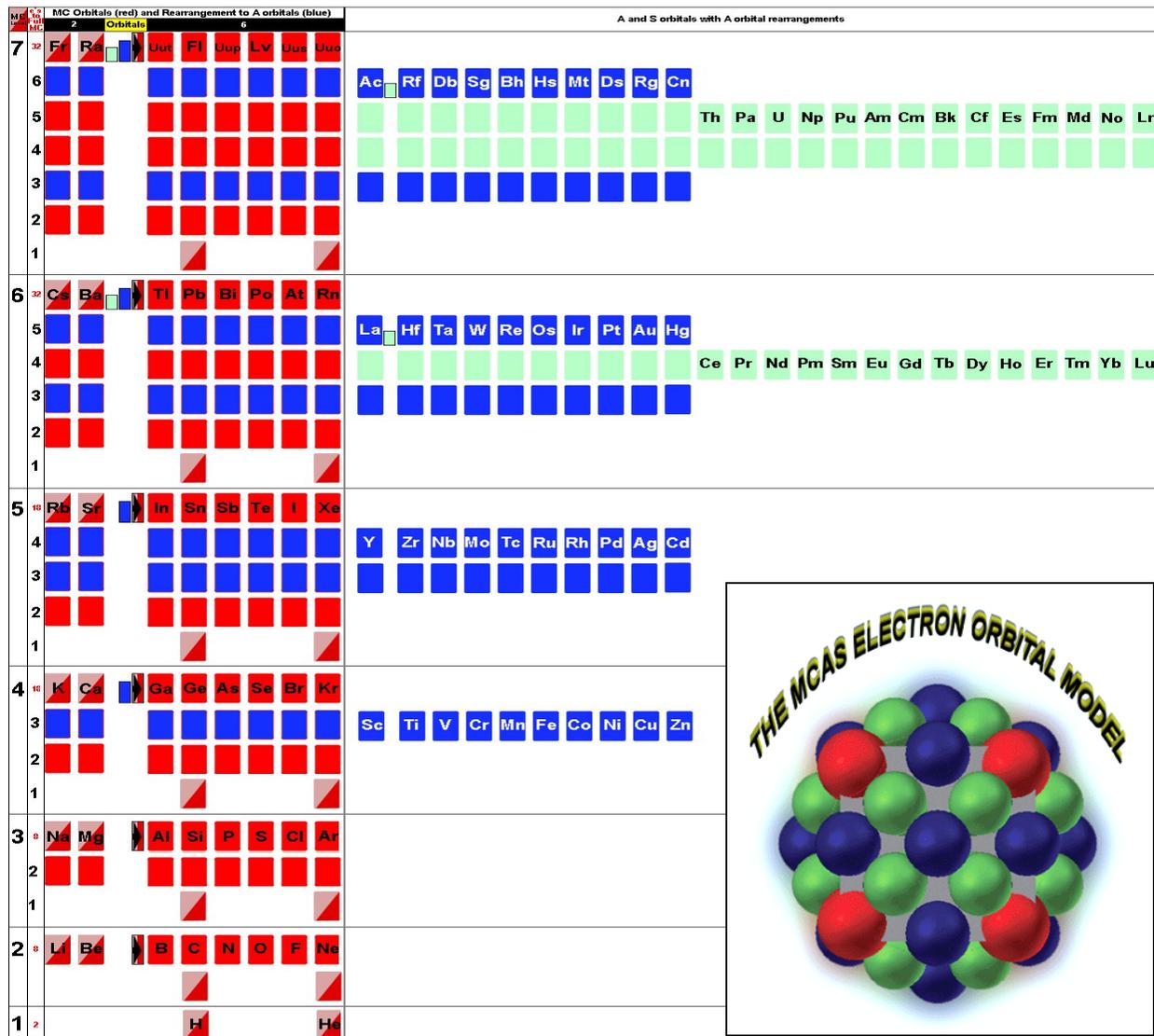
When electrons are too numerous for two quartets (8 total lobes), other orbital space can be used. Simplicity would have the next order of orbitals distributed uniformly amongst the 8 occupied lobes. Simplicity would also have the electrons occupying orbital space not too dissimilar in shape. This is 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 below.



¹ Why do Electrons (Orbitals) Have Discrete Quantum Numbers?, <http://vixra.org/abs/1210.0133>, Joel M Williams

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**q-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.

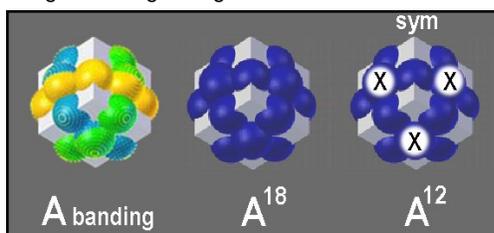
The image below demonstrates how the elements are formed via the **MCAS** model starting with the smallest, **H**(ydrogen) at the bottom and building electron numbers upwards. The unlabeled orbitals below indicated elements are those when all the **C**-orbitals of a period are filled to create the "inert" 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. 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.

- Electron filling at the 3rd period follows the scheme of the 2nd. Again the orbitals to be filled are the two 4-lobed Cubic orbital sets; electron movement is opposite that of those in the 2nd level whose orbital spaces are filled symmetrically (C⁴C⁴). This contrasts with the current spdf model that has two different types.
- At the 4th period, two electrons can be placed opposite one another in the two 4-lobed Cubic orbital sets. Additional electrons, however, can be accommodated in Anticubic orbitals more favorably than adding them to the remaining Cubic orbitals. The image below should help in understanding the filling that gives the “transition series” its properties.



The Anticubic arrangement bands the Cubic 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 higher level Cubic lobes are filled, 8 electrons must be obtained from elsewhere. These are provided by what would have been the previous Cubic electrons of the same level. Favorable energetics is derived when the Anticubic lobes are filled symmetrically: A¹⁸ (completely) and A¹² (face-deficient). The Anticubic 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-Madelung².

Orbital Filling of Transition Elements – spdf vs MCAS			
Scandium	4s ² 3d ¹ 4M ² /3(C8A1)	Yttrium	5s ² 4d ¹ 5M ² /4(C8A1)
Titanium	4s ² 3d ² 4M ² /3(C8A2)	Zirconium	5s ² 4d ² 5M ² /4(C8A2)
Vanadium	4s ² 3d ³ 4M ² /3(C8A3)	Niobium	5s ¹ 4d ⁴ (??) 5M ¹ /4(C8A3)
Chromium	4s ¹ 3d ⁵ 4M ¹ /3A ¹²	Molybdenum	5s ¹ 4d ⁵ 5M ¹ /4A ¹²
Manganese	4s ² 3d ⁵ 4M ² /3A ¹³	Technetium	5s ² 4d ⁵ 5M ² /4A ¹³
Iron	4s ² 3d ⁶ 4M ² /3A ¹⁴	Ruthenium	5s ¹ 4d ⁷ (??) 5M ¹ /4A ¹⁴
Cobalt	4s ² 3d ⁷ 4M ² /3A ¹⁵	Rhodium	5s ¹ 4d ⁸ (??) 5M ¹ /4A ¹⁵
Nickel	4s ² 3d ⁸ 4M ² /3A ¹⁶ (4M ⁰ /3A ¹⁸)	Palladium	5s ⁰ 4d ¹⁰ 5M ⁰ /4A ¹⁸
Copper	4s ¹ 3d ¹⁰ 4M ¹ /3A ¹⁸	Silver	5s ¹ 4d ¹⁰ 5M ¹ /4A ¹⁸
Zinc	4s ² 3d ¹⁰ 4M ² /3A ¹⁸	Cadmium	5s ² 4d ¹⁰ 5M ² /4A ¹⁸
		Lutetium	6s ² 5d ¹ 6M ² /5(C8A1)
		Hafnium	6s ² 5d ² 6M ² /5(C8A2)
		Tantalum	6s ² 5d ³ 6M ² /5(C8A3)
		Tungsten	6s ² 5d ⁴ (??) 6M ² /5A ¹²
		Rhenium	6s ² 5d ⁵ 6M ² /5A ¹³
		Osmium	6s ² 5d ⁶ 6M ² /5A ¹⁴
		Iridium	6s ² 5d ⁷ 6M ² /5A ¹⁵
		Platinum	6s ¹ 5d ⁹ (??) 4M ² /3A ¹⁶
		Gold	6s ¹ 5d ¹⁰ 6M ¹ /5A ¹⁸
		Mercury	6s ² 5d ¹⁰ 6M ² /5A ¹⁸

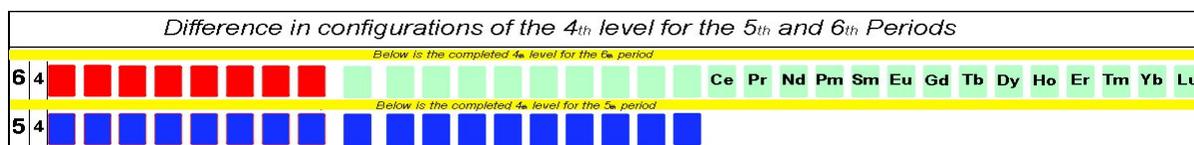
For the transition elements of the 4 period, the A-orbital filling with the MCAS model is fairly straight forward. Unlike the spdf model, where the only way to have 6-unpaired electrons is to shift a 4-s to a 3-d orbital, the MCAS filling is normal to a symmetrical A¹². The symmetrical A¹² has one electron 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 the now vacant C-orbital. Copper does not follow the pattern as completing the Anticubic 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 Cubic sets occupied! These elements are also unique in having fully occupied sub layers. The MCAS Cubic orbitals of Cu, Ag, and Au provide a DONOR-RECEPTOR (one electron in a high-energy orbital and a vacant tetrahedral orbital hole) network that is unrivaled. They, thus, conduct electricity (flowing electrons) nicely.

² http://en.wikipedia.org/wiki/Electron_configuration

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" being of higher energy than others 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.

- The transition elements of the 5th period have their 4th level Anticubic orbitals overlaying those of the filled 3rd level Anticubic 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 A12 and A18 symmetry drivers holding (Molybdenum and Silver). Palladium also has the A18 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.
- The transition elements of the 6th period have their 5th level Anticubic orbitals overlaying those of the filled 3rd level Anticubic orbitals, but with a greater level (energy) separation than that in the 5th period. The aufbau is, thus, more similar to that of the 4th period. The electrons in the 4th level Anticubic 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 Anticubic orbitals can load asymmetrically, although it appears this rarely happens.

When more electrons must be managed than the Anticubic 18 orbitals can handle, another arrangement of the electrons is necessary. After the 5th Anticubic level is begun in the 6th period, electrons are then added to the 4th level. Now, however, unlike the 18-lobes of the Anticubic 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.



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

With the electron packing around the nuclei described, it is time to show how all of this information is compressed into the "uncluttered" and familiar periodic table.

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 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.

