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Atomic Orbitals: Explained with Classical Mechanics

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Summary

Physics separates the study of motion into two branches based on the size of an object in motion: classical mechanics for objects typically larger than an atom and quantum mechanics for atoms and subatomic particles. Quantum mechanics surfaced, in part, to solve the failure of classical mechanics' explanation of the electron and its atomic orbital. Early attempts to explain the electron's motion using classical methods failed because of assumptions that the electron orbits an atomic nucleus similar to a planet orbiting the Sun.

When revisiting the structure of the proton in terms of a five-quark structure known as the pentaquark, found in recent proton collision experiments, it is possible to model the electron's orbital distance, ionization energy and shape based on classical mechanics. In a branch of classical mechanics known as statics, an object is at rest where the point of the resultant forces is equal, otherwise known as the point where the sum of forces is zero. This paper accurately models the electron's orbital distance in an atom based on a pentaquark structure of the proton in which the orbiting electron is both attracted by an anti-quark and repelled by quarks in the proton.

The calculations precisely describe the location of a single electron around a single proton (hydrogen). The Bohr radius and the probability cloud of the electron is explained for hydrogen. Then, an energy value is calculated for a photon that is absorbed to ionize the electron. Finally, the equations in this paper are expanded to calculate the orbital distances and ionization energies for the first 20 elements from hydrogen to calcium.

Two methods were used to compare the results. The first method compares the calculated results with measured atomic orbital distances. The second method uses ionization energies, which are more precise measurements than distance measurements. The calculated results from both methods are charted against measured results from experiments.

Using this new model of the proton, a logical explanation is provided for the quantum jumps of an electron based on a change in the repelling force that is modified due to the alignment of protons in a nucleus for different atomic elements. Two sections of this paper are dedicated to the proposed proton alignment that explains various orbital distances, energy levels, shapes and the periodic sequence seen in elements.

This paper was originally published as Atomic Orbitals: Explained and Derived by Energy Wave Equations in 2019.¹ It has been updated to simplify the calculations of atomic orbital distances and energies using only classical equations and constants. The methods, however, remain the same as the original paper.

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1. Atomic Orbitals – Summary of Calculations

The paper provides the framework for the calculation of the electron's position in the atom, and its associated energy levels, using only classical mechanics. It removes the need to have a separate set of quantum rules and equations for the electron's behavior.

The classical explanation of the electron's position in an atomic orbit is that it is being pulled and pushed at the same time – pulled by a spherical, attractive force and pushed by an axial, repulsive force. The Bohr model assumes that there is only an attractive charge in the atom's nucleus similar to the gravitational pull of the Sun. When this assumption is revisited to consider an attractive *and* repulsive force, it is possible to:

- 1) Calculate the distances of each orbital
- 2) Calculate the energy levels of each orbital
- 3) Explain the probability cloud and behavior of the electron in an orbital

The details of the equations and their derivations to arrive at orbital distances are provided in Section 2. First, the results are summarized in Fig. 1.1 to illustrate initial proof of this revised model of the atom. In this chart, the value that is determined using classical equations is compared to the measured or calculated value for the first twenty elements – hydrogen to calcium.²

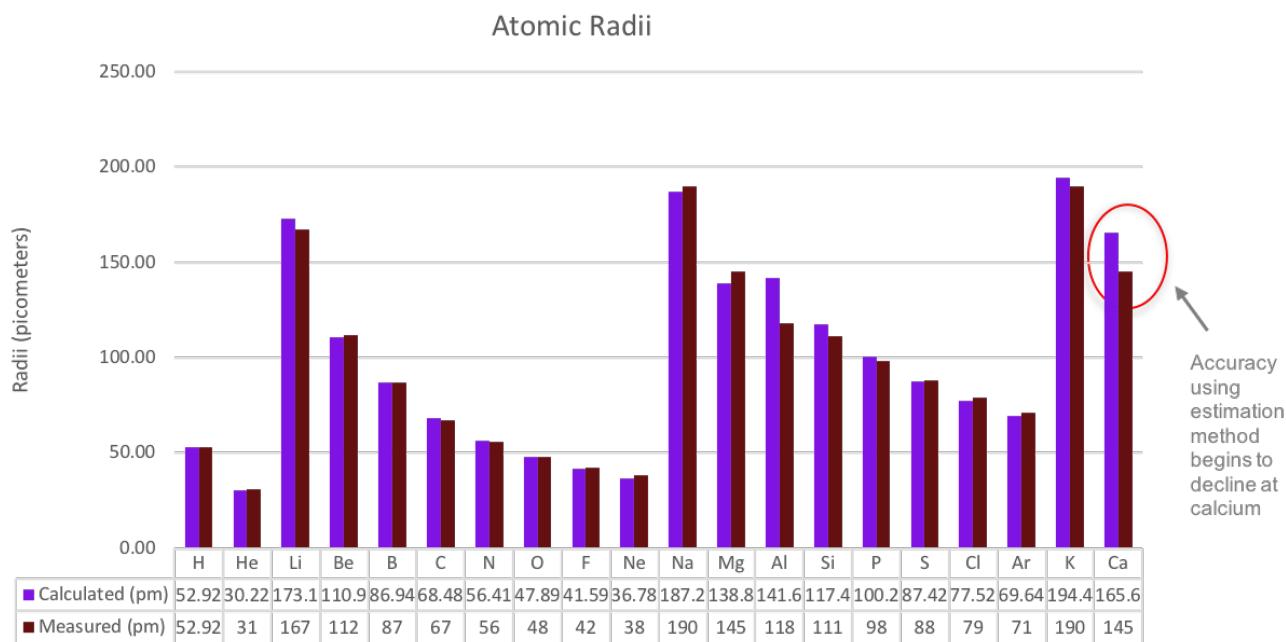


Fig 1.1 – Atomic orbital distances

There are some variations due to two reasons: 1) the measurement of atoms from some experiments may not be precise, and 2) the angles of electrons were estimated and solved using Mathcad and the method begins to decline as the number of electrons in orbit increases or the distance to the nucleus decreases. This will be further explained in Section 2.

Fig 1.1 would not have been sufficient proof alone as it only calculated and compared the largest orbital distance for 20 elements. However, orbital distances were calculated using this classical method for all of the subshells in an atom (1s, 2s, 2p, 3s, 3p, 4s) and also for ionized elements through calcium. Since experimental evidence of orbital distances

for these subshells do not exist, they can be compared to ionization energies instead. Ionization energies depend on an electron's distance from the nucleus.

Section 2 provides the derivations and equations for ionization energies using the orbital distances that are calculated using wave equations. Similar to above, the results are being presented first in this section to show the accuracy of the method. In Fig. 1.2, the measured ionization energies of the first ten neutral elements are compared to calculated results.³ The measured results are the photon energies that are required to ionize an electron in the outermost orbital.

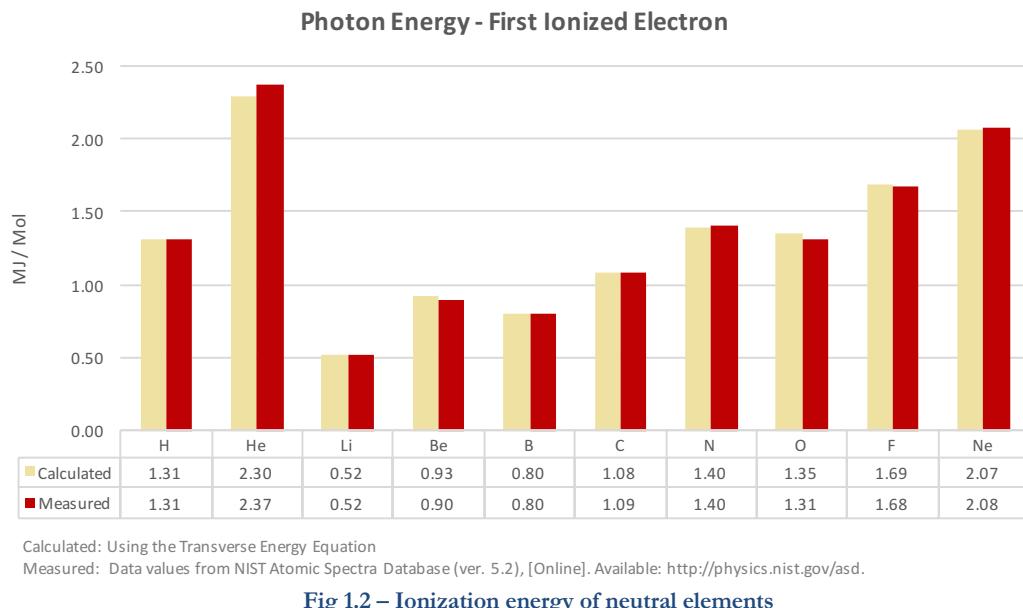


Fig 1.2 – Ionization energy of neutral elements

While Fig. 1.2 shows the ionization energy of the first electron (outermost orbital), the calculations can also be performed for electrons in any orbital. Fig 1.3 shows the ionization energy of the electron in the closest orbital to the nucleus (1s) and is compared to results from spectroscopy experiments.

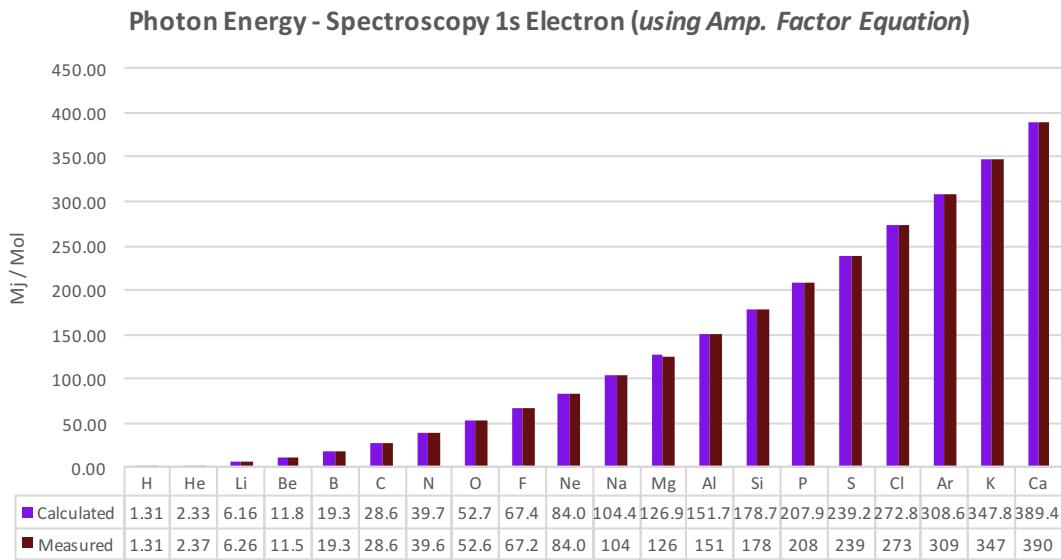


Fig 1.3 – Ionization energy of 1s electron of neutral elements (Spectroscopy). Uses Amplitude Factor Equation – 1s Orbital.

Orbital distances were also calculated for ionized elements. Because the classical explanation of atomic orbitals is based on the interaction of each and every electron on other electrons, in addition to the nucleus, they have been grouped into atoms with a similar electron structure. For example, Fig. 1.4 lists the ionized elements with only one electron in orbit ($1s^1$). This is the simplest arrangement as the only force on the electron is from the nucleus. For helium, it is $He1+$. For heavily ionized calcium, it is $Ca19+$. In Fig 1.4, the calculated orbital distances and ionization energies agree with the measured results.

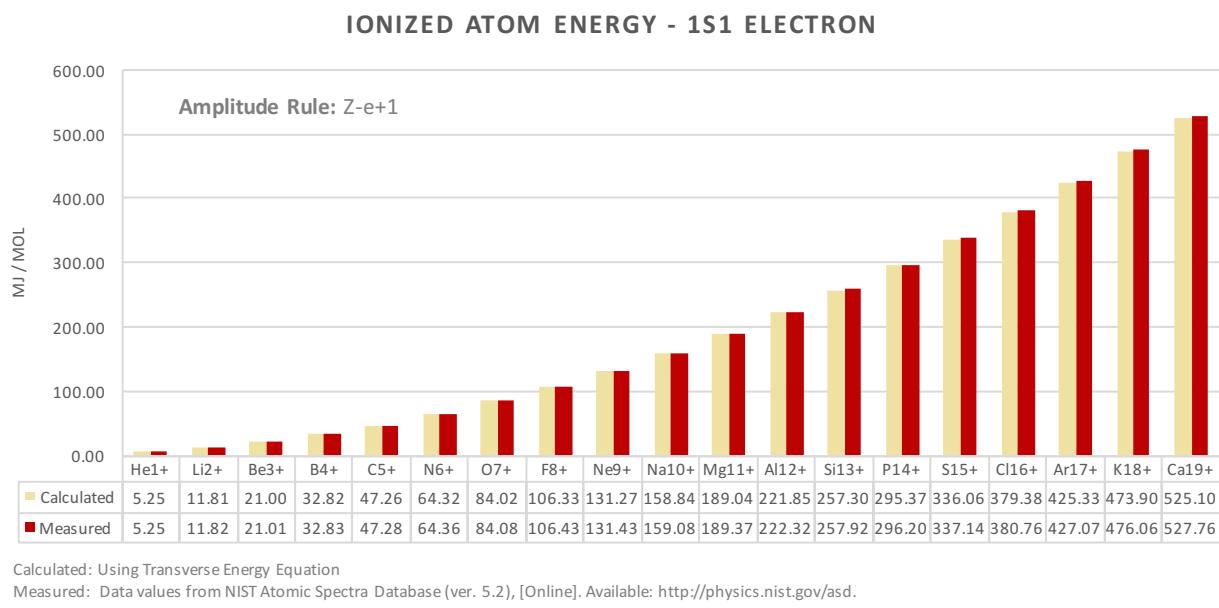


Fig 1.4 – Ionization energy of ionized elements with 1 electron

Fig 1.5 shows the next simplest configuration of electrons, with two electrons in orbit ($1s^2$). Again, the results agree, but show slight deviation as the elements become more complex and have more protons in the nucleus.

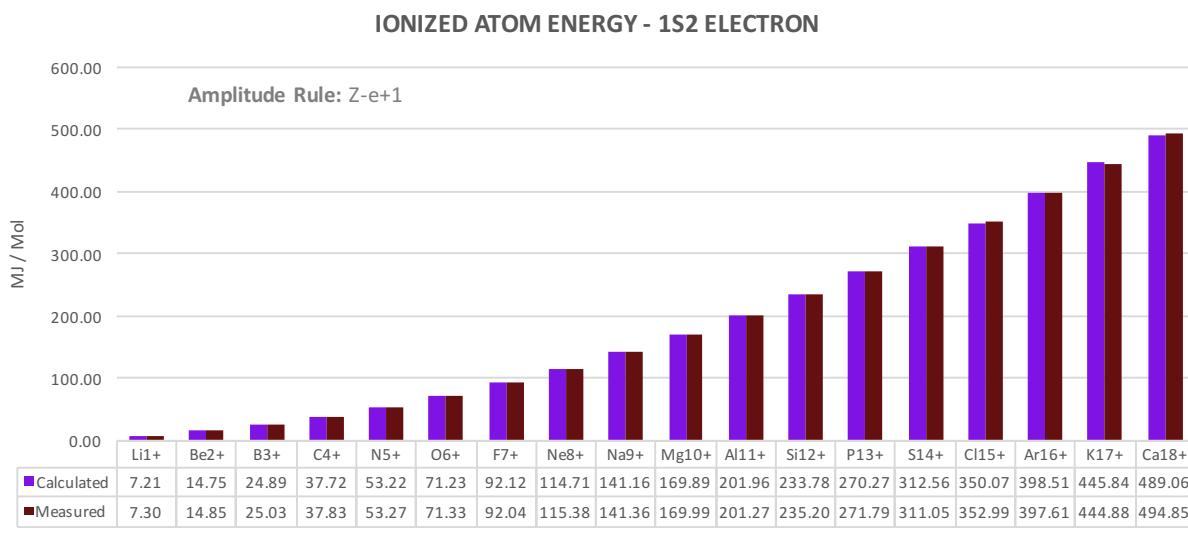


Fig 1.5 – Ionization energy of ionized elements with 2 electrons

Finally, in Fig. 1.6, the ionization energies for the second orbital (from $2s^1$ to $2p^6$) are provided. They are shown in summary form in this figure, but **Appendix C includes the details for each of these charts**. By $2p^6$, the electron angle estimation begins to show further deviation, which will be explained in further detail in Section 2.

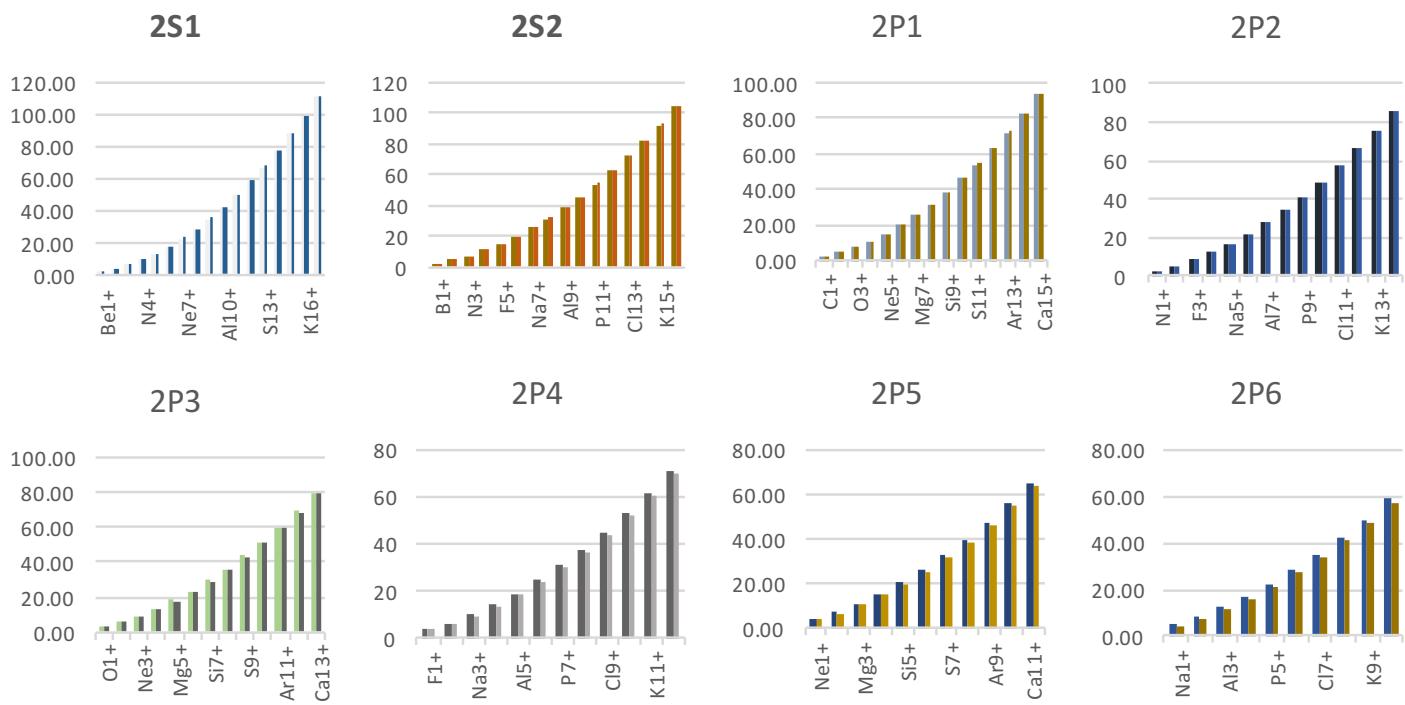


Fig 1.6 – Ionization energy of ionized elements with 3 to 10 electrons

In total, more than 450 calculations were performed for varying atomic configurations of electrons in orbitals for neutral and ionized elements from hydrogen to calcium. And more than 150 calculations were performed for ionization energies for the same atoms. A summary of all calculations results and their comparisons against measurements have been placed in the Appendix of this paper. The calculations agree with measured results. When there are deviations, there is a noticeable trend that appears as elements become more complex with increasing electrons and shorter distances to the nucleus. With greater accuracy in computer modeling of electron angles, it is expected that these deviations should disappear.

In addition to orbital calculations and ionization energies, an explanation is provided for orbital shapes in Section 3. Orbital shapes are attributed to a tetrahedral nucleus structure and an arrangement of protons that cause a greater repulsion factor when protons and spins are aligned. This same tetrahedral structure is then expanded upon in Section 4 to explain the sequence of the Periodic Table of Elements.

1.1. Constants and Variables

Constants and Variables

The following are the constants and variables used in this paper:

Symbol	Definition	Value (units)
Constants		
E_e	Electron energy (rest)	8.1871×10^{-14} ($\text{kg m}^2/\text{s}^2$)
r_e	Electron radius (classical)	2.8179×10^{-15} (m)
a_0	Bohr radius	5.2918×10^{-11} (m)
α_e	Fine structure constant	0.00729735 (dimensionless)
N_A	Avogadro's number	6.0221×10^{23} (dimensionless)
Variables		
Z	Proton count	variable - dimensionless
e	Electron count	variable - dimensionless
Q	Particle count	variable - dimensionless
δ	Amplitude factor	variable - dimensionless

Table 1.1.1 – Constants and Variables

Q and δ

This paper introduces two variables not common in classical equations. Q is used for the number of protons and electrons, sometimes only in alignment. δ is used to calculate constructive and destructive wave interference, as a measurement of wave amplitude relative to a stable particle system. Both variables are described in more detail later in this paper.

2. Orbital Distances and Energies

This section provides the derivation of classical equations to calculate the orbital distances and ionization energies of elements from hydrogen to calcium that were graphed and compared against measured results in Section 1.

2.1. Orbital Force Equation

For more than a century, the Bohr model has explained the atom as a collection of electrons orbiting around an atomic nucleus, similar to planets in the solar system circling the Sun.⁴ In fact, this is why they continue to be called “atomic orbitals”. This presumes that the electron has a specific velocity that allows it to stay in orbit, without being pulled into the nucleus. However, this model fails to explain the quantum jumps of the electron or the probability cloud that is found in experiments. The electron does not take a predictable path around the nucleus like the Earth takes around the Sun. This, amongst other observations, led to a separate branch of science to predict the behavior of subatomic particles known as quantum mechanics.⁵ Strangely, the world of particles seems to behave under a different set of rules for objects that are larger than an atom.

In Section 1, an introductory explanation of the electron’s orbital distance was described as a nucleus that has both a spherical, attractive force and an axial, repulsive force. The electron is being both pushed and pulled by a proton and the orbital is the point where the sum of the forces on the electron is zero.

This explanation requires a model of the proton that is consistent with the recently discovered pentaquark model of the proton at CERN, which includes four quarks and one anti-quark.⁶

Attractive Force

In Fig 2.1.1, a proton is described with an anti-quark in the center of four tetrahedral quarks. The anti-quark has an attractive force on a nearby electron. This is a standard Coulomb electric force (F_1) that is spherical and decreases with the square of distance, very similar to a positron-electron relationship which is attractive due to destructive, longitudinal wave interference between two particles.

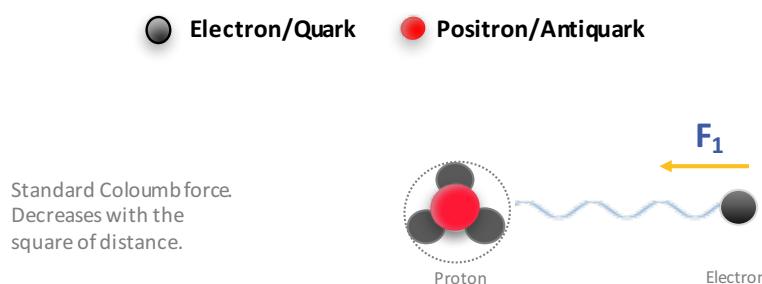


Fig 2.1.1 – Attractive force of proton and electron

Repelling Force

The tetrahedral quarks in the proton are bound by an attractive, strong force known as gluons within the proton. The force is only attractive within the standing wave structure of the proton where quarks are placed at nodes on standing waves. Beyond the standing wave structure, it is a repulsive force on an orbiting electron. Like a dipole magnet, it

can be thought of as a declining, strong force, which is axial and declines with the cube of distance. This force (F_2) is illustrated in Figure 2.1.2.

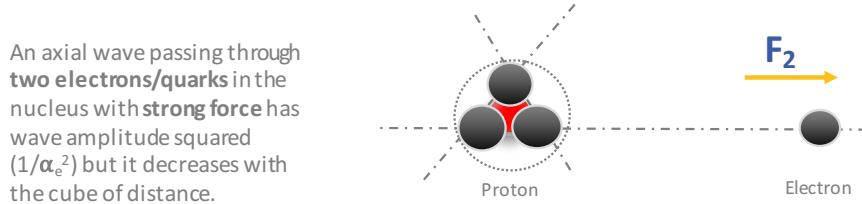


Fig 2.1.2 – Repelling force between proton and electron

For a single proton and electron, the attractive force can be calculated at various distances as a decline of energy (wave amplitude), based on the electron's energy (E_e), and then declining proportionally from the electron's radius (r_e) to the distance being measured (r). And the repelling force is calculated as the electron's energy, passing through two wave transformations (two quarks in alignment) of the strong force, increasing in wave amplitude along the axis proportional to the fine structure constant (α_e). Thus, these classical terms for electron energy, electron radius and fine structure constant will appear throughout this paper describing these forces classically. Ultimately, they are derived in their true form, later in the paper, as wave constants. The details of these classical forms and equations are found in the *Forces* paper.

The decline of wave amplitude from the proton's core of the attractive wave (blue) and the repulsive wave (green) are calculated and graphed below in Fig. 2.1.3. At the Bohr radius, the square of wave amplitude from both waves are equal.

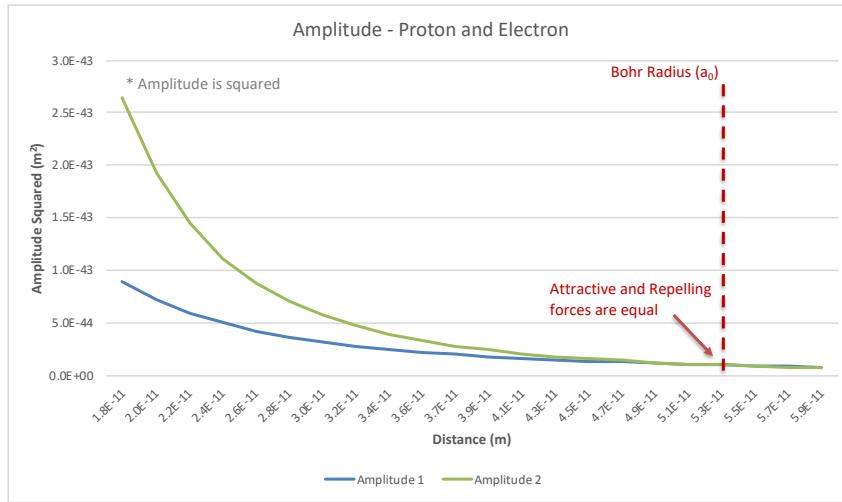


Fig 2.1.3 – Amplitude is equal at the Bohr radius for the attractive and repelling forces

Bohr Radius

The orbital distance of a single proton and electron is known as the Bohr radius.⁷ This is the orbital distance for hydrogen. The following is the derivation in **classical terms**. To simplify equations that will be used to set attractive and repulsive forces to be equal, the electric force, strong force and orbital force equations are written in terms of the electron's energy (E_e) and classical radius (r_e), by using a particle count (Q) instead of charge (q). This representation of the electric (Coulomb) force, the strong force and the orbital force are:

$$F_e = E_e \frac{Q_1 r_e Q_2}{r} \quad (2.1.1)$$

Electric force – classical form

$$F_s = E_e \frac{Q_1 r_e Q_2}{\alpha_e r} \quad (2.1.2)$$

Strong force – classical form

$$F_o = E_e \frac{Q_3 r_e Q_4 r_e Q_2}{\alpha_e r \alpha_e r r} \quad (2.1.3)$$

Orbital force – classical form

The electric force is the Coulomb force, declining at the square of distance. The strong force is known to be stronger, relative to the electric force, at the inverse of the fine structure constant. The orbital force is not a known force in modern physics and requires further explanation in this paper. The orbital force is an axial force as the wave passes through two quarks before reaching an electron. Each quark experiences an increased wave amplitude seen in the strong force, which is the fine structure constant ($1/\alpha_e$), but it is the square of the strong force before declining with the cube of distance. This is similar to static dipole magnets that also decline with the cube of distance.

The variable Q used in these equations is a count of particles and is dimensionless, as opposed to a variable with units of charge. For the electric force, the effect is the same as charge is based on the number of particles. However, for particles that need to be in alignment to determine the force, such as the strong force between two quarks and the proposed orbital force, Q is also used as a particle count when in alignment. Q_3 and Q_4 are the particle counts of quarks in alignment on an axis in the direction of the electron (Q_2). This is expressed mathematically in Eq. 2.1.3, and now visually in the figure below.

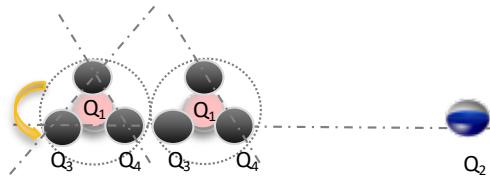


Fig 2.1.4 – Components of the orbital force

A short summary of these particle counts (Q):

- Q_1 – Number of protons in the atom for the spherical attractive force. It is the proton count (Z) in an atom.
- Q_2 – Number of electrons. Since only one electron is calculated for ionization, $Q_2=1$ in all cases in this paper.
- Q_3 and Q_4 – Number of “quarks” per proton in alignment. $Q_3=Q_4$ in all cases. It is the principal quantum number (n), but the variable n is not used in wave equations due to n being used for wavelength counts.

Because Q_2 is always one, and Q_1 in the case of an atom is the proton count (Z), for the purposes of this paper, the electric force can be reduced to a shorthand notation below. Because there will eventually be many different forces in an atom from surrounding electrons, the forces will have a numbering sequence. F_1 will be assigned to the attractive force.

$$F_1 = F_e = E_e r_e \left(\frac{Z}{r^2} \right) \quad (2.1.4)$$

Electric force – shorthand

And because Q_3 and Q_4 are always equal, it is Q^2 . It is simplified to just Q^2 for shorthand, where Q is the number of protons in alignment (i.e. the principal quantum number). Again, Q_2 is always one, so the orbital force can be reduced to a shorthand notation below. F_2 will be assigned to the orbital force.

$$F_2 = F_o = \frac{E_e r_e^2}{a_e^2} \left(\frac{Q^2}{r^3} \right) \quad (2.1.5)$$

Orbital force – shorthand

The calculation of any electron distance in any atomic configuration will be the location where the **sum of all forces is zero**, expressed in the next equation, where x is a numerical value given to distinguish each force such as F_1 and F_2 above, and y is the total number of forces acting on the electron being measured.

$$\sum_{x=1}^y F_x = 0 \quad (2.1.6)$$

Orbital distance – Sum of forces is zero

The Bohr radius is the simplest electron location to derive because it has a single proton and electron and thus only two forces to calculate. This is the location where the electron settles into position – when along the axis of proton alignment as illustrated in Fig. 2.1.2.

$$F_1 + F_2 = 0 \quad (2.1.7)$$

Substituting Eqs. 2.1.4 and 2.1.5 into Eq. 2.1.7 and then simplify.

$$E_e r_e \left(\frac{Z}{r^2} \right) + \frac{E_e r_e^2}{a_e^2} \left(\frac{Q^2}{r^3} \right) = 0 \quad (2.1.8)$$

The variables in this equation for a single proton and electron are $Z=1$ and $Q=1$. There is only one proton in hydrogen, so it has Z number of 1. And there is only one proton in alignment along an axis. Substituting these variables into Eq. 2.1.8 and then solving for distance (r) yields the Bohr radius (a_0).

- $Z = 1$
- $Q = 1$

$$E_e r_e \left(\frac{(1)}{r^2} \right) + \frac{E_e r_e^2}{a_e^2} \left(\frac{(1)^2}{r^3} \right) = 0 \quad (2.1.9)$$

$$\frac{E_e r_e^2}{\alpha_e^2} \left(\frac{1}{r^3} \right) = E_e r_e \left(\frac{1}{r^2} \right) \quad (2.1.10)$$

$$a_0 = r = \frac{r_e}{\alpha_e^2} = 5.2918 \cdot 10^{-11} \text{ (m)} \quad (2.1.11)$$

Bohr radius

After solving for r in Eq. 2.1.11, it is found to be the **Bohr radius** ($a_0 = 5.2918 \times 10^{-11}$ meters).⁸

Electric Force and Energy – Electron energy and radius form

Eq. 2.1.1 is rewritten for the more familiar Coulomb's law, as it generates the same results. But whereas the electron energy (E_e) and radius (r_e) are the constants in the equation below, they are not equivalent to Coulomb's constant (k) because the Q is a count of particles, not a charge. Yet the force results are the same when using Eq. 2.1.14 and comparing it to Coulomb's equation.

$$F_e = E_e r_e \left(\frac{Q_1 Q_2}{r^2} \right) \quad (2.1.14)$$

Electric Force

The reason for defining the electric force equation (F_e) in these terms is because the calculation of ionization energies (E_t) will use a similar format. However, note three differences to calculate ionization energies: 1) it is half ($1/2$) the electron's energy and radius, and 2) it is divided by a distance (r) and not squared like it is in the force calculation, and 3) it introduces a new variable for constructive wave interference (δ). An explanation is provided in the next section and then the calculations for atoms from hydrogen to calcium are provided in Section 2.5.

$$E_t = \frac{1}{2} E_e r_e \left(\frac{\delta}{r} - \frac{\delta}{r_0} \right) \quad (2.1.15)$$

Ionization Energy Equation

To solve for photon energy, the variables for initial distance (r_0), final distance (r) and amplitude factor (δ) must be known. This paper calculates ionization energies of electrons, so the final distance is set to infinity since the electron leaves the atom and its distance is negligible. So, the two variables that need to be calculated to compute photon energy is the electrons orbital distance (r_0) and the constructive wave interference that particles in the atom have on the affected electron (δ). The next figure illustrates these two variables that affect photon (ionization) energy.

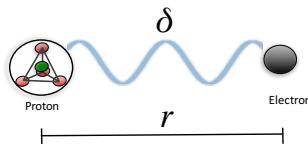


Fig 2.1.5 – Variables of the Ionization Energy Equation

The method to calculate wave interference (δ) is described in the next section, with calculations in Section 2.4. The method to calculate electron distance (r) is described in Section 2.3 with calculations in Section 2.4. Finally, the calculated variables are then used for the ionization energies of atoms that are found in the summary section of this paper. They are detailed in Section 2.6 with example calculations.

2.2. Wave Interference Rules

In the electric force equation (Eq. 2.1.14), the variables are the count of particles in two different groups (Q_1 and Q_2) separated at a distance (r). The method works for two groups by matching calculations of various particle counts and distances when compared to Coulomb's law. It can also be used to calculate the electric force on particles in the atom, but it becomes much more complex due to different electrons in an atomic orbital at various distances and angles relative to the nucleus.

To simplify this complexity, a variable is introduced to calculate the constructive wave interference effect on a given electron in an atom. The variable is called the amplitude factor (δ) and was introduced in the previous section. It replaces Q_1 and Q_2 in the energy equation (Eq. 2.1.15) as the constructive wave interference is now more complex than two particle groups. It is a variable that calculates the change in wave interference relative to a single proton and electron.

For example, in the previous example for the Bohr radius, a single proton and electron was used. In the electric force, $Q_1=1$ (proton) and $Q_2=1$ (electron). This results in an amplitude factor of one ($\delta=Q_1*Q_2=1$). For ionized helium (He^+) which has only one electron, it is $Q_1=2$ (two protons) and $Q_2=1$ (electron) for an amplitude factor of two ($\delta=Q_1*Q_2=2$). This is illustrated in the picture below.

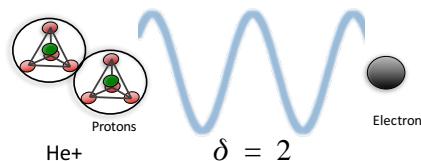


Fig 2.2.1 – Ionized helium amplitude factor is 2.

But the amplitude factor is introduced as a simpler way to calculate multiple particles at different distances. For example, neutral helium (He) has two electrons, as shown in the next figure. A single equation for the electric force cannot be used as the particles are separated into three groups, thus Q_1 and Q_2 cannot be used. The amplitude factor is introduced as a simpler way to calculate the effect of wave interference on a single particle. For example, neutral helium has an amplitude factor of one. The rules will be explained in this section, along with special rules that explain the quantum leaps of electrons.

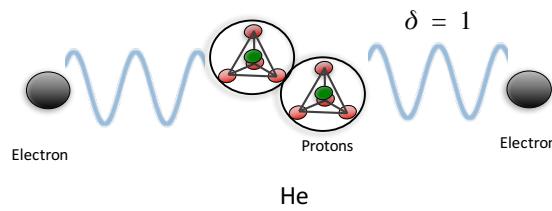


Fig 2.2.2 – Helium amplitude factor is 1.

An orbiting electron in an atom makes jumps between energy levels, known as quantum leaps or jumps.^{Error! Bookmark not defined.} The atom creates a photon when an electron moves to a lower energy level and absorbs a photon when an

electron moves to a higher energy level or leaves the atom (ionization). This is described in the next figure. There are two reasons for this quantized energy that will be explained in this section, both of which are related to a proton's spin.

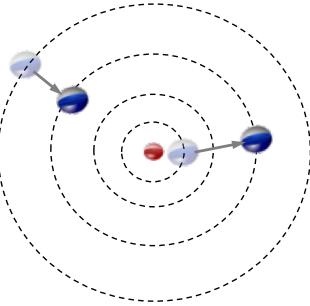


Fig 2.2.3 – Electron quantum orbital jumps

Protons have a similar spin as electrons. In the revised pentaquark model of the proton, there are four tetrahedral quarks and an anti-quark in the middle. The tetrahedral quarks cancel spin ($+ \frac{1}{2}, + \frac{1}{2}, - \frac{1}{2}, - \frac{1}{2}$), leaving the anti-quark/positron in the center that is responsible for the spin. It has value $+ \frac{1}{2}$ or $- \frac{1}{2}$. The anti-quark/positron reflects longitudinal waves that is responsible for the electric force, but its spin also creates a second, transverse wave as illustrated in Fig. 2.2.4 in red.

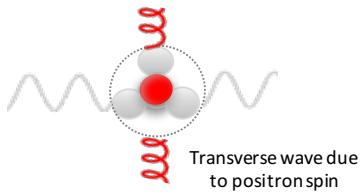


Fig 2.2.4 – Proton's spin (anti-quark/positron spin in the center)

There are two directions for spin, otherwise referred to as spin-up or spin-down in physics. Since quantum jumps are related to the arrangement of protons in the nucleus, which is affected by their tetrahedral structure, the following icons are used in this theory:

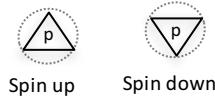
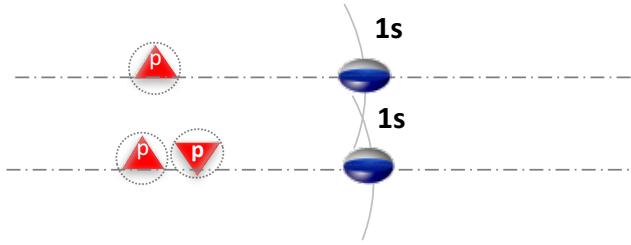


Fig 2.2.5 – Proton's icons for spin-up and spin-down showing tetrahedral quark alignment

Quantum Leap – Cause #1

The first cause of the quantum leap is a wave passing through two or more spin-aligned protons. This causes an increase in the axial force, repelling the electron further, proportional to the square of the protons in alignment.

No Increase: Only one proton in alignment



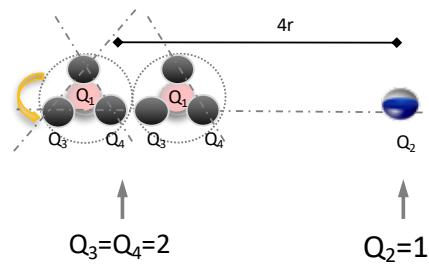
No Increase: Two protons in alignment, but opposite spin.
The gluons need to be aligned for the axial force.

Increase to 2s: Two same-spin protons in alignment.
Gluons aligned to increase the repelling force to $2^2 = 4$ times the force as a single proton.



Fig 2.2.6 – Cause #1 of quantum leaps: Two or more spin-aligned protons

In Fig. 2.2.6, three examples are shown. First, is a wave passing through only one proton. It passes through two quarks in the tetrahedral vertices, creating an axial, repelling force to the 1s orbital. In the second example, two protons are in alignment, but the tetrahedral vertices of these protons are not in alignment, due to opposite spins. It therefore repels to the 1s orbital distance. However, in the last example, two spin-aligned protons now have a wave that passes two protons that have their axial force aligned. This forces the electron to the 2s orbital, as further illustrated in Fig. 2.2.7.



Protons with gluon in alignment is two. Q_3 and Q_4 are two. Q_2 is one (electron).

Fig 2.2.7 – Tetrahedral quark alignment of two protons causing the 2s orbital

The orbital force from Eq. 2.1.5 is now revisited with the updated particle count Q_3 and Q_4 , which represents the number of protons in alignment which is two. It is $Q_3 * Q_4$, or 2^2 . Reminder, Q is used as the shorthand notation since the particles will always be equal, so it's Q^2 .

$$F_o = \frac{E_e r_e^2}{\alpha_e^2} \left(\frac{(2)^2}{r^3} \right) \quad (2.2.1)$$

This becomes the common cause of various orbitals with differing energies and is dependent on the structure and arrangement of the protons in the atomic nucleus. For example, hydrogen (one proton) has an electron at the 1s orbital in its ground state. Helium (two protons) also has an electron at the 1s orbital because there are two protons with opposite spin. Lithium (three protons) now has two same-spin protons, so one electron in the axial direction of these two protons will be at the 2s orbital.

It is also the cause of the number of electrons in each shell. Because it is an axial wave from the proton, its energy is split in two direction. This leaves room for an electron to settle on both sides of the nucleus. Then, the next orbitals are based on the number of same-spin protons in alignment, following the pattern $2Q^2$. Solving for up to four same-spin protons in alignment yields:

- $2(1)^2=2$
- $2(2)^2=8$
- $2(3)^2=18$
- $2(4)^2=32$

The numbers 2, 8, 18 and 32 are the total number of electrons in the first four shells including all the subshells (s, p, d and f).

Quantum Leap – Cause #2

A second cause of the quantum leap can be attributed to an energy gain in the spin of the proton. Hydrogen, for example, has an electron at the 1s orbital (Bohr radius) at ground state. This is shown in the next figure.

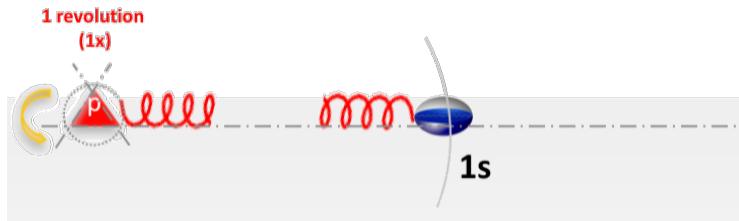


Fig 2.2.8 – Hydrogen electron at ground state (1s)

If it absorbs a photon (energy), then it affects the axial force, which in turn affects the orbital distance. For example, if the transverse wave of a photon causes the proton's spin to rotate at 2 revolutions per cycle (longitudinal wavelength), then the repelling, axial force is now 2x stronger for each tetrahedral quark in alignment.

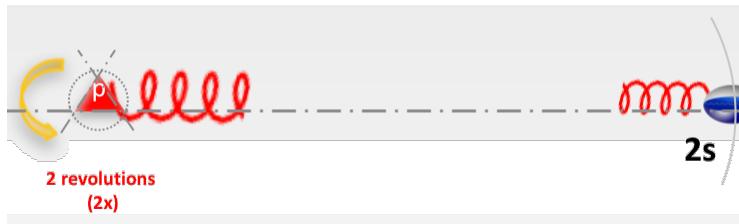


Fig 2.2.9 – Hydrogen electron energized to 2s orbital when proton spins at 2 revolutions per wavelength

The reason for the quantum jumps in this case is due to resonance. Energy gain in spin energy can cause an electron to change orbitals or ionize, but the spin energy must resonate with the longitudinal wave energy to continue spinning. Spin is synchronized by longitudinal wave frequency (wave center off node is the cause for spin). It is a **resonance frequency** and it needs to be an integer of a periodic function. An analogy is a carousel. The longitudinal wave frequency must match the spinning frequency of the carousel to effectively push the horse at the right time. Otherwise, energy passes through and is not converted to spin energy.

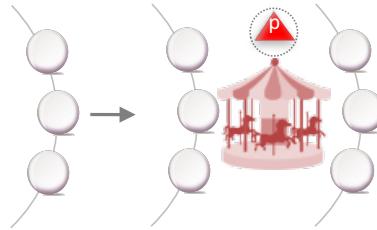


Fig 2.2.10 – Resonance example: longitudinal wave passes through carousel without pushing horse if not at the right frequency

Longitudinal wave amplitude can increase and cause faster spin, but it can only be 1x, 2x, 3x, etc in integers, because the rotation must match the periodic frequency of longitudinal waves. E.g. 2x wave amplitude is 2x rotational spin; but 1.5x wave amplitude is still only 1x rotational spin. Thus, the electron would fall back to the 1s orbital, vibrating into position and creating a new photon with this transverse energy as it settles back to 1s.

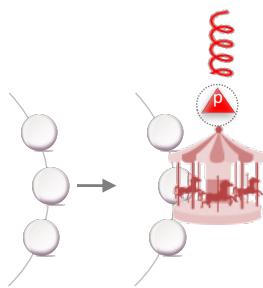


Fig 2.2.11 – Resonance example: longitudinal wave pushes horse, transferring longitudinal energy to transverse energy

This explanation of spin and resonance frequency can now be modeled mathematically. A single proton and electron are now shown in the next figure, with a 2x proton spin. If the energy is sufficient to reach two revolutions per longitudinal wavelength (2x), it can now continue to spin at that frequency.

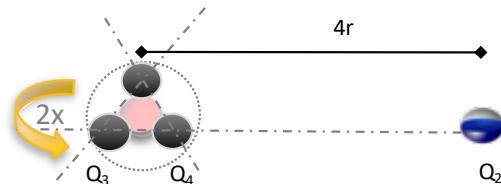


Fig 2.2.12 – Repelling force equation for proton with 2x spin

The fine structure (α_e) is the wave amplitude change between quarks for the strong force, which is now modified to be 2x greater for each quark in axial alignment. Note that it is the inverse of the fine structure constant that is the increase in wave amplitude (i.e. the increase is $\alpha_e/2$). The equation for 2x spin is:

$$F_o = \frac{E_e r_e^2}{\left(\frac{\alpha_e}{2}\right)^2} \left(\frac{(Q)^2}{r^3} \right) \quad (2.2.2)$$

Although the equations to arrive at the force are different, the net result is exactly the same force for both Cause #1 and Cause #2. This model is further proven with the Zeeman effect⁹ where spectral lines are different under a

magnetic field on an atom. The increased spin on particles changes the resonance frequency, thus changing the orbital distance. A constant magnetic force is a transverse wave that either increases or decreases the proton's spin depending on the direction of proton's spin relative to the magnetic spin. This causes the electron to be further from the nucleus (when proton spin and magnetic spin are aligned) or closer to the nucleus (when proton and magnetic spin are opposite). This is illustrated in Fig. 2.2.13.

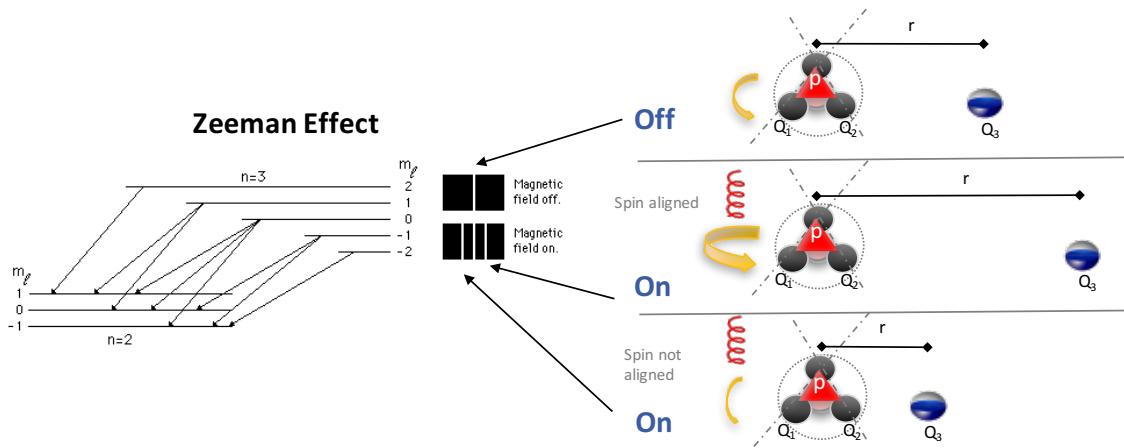


Fig 2.2.13 – Proton under magnetic influence changes the orbital distance (spectral lines) known as the Zeeman Effect

Amplitude Factor Rules

Proton count, proton alignment and increased proton spin are just some of the factors to consider for the effect of constructive wave interference on a single electron being measured. The other factors are the other electrons in an atom, which will repel an electron. This section details the rules to calculate the amplitude factor (constructive wave interference) for all particles in the atom.

When one or more particles are located in two groups at a single distance (r), the rule for amplitude factor is simple. The waves are added or subtracted based on the positive or negative charge of the particle where a single proton-electron combination is one. This is the case for electrons in the 1s orbital as there is only one distance, regardless of the number of protons in the nucleus or electrons in orbit (although there is a maximum of two electrons in 1s). The amplitude factor rule is shown in Fig. 2.2.15, where Z is the number of protons and e is the number of electrons.

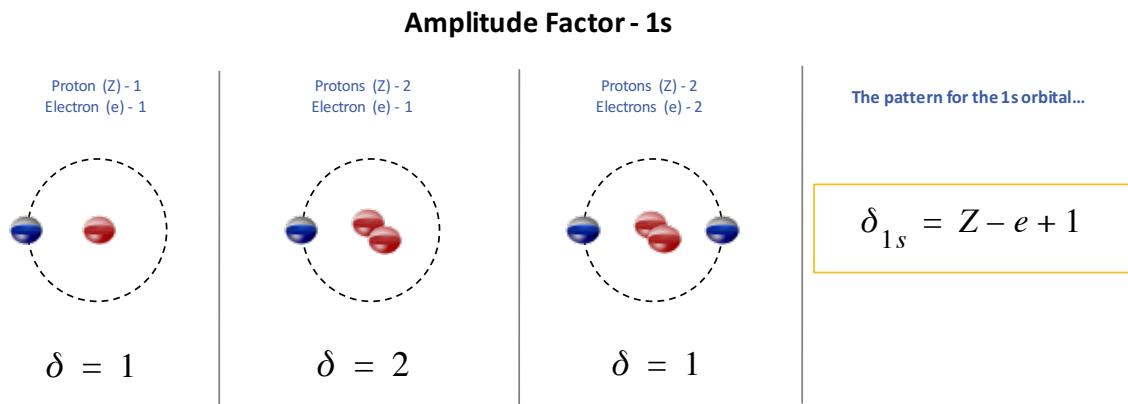


Fig 2.2.15 – Amplitude Factor Rule - 1s Orbital

Amplitude Factor Equation – 1s* Orbital

A pattern emerged for the 1s orbital, neutral and ionized elements, from hydrogen to calcium that made it possible to calculate a special amplitude factor without having to know electron distance. When this special amplitude factor is used, the Bohr radius is substituted into the Ionization Energy Equation as the initial orbital distance (r_0). This equation was given a special name **Amplitude Factor Equation – 1s Orbital** as it can only be used for the 1s orbital. This equation is Eq. 2.5.1.

$$\delta = \left((Z) - \frac{4}{3} \left(\frac{e_1 - 1}{2} + \frac{e_2}{8} + \frac{1}{2} \left(\frac{e_3}{8} \right) + \frac{1}{3} \left(\frac{e_4}{8} \right) \right) \right)^2 \quad (2.2.3)$$

Amplitude Factor Equation – 1s Orbital

Amplitude Factor Equations – 1s to 3p Orbitals

Beyond the 1s orbital, it becomes more complicated as electrons have varying distances, yet they affect each other. However, the amplitude factor resembles the shape and structure of the orbitals (which will be addressed further in Section 3). There is a pattern for s subshells and p subshells, and further, the p subshell is split into two parts based on the spin of the proton $2p^{[1-3]}$ (spin up) versus $2p^{[4-6]}$ (spin down).

Orbital	Shape	Amplitude Factor
1s		$\delta_{1s} = Z - e + 1$
2s		$\delta_{2s} = Z - e + \left(1 + \frac{1}{r_x} \right)$
2p ^{[1-3]*}		$\delta_{2p(1-3)} = Z - e + \frac{1}{2} \left(1 + \frac{1}{r_x} \right)$
2p ^{[4-6]**}		$\delta_{2p(4-6)} = Z - e + \frac{1}{2} \left(\frac{1}{2} + \frac{1}{r_x} \right)$
3s		$\delta_{3s} = Z - e + \left(1 + \frac{1}{r_x} \right)$
3p ^{[1-3]*}		$\delta_{3p(1-3)} = Z - e + \frac{1}{2} \left(1 + \frac{1}{r_x} \right)$
3p ^{[4-6]**}		$\delta_{3p(4-6)} = Z - e + \frac{1}{2} \left(\frac{1}{2} + \frac{1}{r_x} \right)$

*Spin up protons; ** Spin down protons

Table 2.2.1 – Amplitude factor rules by orbital

The rules can be used for the first twenty elements up to calcium. The calculations of amplitude factors for each orbital are presented in tabular format with example calculations in Section 2.5.

2.3. Electron Angle and Distance Rules

Orbital distances beyond hydrogen, calculated as the Bohr radius in Section 2.1, become more complex because of constructive wave interference from other electrons in the atom. The distances and angles of the other electrons are required to compute the final orbital distance of the affected electron. A method to calculate these angles and distances (illustrated in the next figure) is explained in this section.

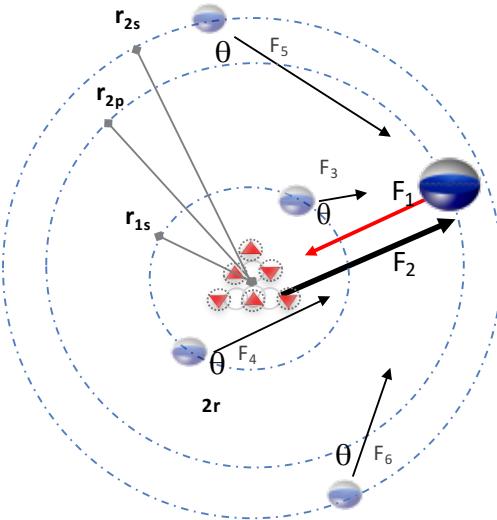


Fig 2.3.1 – Complex interaction of forces on an affected electron. The distances and angles of each particle are required.

Electron Angle Rule

Because of tetrahedral alignment from the quarks in the proton, most angles are at 0° or 60° in relation to the proton. As orbitals become more complex, they are computed as an average of these angles. The angle is in relation to the proton because the sum of forces that is calculated in the equations is the linear direction between the atom's nucleus and the affected electron.

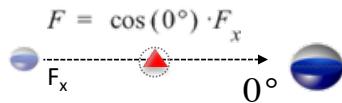
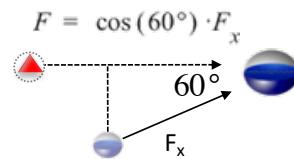


Fig 2.3.2 – Electron angles in relation to the proton

The s orbitals have a common angle:

$$\theta_s = \cos(60^\circ) \quad (2.3.1)$$

The p orbitals are a mix of these two angles*:

$$\theta_p = \frac{\cos(60^\circ) + \cos(0^\circ)}{2} \quad (2.3.2)$$

There are a few exceptions that have this angle**:

$$\theta_x = \frac{2\cos(60^\circ) + \cos(0^\circ)}{3} \quad (2.3.3)$$

* The angles are averaged across the entire solution

** When sodium and magnesium begin building the 3s orbital, they have this angle

Electron Distance Rule

The axis between the nucleus and the electron being measured is the line where the forces will be calculated (where the sum of the forces is zero). The attractive force (F_1) and proton's repulsive force (F_2) are on this axis. Each additional electron in the atom has a repulsive force that may be on a different axis and its distance is computed based on its orbital and the electron angle from the previous section.

F₁ and F₂ are from the nucleus and the radius to the electron is:

$$r = r_x \quad \text{where } x = 1s, 2s, 2p, 3s, \text{ etc.}$$

F₃ and greater are from electrons that have the contribution of their force along the axis measured by:

$$r = \cos(\theta_y) \cdot r_y + r_x$$

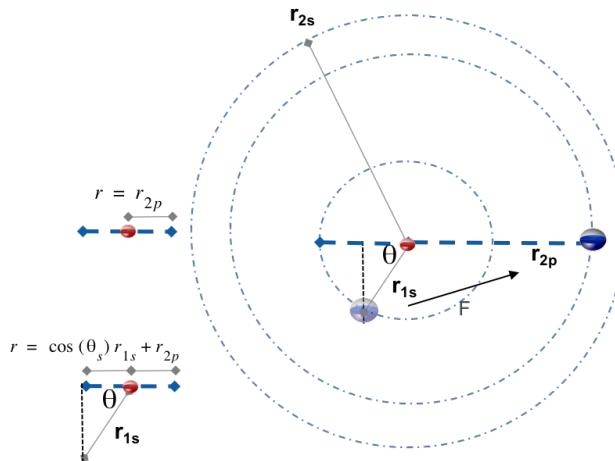
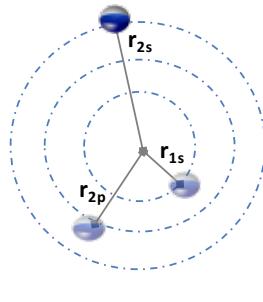


Fig 2.3.3 – Electron distances in relation to the affected electron (being calculated for orbital distance)

Each electron affects all others and so all distances need to be solved simultaneously. The equations in this paper were arranged to be solved with Mathcad to generate the orbital distances for each electron in an atom (illustrated in Fig. 2.3.4). This solution provides the radius in terms of a **ratio to the Bohr radius**.



To do this, radii were solved using Mathcad solver with multiple equations to resolve multiple unknown radii.

For each group of electrons in an orbit (e_y) the equation expands to the right

$$\frac{Z}{r_x^2} = \frac{Q^2}{r_x^3} + \frac{e_{y1}}{(r_x + \cos(\theta_{y1}) \cdot r_{y1})^2} + \frac{e_{y2}}{(r_x + \cos(\theta_{y2}) \cdot r_{y2})^2} + \frac{e_{y3}}{(r_x + \cos(\theta_{y3}) \cdot r_{y3})^2} + etc$$

Unknown: r_{1s}, r_{2s}, r_{2p}

A separate equation is needed for each radius to be solved for. I.e. For 3 radii, $r_x = 1s, 2s, 3p$ (3 equations)

Fig 2.3.4 – Equation format used in Mathcad to simultaneously solve electron distances in an atom

The following is the derivation of the Mathcad equations from above. To simplify the complex Mathcad solution, the electric force and orbital force equations were simplified to only the orbital radii as the unknowns. The Bohr radius was removed from F_2 but is added back after the solution of radius (r_x) to get to meters. Thus, the Mathcad solution provides a ratio of distance to the Bohr radius.

Derivation steps:

- Additional electrons in an atom have a repulsive effect on the electron being measured. It is the electric force of two electrons (Q_1 and Q_2) at a distance r , as expressed earlier in the classical form of the electric force. A second electron will have a force labelled here as F_3 . Additional electrons will each have their own force (F_4, F_5 , etc).

$$F_3 = E_e \frac{Q_1 r_e Q_2}{r} \quad (2.3.1)$$

- Q_2 is the electron being measured and it is always one ($Q_2=1$). Q_1 is a single electron, but for the purposes of simplifying an equation, electrons that reside at the same distance from the measured electron will be grouped together. Q_1 is set to the number of electrons (e) grouped at this distance.

$$Q_1 = e_y \quad (2.3.2)$$

- The sum of all forces is taken along the axis designated as the x-axis, between the atom's nucleus and the electron being measured. However, the other electrons in the atom that affect the electron being measured may not be on this axis. The force along this axis depends on the angle as illustrated in Fig. 2.3.3. Thus, the distance (r) is modified to account for this angle, where r_x is the axis between the atom's nucleus and the measured electron, and r_y is perpendicular to this axis.

$$r = (r_x + \cos(\theta_y) r_y) \quad (2.3.3)$$

- Since Q_2 is 1, and the other variables are found in Eqs. 2.3.2 and 2.3.3, they are substituted into Eq. 2.3.1:

$$F_3 = E_e \frac{e_y r_e}{(r_x + \cos(\theta_y) r_y)^2} \quad (2.3.4)$$

5) The force for F_3 and all forces that follow, will always be repulsive since it is electrons affecting electrons. Expanding on Eq. 2.1.10, where the sum of the forces is zero, the force is placed on the right side of the equation for all forces that have a repulsive effect. It is then simplified by removing consistent terms in each equation.

$$F_1 = F_2 + F_3 = E_e r_e \left(\frac{Z}{r_x^2} \right) = \frac{E_e r_e^2}{\alpha_e^2} \left(\frac{Q^2}{r_x^3} \right) + E_e \frac{e_y r_e}{(r_x + \cos(\theta_y) r_y)^2} \quad (2.3.5)$$

$$\frac{Z}{r_x^2} = \frac{r_e Q^2}{\alpha_e^2 r_x^3} + \frac{e_y}{(r_x + \cos(\theta_y) r_y)^2} \quad (2.3.6)$$

6) The Bohr radius (a_0) is found in the terms of the orbital force as the electron radius and fine structure constant squared. It is **removed temporarily** from the equation to make the solution for Mathcad easier to compute for simultaneous equations. *By removing it here, it must be re-added back to the equation at the end to be complete.*

$$a_0 = \frac{r_e}{\alpha_e^2} \quad (2.3.7)$$

$$\frac{Z}{r_x^2} = \frac{Q^2}{r_x^3} + \frac{e_y}{(r_x + \cos(\theta_y) \cdot r_y)^2} \quad (2.3.8)$$

7) The steps for Eqs. 2.3.1 to 2.3.8 are identical for other electrons in different orbitals that affect an electron. They will always be repulsive, so each one is added to the equation where the sum of forces is zero. It can be given the following format, where j is the total number of orbitals. An example of this equation when expanded was illustrated in Fig. 2.3.4.

$$\frac{Z}{r_x^2} = \frac{Q^2}{r_x^3} + \sum_{i=1}^j \frac{e_{y(i)}}{(r_x + \cos(\theta_{y(i)}) \cdot r_{y(i)})^2} \quad (2.3.9)$$

Orbital distance solution – function of Bohr radius*

*The solution requires solving the equation simultaneously for each electron in the atom, as each electron distance will affect another electron. For this reason, it was simplified to the equation above, and with the Bohr radius temporarily removed. This means that when solving the solution for orbital distance (r), that it is a function of the Bohr radius which must be multiplied back into the solution. The distance r_x is a *dimensionless* value, such that:

$$r = a_0 r_x \quad (2.3.10)$$

Orbital distance

These explanations and the derivations of these equations for force will now be used in the calculations of orbital distances in the next section.

2.4. Calculating Orbital Distances

Using the method established in the previous section, orbital distances were calculated for each electron in each orbital for elements from hydrogen to calcium, including their ionized elements. These calculated orbital distances were validated by two methods:

1. Comparing calculated distances against the known distance of the largest orbital radius (Fig. 1.1).
2. Comparing calculated distances against ionization energies of all orbitals, using the Ionization Energy Equation, which requires electron distance (Fig. 1.2 to 1.6 and further in Appendix C).

In this section, the details of the calculations and how to reproduce these results are provided.

Hydrogen

A single proton and electron at the ground state is known as the Bohr radius, which was derived earlier. Here it is repeated as the method will need to be reproduced and translated into equations for Mathcad.

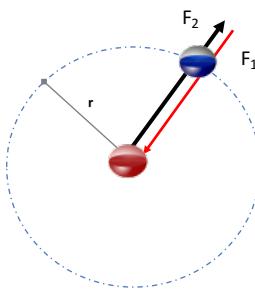


Fig 2.4.1 – Hydrogen: The attractive force and repulsive force of an electron in orbit

The following are the variables for hydrogen using the orbital distance solution in Eq. 2.3.9. The equation only requires two forces since there is a single proton and electron.

- $Z = 1$
- $Q = 1$

$$\frac{(1)}{r_x^2} = \frac{(1)^2}{r_x^3} \quad (2.4.1)$$

$$r_x = 1 \quad (2.4.2)$$

As a reminder, when using the simplified version for solving simultaneous equations, the Bohr radius (a_0) was removed for Eq. 2.3.9, so the final solution uses Eq. 2.3.10, multiplying the Bohr radius back in.

$$r_{1s} = a_0(1) = 5.2918 \cdot 10^{-11} \text{ (m)} \quad (2.4.3)$$

Helium

Helium adds a second electron which is also in the 1s orbital, placed in the position as shown in Fig. 2.4.2.

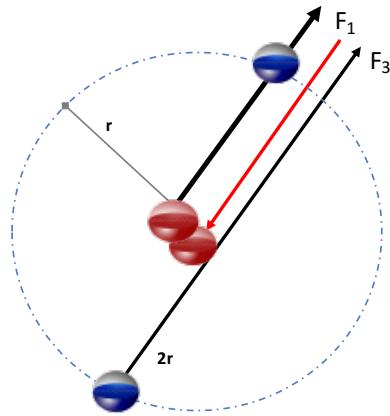


Fig 2.4.2 – Helium: Similar to hydrogen, but now with two protons and one extra electron

An additional force (F_3) must now be applied to Eq. 2.3.9. Because the second electron is along the axis and is equidistant from the nucleus, it can be expressed as a total distance of $2r$ from the first electron. Thus, although a new force is added to the equation, there is still one variable in the equation to solve for. Helium is the last instance where this will occur. Beginning with lithium, multiple equations need to be solved simultaneously for two or more distances. The following are the variables for helium to insert into Eq. 2.3.9. There are two protons in the nucleus ($Z=2$), but there is only one same-spin proton aligned on the axis ($Q=1$). There is one additional electron (e_y) at a distance of $2r$.

- $Z = 2$
- $Q = 1$
- $e_{y1} = 1$

$$\frac{(2)}{r_x^2} = \frac{(1)^2}{r_x^3} + \frac{(1)}{(r_x + r_x)^2} \quad (2.4.4)$$

Solving for r_x in the equation above simplifies to $4/7$, or 0.571. Then, using Eq. 2.3.10, the Bohr radius is multiplied back for the final orbital distance for helium.

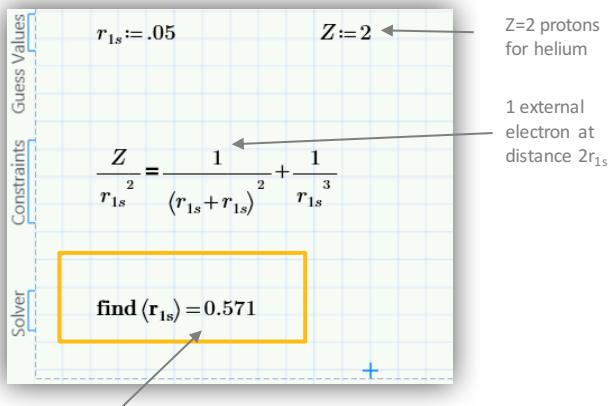
$$r_x = \frac{4}{7} = 0.571 \quad (2.4.5)$$

$$r_{1s} = a_0 (0.571) = 3.02 \cdot 10^{-11} (m) \quad (2.4.6)$$

The orbital distance for helium 1s is calculated to be **30.2 pm** (in picometers). This is compared with an estimated radius of 31 pm from experiments.¹⁰

Helium – Mathcad Solution

Beyond helium, it is too difficult to manually calculate simultaneous equations because the electrons begin to have two or more distances beginning with lithium ($Z=3$). Therefore, helium is replicated now using the Mathcad equations (Eq. 2.3.9) to prove the same results as the manual calculation above.



Distance: 0.571 of Bohr radius. To convert to meters, multiply by Bohr radius. **30.2 pm.**

Fig 2.4.3 – Helium: Mathcad solution of 1s orbital distance (ratio of Bohr radius)

Using the results from Mathcad (Eq. 2.4.3), the result is the same as the manual method – **30.2 pm**.

$$r_{1s} = a_0 (0.571) = 3.02 \cdot 10^{-11} (m) \quad (2.4.7)$$

Lithium – Mathcad Solution

The equations become more complex beginning with lithium ($Z=3$) because it begins a new orbital (2s). Therefore, a second equation is required to simultaneously solve the 1s and 2s orbital distances. Each new orbital requires a new equation and appends more repulsive electrons to each equation being solved. These explanations are annotated along with the Mathcad solution in Fig. 2.4.4.

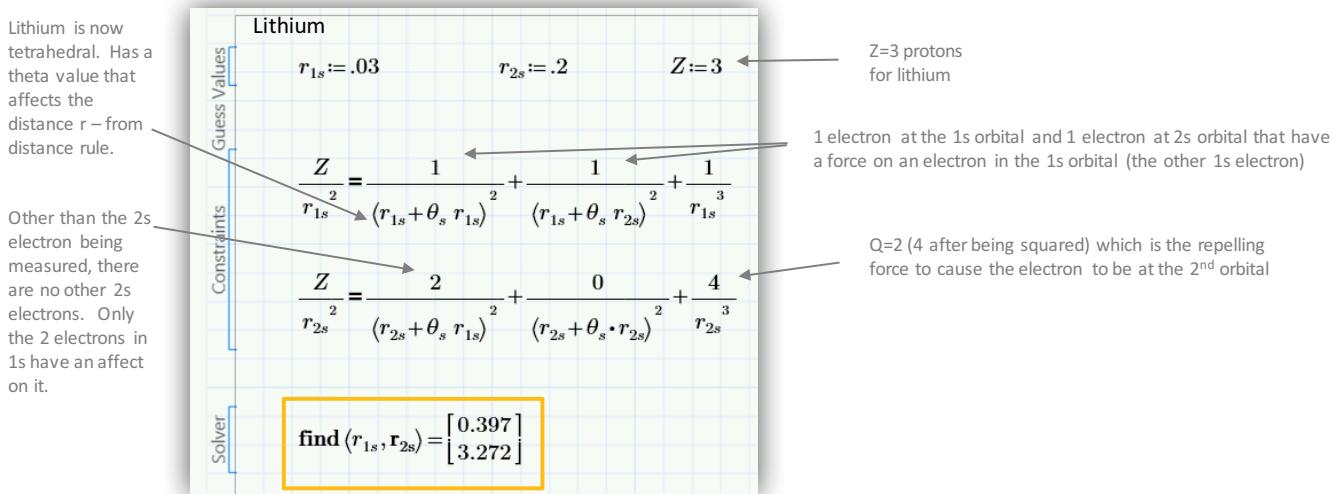


Fig 2.4.4 – Lithium: Mathcad solution of 1s and 2s orbital distances (ratio of Bohr radius)

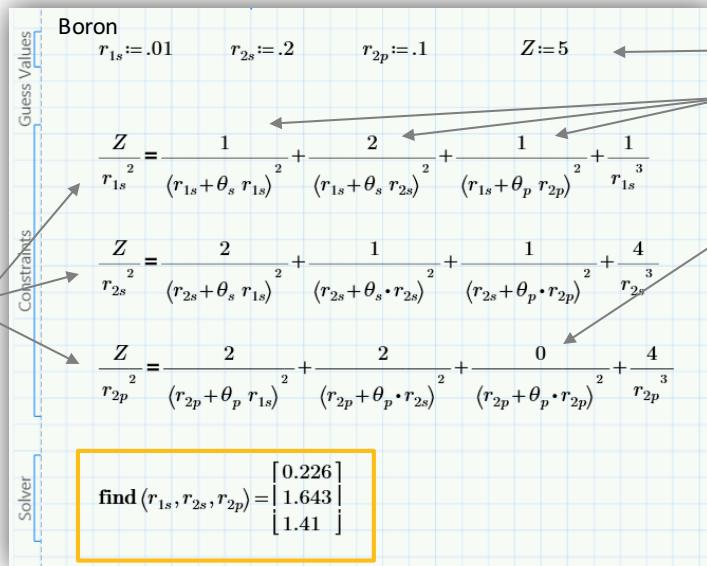
The solution provides the 1s and 2s orbital distances as a ratio of the Bohr radius as 0.397 and 3.272 respectively. In picometers, these distances are 21 pm and 173 pm. The largest distance (2s) was then plotted in the graph in Fig. 1.1.

$$r_{1s} = a_0 (0.397) = 2.10 \cdot 10^{-11} \text{ (m)} \quad (2.4.8)$$

$$r_{2s} = a_0 (3.272) = 1.73 \cdot 10^{-10} \text{ (m)} \quad (2.4.9)$$

Boron – Mathcad Solution

Boron is the next example, as it now begins the transition to the 2p orbital. Since this is a third distance to calculate, a third equation is added and each equation expands to the right to include the effect of the electron at the 2p orbital distance. Also, this is the first time that the electron angles for the p orbital (θ_p) needs to be considered. Again, annotations in Fig. 2.4.5 explain the changes at boron to construct the equations that yield the orbital distances.



Z=5 protons for boron

The pattern continues to add new electrons at common distances that have an effect on the electron being measured in the orbital. E.g. at 1s, only one electron affects it at 1s, but Boron now has 2 in 2s and 1 in 2p that affect it.

At 2p, there is only one electron and it is the one being measured. So zero (0) other electrons in the orbital affect it.

Fig 2.4.5 – Boron: Mathcad solution of 1s, 2s and 2p orbital distances (ratio of Bohr radius)

The solution provides the 1s, 2s and 2p orbital distances as a ratio of the Bohr radius as 0.226, 1.643 and 1.41 respectively. In picometers, these distances are 11.9 pm, 86.9 and 74.6 pm. The largest distance (2s) was then plotted in the graph in Fig. 1.1.

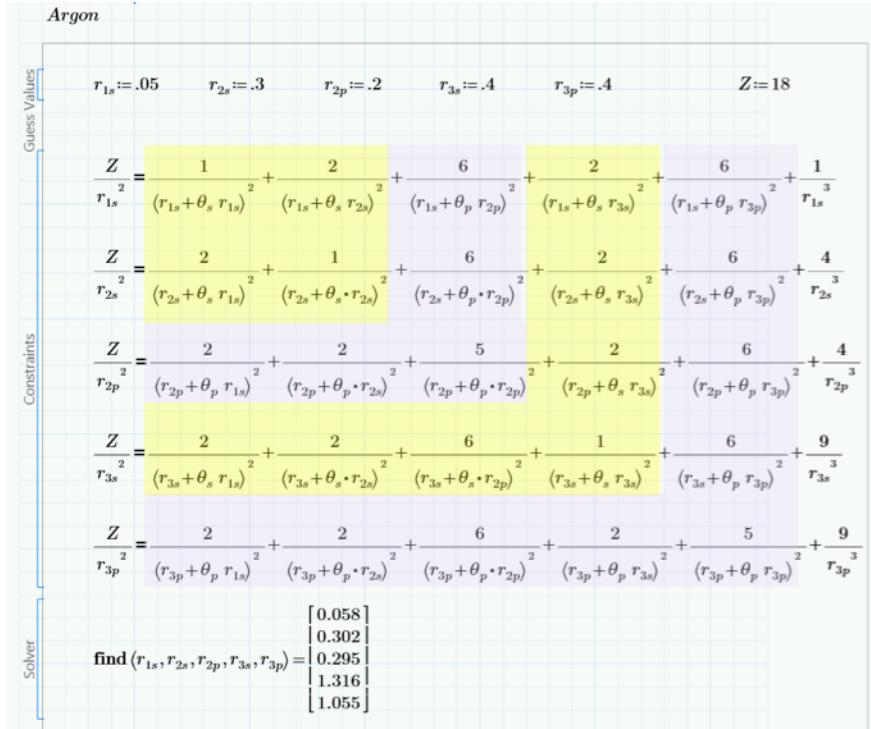
$$r_{1s} = a_0 (0.226) = 1.20 \cdot 10^{-11} \text{ (m)} \quad (2.4.10)$$

$$r_{2s} = a_0 (1.643) = 8.69 \cdot 10^{-11} \text{ (m)} \quad (2.4.11)$$

$$r_{2p} = a_0 (1.41) = 7.46 \cdot 10^{-11} \text{ (m)} \quad (2.4.12)$$

Argon – Mathcad Solution

The pattern continues for equations and electron angles. Argon, with 18 protons, now includes five orbital distances for 1s, 2s, 2p, 3s and 3p. Mathcad now simultaneously solves 5 unknowns (orbital radii) using 5 equations. The electron angles have been color coded in Fig. 2.4.6 because there is a distinct pattern.



Notice the pattern for electron angles. They have been color coded yellow and purple.

$$\theta_s \quad \theta_p$$

The pattern holds true except when 3s and 4s orbitals immediately start filling (Na, Mg) and (K, Ca).

Fig 2.4.6 – Argon: Mathcad solution of 1s, 2s, 2p, 3s and 3p orbital distances (ratio of Bohr radius)

The complete set of Mathcad solutions for all neutral elements from hydrogen to calcium are provided in Appendix A. The ionized elements from hydrogen to calcium were also calculated and put into the tables in Appendix B, although their Mathcad solutions were not provided. Ionized elements simply need to change the Z variable in the Mathcad solution to obtain the ionized element distance. For example, Li⁺ uses the configuration and Mathcad solution for He since they both have two electrons. However, the Z value is modified to be Z=3, which is lithium.

Orbital Distance Calculations

The values of each orbital for hydrogen to calcium generated by Mathcad are summarized into Table 2.4.1. A reminder that these orbital distance results are a ratio of Bohr radius (a_0). For example, the hydrogen 1s orbital distance is $a_0 * 1 = 52.92$ pm (in picometers).

	H	He	Li	Be	B	C	N	O	F	Ne	Na	Mg	Al	Si	P	S	Cl	Ar	K	Ca
1s	1.00	0.57	0.40	0.29	0.23	0.19	0.16	0.14	0.12	0.11	0.10	0.09	0.08	0.08	0.07	0.07	0.06	0.06	0.05	
2s																				
2p																				
3s																				
3p																				
4s																				

Table 2.4.1 – Orbitals Distances: Neutral elements from hydrogen to calcium (ratio of Bohr radius)

The results of the largest orbital distance (the largest s subshell) for neutral elements were plotted in Fig 1.1 and compared against measured results. The remaining orbital distances were used in ionization energy calculations to compare against measured results in Figs. 1.2 to 1.5.

The orbital distances for ionized elements were also calculated and have been placed into tables in Appendix B.

2.5. Calculating the Wave Amplitude Factor

Two examples are provided for calculating wave amplitude factors using the rules in Table 2.2.1 (Section 2.2). Most of the rules require knowing the electron's distance, so the table in Section 2.4 is consulted to calculate values. There is an exception for the 1s orbital, and a special case where the amplitude factor can be calculated and the distance set to the Bohr radius.

Boron – 1s*

The amplitude factor of boron is calculated for the 1s electron. This special case allows only the amplitude factor to be calculated using the Amplitude Factor Equation – 1s orbital, from Eq. 2.2.3, and is labeled 1s* in the next table. It will be used in the example energy calculation in Section 2.6. The variables for boron for this equation are:

- $Z = 5$ (protons)
- $e_1 = 2$ (electrons in the first shell)
- $e_2 = 3$ (electrons in the second shell)

$$\delta_{B1s} = \left((5) - \frac{4}{3} \left(\frac{(2)-1}{2} + \frac{(3)}{8} + \frac{1}{2} \left(\frac{0}{8} \right) + \frac{1}{3} \left(\frac{0}{8} \right) \right) \right)^2 = 14.69 \quad (2.5.1)$$

The value of 14.69 was placed into Table 2.5.1 under the column for boron (B) and the row for Amp. Fac. Eq. 1s*. The remaining values of each of the elements in that row for this special case was calculated using the same method.

Boron – 2p

The amplitude factor of neutral boron for the 2p electron is calculated using the standard method – as opposed to 1s orbitals which can be calculated using the special method above. For boron, Table 2.2.1 is used for the equation for the $2p^{[1-3]}$ orbital, since boron fills out the first p orbital. The equation is shown below in Eq. 2.5.2, and then completed with the variables for boron. Note, unlike the special equation above, only the total electron count (e) in the atom is needed and not individual shells. Then, the distance relative to the Bohr radius (r_x) is found in Table 2.4.1.

- $Z = 5$ (protons)
- $e = 5$ (total electrons)
- $r_x = 1.41$ (from Boron 2p distance in Table 2.4.1)

$$\delta_{B2p} = Z - e + \frac{1}{2} \left(1 + \frac{1}{r_x} \right) \quad (2.5.2)$$

$$\delta_{B2p} = (5) - (5) + \frac{1}{2} \left(1 + \frac{1}{(1.41)} \right) = 0.8546 \quad (2.5.3)$$

The value of 0.8546 was placed into Table 2.5.1 under the column for boron (B) and the row for 2p. The remaining values of each of the elements in the table, with the exception of 1s*, was calculated using this same method.

Amplitude Factors Calculations

After calculating all neutral elements from hydrogen to calcium, using the method described above, the results were organized and placed into Table 2.5.1. The amplitude factors can also be calculated for ionized elements by modifying the number of protons (Z) or electrons (e) in the equations described above.

	H	He	Li	Be	B	C	N	O	F	Ne	Na	Mg	Al	Si	P	S	Cl	Ar	K	Ca
1s	1.00	1.00	1.89	2.63	3.32	4.05	4.78	5.47	6.20	6.94	7.65	8.43	9.15	9.87	10.56	11.36	12.10	12.93	13.64	14.42
2s			1.31	1.48	1.61	1.77	1.94	2.10	2.27	2.44	2.69	2.93	3.16	3.39	3.62	3.85	4.08	4.31	4.55	4.79
2p				0.85	0.94	1.02	0.85	0.94	1.02											
3s											1.28	1.38	2.37	2.45	2.53	2.61	2.68	2.76	2.87	2.98
3p												0.78	0.82	0.86	0.65	0.69	0.72			
4s																		1.27	1.32	
Amp Fac. Eq.																				
1s*	1.00	1.78	4.69	9.00	14.69	21.78	30.25	40.11	51.36	64.00	79.51	96.69	115.56	136.11	158.34	182.25	207.84	235.11	264.97	296.60

Table 2.5.1 – Amplitude Factors: Neutral Elements from Hydrogen to Calcium;
1s* is calculated with Amplitude Factor Equation and uses the Bohr radius as initial orbital distance (r_0)

Now, using the amplitude factors for constructive and destructive wave interference and orbital distances, the photon energy required for electron ionization can be calculated in the next section.

2.6. Calculating Ionization Energy

The results of photon ionization energies using the orbital distances calculated via classical methods were placed in Section 1 in Figs. 1.2 to 1.5, with further details in Appendix C. In this section, example calculations are provided with the steps to reproduce the results.

Photon energy is a transverse wave which is calculated using the Ionization Energy Equation in Eq. 2.1.15. The three variables are the initial electron distance (r_0), final distance (r) and the amplitude factor (δ), but for ionization energy, the final distance is set to infinity so only two variables are required: r_0 and δ .

The same examples from Section 2.5 are used here for boron. The remaining calculations use the same methodology.

Boron – 1s*

The ionization energy of the 1s electron in boron is calculated as follows. For the 1s orbital, the special case can be used of the Amplitude Factor Equation – 1s orbital, where the distance (r_0) is set to the Bohr radius. The Ionization Energy Equation (Eq. 2.1.15) is used with this distance and with the special 1s* amplitude factor from Table 2.5.1:

- $\delta_{B1s} = 14.69$ (from Table 2.5.1 – 1s* value)
- $r_0 = a_0$

$$E_t = \frac{1}{2} E_e r_e \left(\frac{\delta_{B1s}}{\infty} - \frac{\delta_{B1s}}{a_0} \right) = -3.2 \cdot 10^{-17} (J) \quad (2.6.1)$$

The results are in joules ($\text{kg}^* \text{m}^2/\text{s}^2$), but the comparisons against measured results are in megajoules per mole. The conversion uses Avogadro's constant ($N_A = 6.02214 \times 10^{23}$) and is divided by 10^6 to arrive at the equivalent in MJ/mol.

$$E_t = \frac{1}{2} E_e r_e \left(\frac{\delta_{B1s}}{\infty} - \frac{\delta_{B1s}}{a_0} \right) \left(\frac{N_A}{10^6} \right) = -19.3 \left(\frac{\text{MJ}}{\text{mol}} \right) \quad (2.6.2)$$

After converting from joules to megajoules per mole, the calculated result is **-19.3 MJ/mol**. This matches the measured result for Boron 1s spectroscopy which is -19.3 MJ/mol.¹¹ The negative sign indicates a photon was absorbed. This value was added to the table and graph in Fig 1.3. The remaining calculations for 1s spectroscopy results were repeated for elements from hydrogen to calcium.

Boron – 2p

The second example is the photon energy required to ionize an electron in the 2p subshell of boron. Using the Ionization Energy Equation, the final distance (r) is once again set to infinity as shown. The initial 2p orbital distance (r_0) and the amplitude factor for Boron 2p (δ_{B2p}) come from Tables 2.4.1 and 2.5.1 respectively. Reminder that distance is converted to meters by multiplying the value (1.41) by the Bohr radius.

- $\delta_{B2p} = 0.8546$ (from Table 2.5.1 – 2p value)
- $r_0 = a_0 * 1.41$ (from Table 2.4.1 – 2p value)

$$E_t = \frac{1}{2} E_e r_e \left(\frac{\delta_{B2p}}{\infty} - \frac{\delta_{B2p}}{a_0 (1.41)} \right) = -1.32 \cdot 10^{-18} (J) \quad (2.6.3)$$

Convert from joules to MJ/mole using Avogadro's constant:

$$E_t = \frac{1}{2} E_e r_e \left(\frac{\delta_{B2p}}{\infty} - \frac{\delta_{B2p}}{a_0 (1.41)} \right) \left(\frac{N_A}{10^6} \right) = -0.80 \left(\frac{\text{MJ}}{\text{mol}} \right) \quad (2.6.4)$$

After converting from joules to megajoules per mole, the calculated result is **-0.80 MJ/mol**. This matches the measured result for boron which is -.80 MJ/mol.¹² Both values were charted in Fig. 1.2.

These examples show the calculations for two different boron orbital distances. All of the calculations in Figs. 1.2 to 1.6 and in Appendix C are calculated using the same methodology. In the case of boron and many of the examples, the calculations exactly match the measured results. However, there is a trend where the calculated results slowly deviate from measured results. This occurs as the number of electrons increases in an atom or as the distance from the nucleus to the orbital decreases (such as heavily ionized atoms). This is due to the electron angle rule which estimates the angles for each electron and averages them over the solution. By removing these as being variable, it reduced the Mathcad solution to have an equal number of unknowns (orbital radii) as the number of equations. However, to be more accurate, the exact electron angles could be computer modelled and the distances and angles solved for simultaneously with more powerful computer algorithms. This will be required to calculate photon energies beyond calcium.

3. Orbital Shapes

Section 2 describes a method to calculate orbital distances, but it does not explain the strange shapes and probability nature of the electron. Using the proton's pentaquark model, these shapes can be explained based on proton arrangement in an atomic nucleus.

First, tetrahedral numbers are revisited since the nucleus structure appears to be based upon a tetrahedral structure based on evidence in this section and also in Section 4. Tetrahedrons are geometric 3D stability for waves in all directions. The properties of a tetrahedron: the layer height, the number in each layer and the total number is shown in Fig. 3.1. The important number for this section is the number in each layer. These have been mapped to subshells: s, p, d and f.

Tetrahedron Levels			
Orbital	Height	# in Layer	Total #
s	1	1	1
s	2	3	4
p	3	6	10
d	4	10	20
f	5	15	35

↑
Orbitals need to be in pairs to cancel spin, so s orbital is "2" and f orbital is "14".

Fig. 3.1 – Tetrahedral Numbers

3.1. Probability Cloud

The electron has a probability cloud as described in Fig. 3.1.1. It does not have a definitive line for an orbit like the Earth revolves around the Sun.

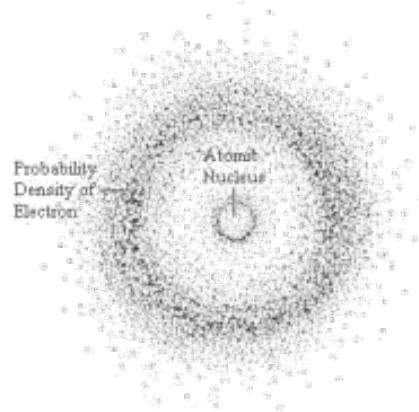


Fig. 3.1.1 – Electron probability cloud ¹³

The electron has a probability cloud because the proton continues to spin, changing the point where the sum of the forces is zero. The axial force repels the electron at certain geometric alignments (six possible axes in the 2 level tetrahedron). The electron continues to be pushed and pulled as the proton spins and the electron encounters the axial force.

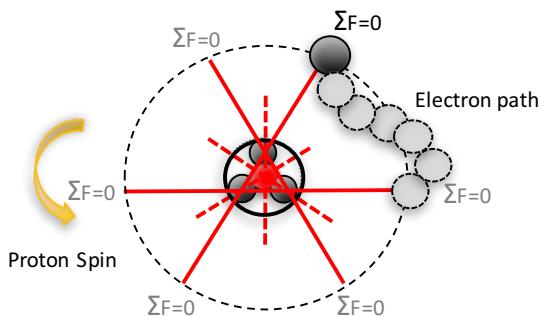


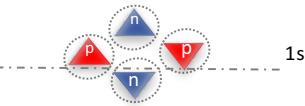
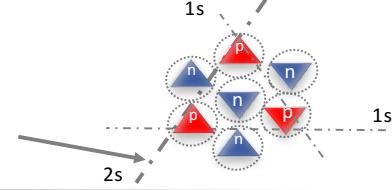
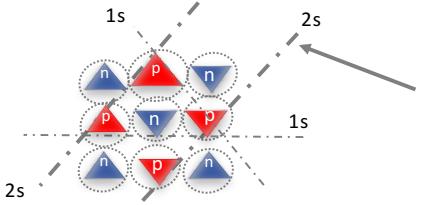
Fig. 3.1.2 – Electron probability cloud generated by proton spin and changing axis of repelling force (F_2)

The “probability” of an electron is seen in experiments. The electron can be in various places, yet the ionization energy values are always exact. This is due to the fact that the attractive electric force (F_1) remains constant, and the ionization energy to remove the electron from this force is therefore also constant. But the repelling force (F_2) depends on the spin of the proton and location of the electron, creating a variation in the measured result of the electron’s distance.

3.2. S Orbital

The explanation of the transition from 1s to 2s and other orbital jumps were described previously in Section 2.2. One of the causes is the alignment of same-spin protons in the atomic nucleus. Helium ($Z=2$) has two opposite spin protons, but lithium ($Z=3$) is the first atomic element with two protons with the same spin. This causes one electron to be pushed out to the 2s subshell. Beryllium has two pairs of protons now with the same spin, thus two electrons are pushed out to the 2s subshell. The proposed nucleon structure for these elements are shown in Fig. 3.2.1.

The nucleon structure is also mapped to a VSEPR molecular geometry class because it is possible that molecules get their shapes as an extension of how the nucleus itself is structured.¹⁴ The first four elements may be planar (2D) in structure given the stability of ^7Li and ^9Be which are proposed in symmetric arrangement in Fig. 3.2.1. These proposed structures would match the known electron configurations in 1s and 2s and also the stability of the elements with these number of protons and neutrons.

Element	Nucleon Structure	VESPR
He		Linear
^7Li		Trigonal Planar
^9Be		Trigonal Planar x2

Legend: Proton (red triangle) Neutron (blue triangle)

Fig. 3.2.1 – Configuration of protons and neutrons for He, Li and Be

Shape

As the proton spins on three axes, it creates a spherical shape. H and He ($Z=1$ and $Z=2$) have no protons with gluons that align (differing spins) and are confined to 1s. Li and Be ($Z=3$ and $Z=4$) begin to have protons that align spin and gluons; this greater axial force pushes electrons to 2s.

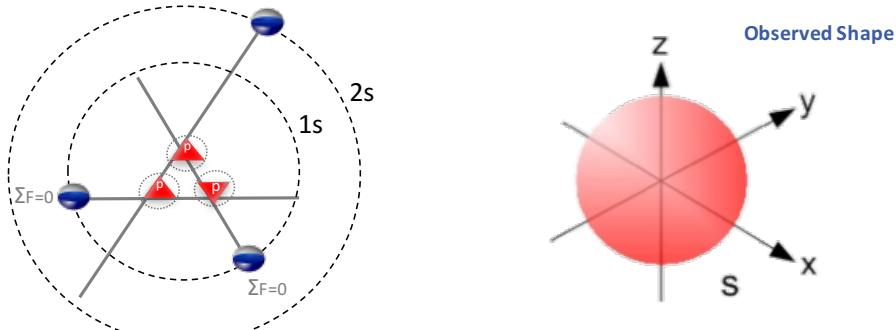
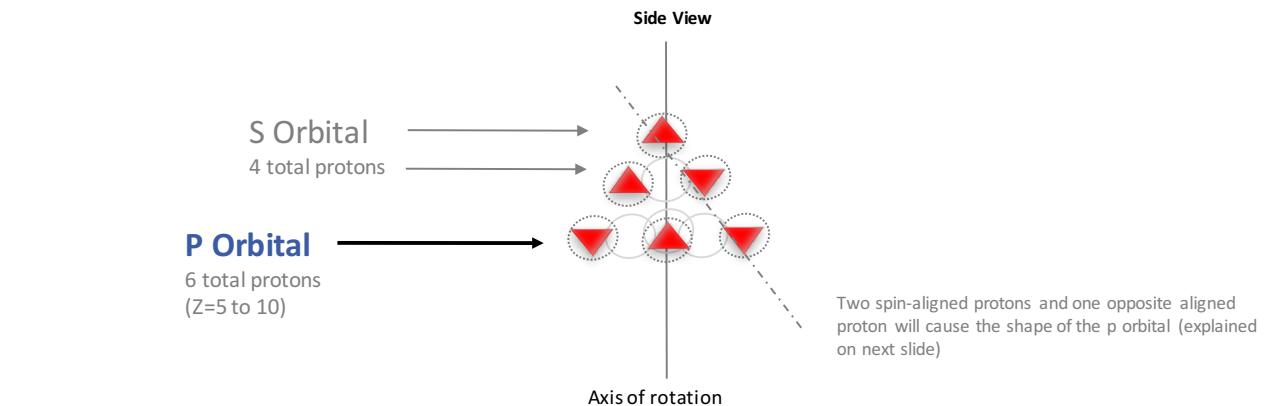


Fig. 3.2.2 – Shape of the s orbital¹⁵

3.3. P Orbital

Beginning with boron, a 3D tetrahedral structure begins to form. It is no longer planar (2D). There are six protons in the 2p subshell (B to Ne). Refer to Fig. 3.1. This is the 3rd level of a tetrahedron. The side view of an atomic element, based on the axis of rotation, is shown in Fig. 3.2.3. The first four protons (H to Be) are now arranged as the first two layers of the tetrahedron.

Beginning with the 2p subshell, neutrons will be excluded from the view for simplicity to visualize the nucleus structure. However, neutrons are assumed to continue to fill the spaces between protons.



Proton (spin up) Proton (spin down) Neutrons continue to separate protons, but only protons will be shown to simplify drawings of elements $Z > 4$.

Fig. 3.2.3 – Protons forming in nucleus. The p orbital has six protons to complete the third level of a tetrahedral structure.

In Fig. 3.2.3, the dashed line is the focus for why the p orbital has a different shape than the s orbital. The p orbital appears as a dumbbell – a spherical shape like the s orbital cut in half. As the atomic nucleus spins, individual protons also spin. There are two times during a rotation that three protons align – 90° and 270° (below).

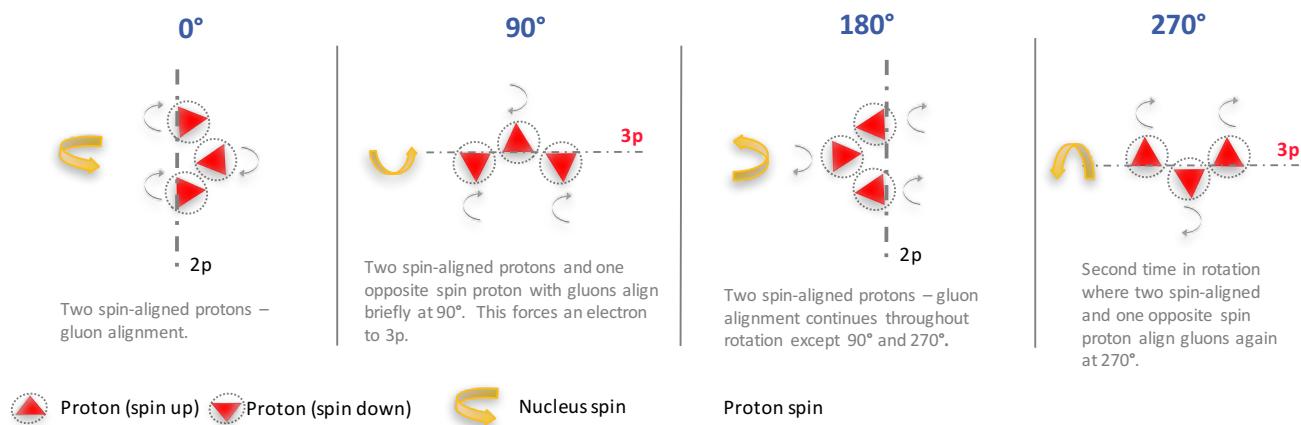


Fig. 3.2.4 – Two points in the proton's spin rotation have an intersection where the axial force aligns for opposite spin protons

Shape

The p orbital is a dumbbell shape because the electron is pushed out twice during the rotation to the $3p$ subshell when an opposite spin proton aligns gluons with two same-spin protons.

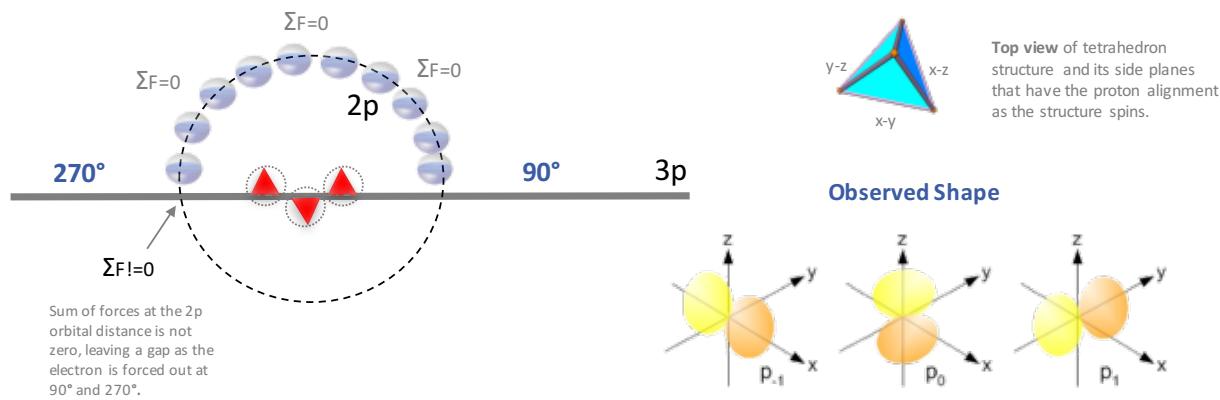


Fig. 3.2.5 – Dumbbell shape of p orbital due to two points in rotation where sum of forces is not at 2p distance

Proton Fill Order

Protons with spins aligned with the atomic nucleus' spin will fill first as there is less energy required before a proton with opposite spin is filled in the nucleus structure. Protons also fill from the center then outwards for geometric stability. Fig. 3.2.6 shows the fill order of atomic elements from boron (B) to neon (Ne) in both the side view of the nucleus and the bottom row (third row) which is being filled with protons.

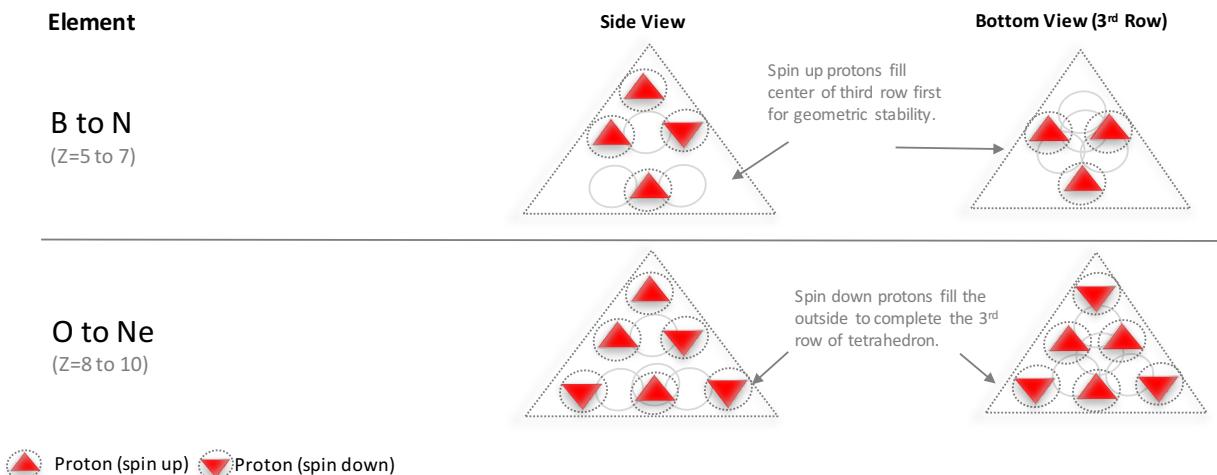


Fig. 3.2.6 – Fill order of p orbital electrons (side view and bottom view shown)

3.4. D Orbital

The d orbital contains 10 electrons. Again, refer to Fig. 3.1. This is the 4th level of the tetrahedron. This is illustrated in Fig. 3.2.7. Note that the 3s and 3p protons are not shown in this tetrahedral view, but are addressed in Section 4.

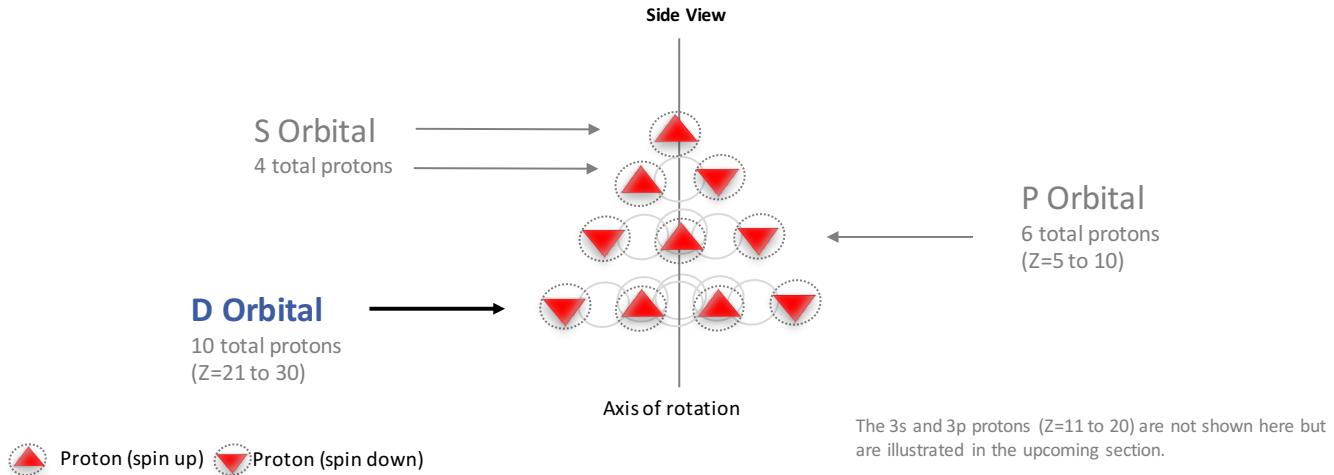


Fig. 3.2.7 – Protons forming in nucleus. The d orbital has ten protons to complete a fourth level of a tetrahedral structure.

With three spin-aligned protons, it would have a spherical shape, yet four times during the rotation it will have gluons that align with a proton of the opposite spin to force an electron out to 4d.

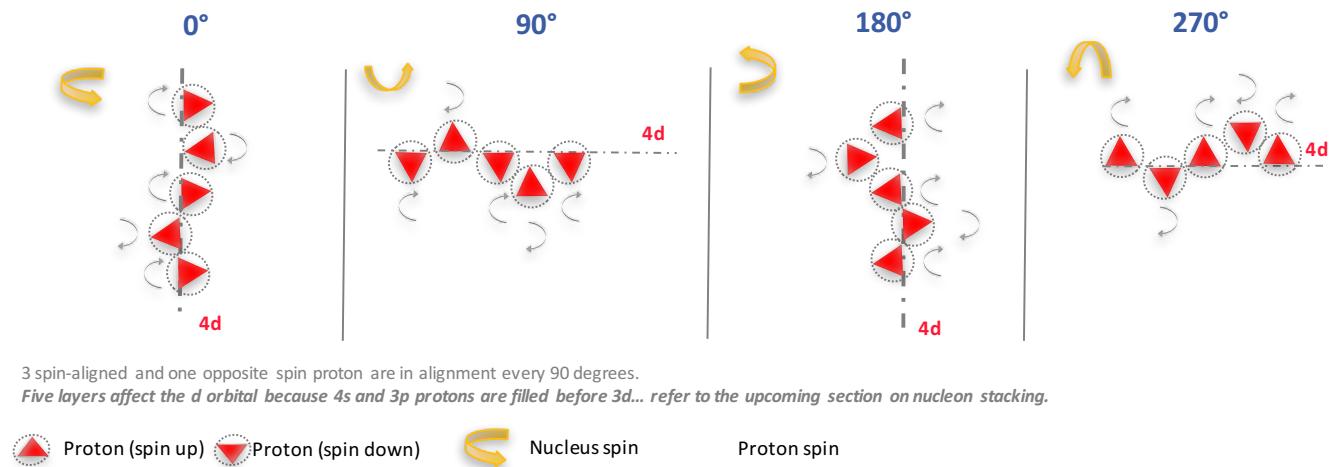


Fig. 3.2.8 – Four points in the proton's spin rotation have an intersection where the axial force aligns for opposite spin protons

Shape

The d orbital is a clover shape because the electron is pushed out four times during the rotation when an opposite spin proton aligns gluons with three spin-aligned protons.

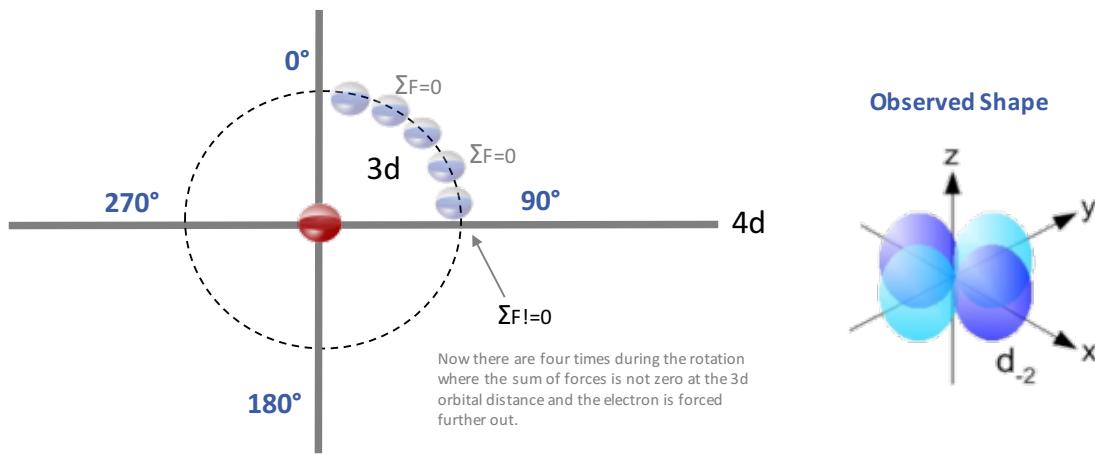


Fig. 3.2.9 – Dumbbell shape of d orbital due to four points in rotation where sum of forces is not at 3d distance

Proton Fill Order

At Z=21, scandium (Sc) is the first element that begins a d orbital. As protons always build from the center then outwards for stability, the first proton is placed in the center (refer to Fig. 3.2.10). In a 4th row of a tetrahedron, this is the first time that a unit is in the center of axis of rotation. This creates a unique shape relative to other d orbital shapes (refer to shape highlighted in yellow).

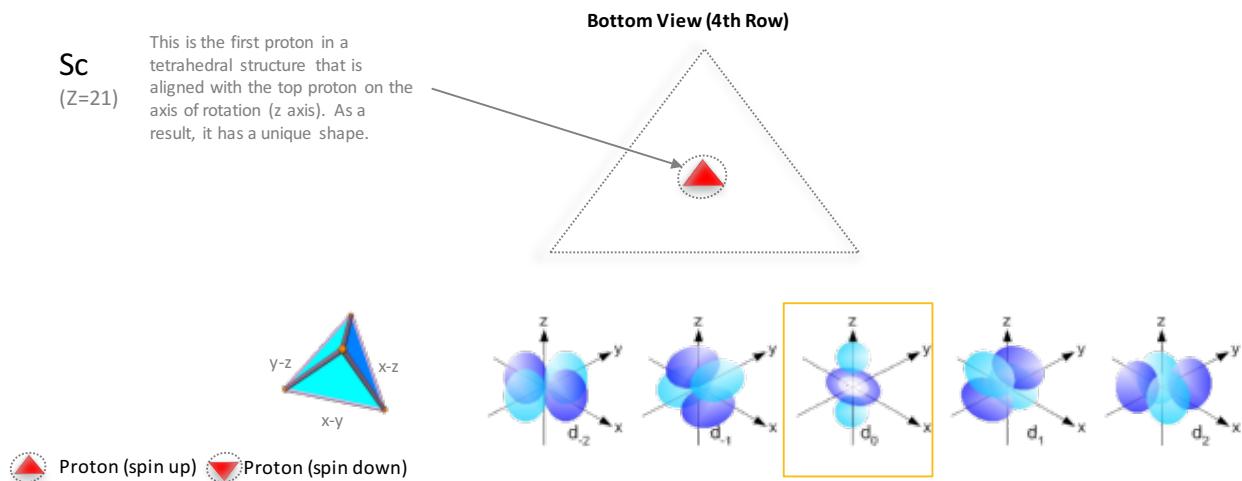


Fig. 3.2.10 – Fill order of the 1st d orbital electron (bottom view shown)

The next three elements build outwards from the center, occupying the three sides of the triangle as shown below. These now have the clover shape as there are four points in the rotation where the repelling, axial force distance changes as shown in Fig 3.2.9. These take place on the x-y, x-z and y-z planes of the tetrahedron while it spins. This is highlighted in yellow below.

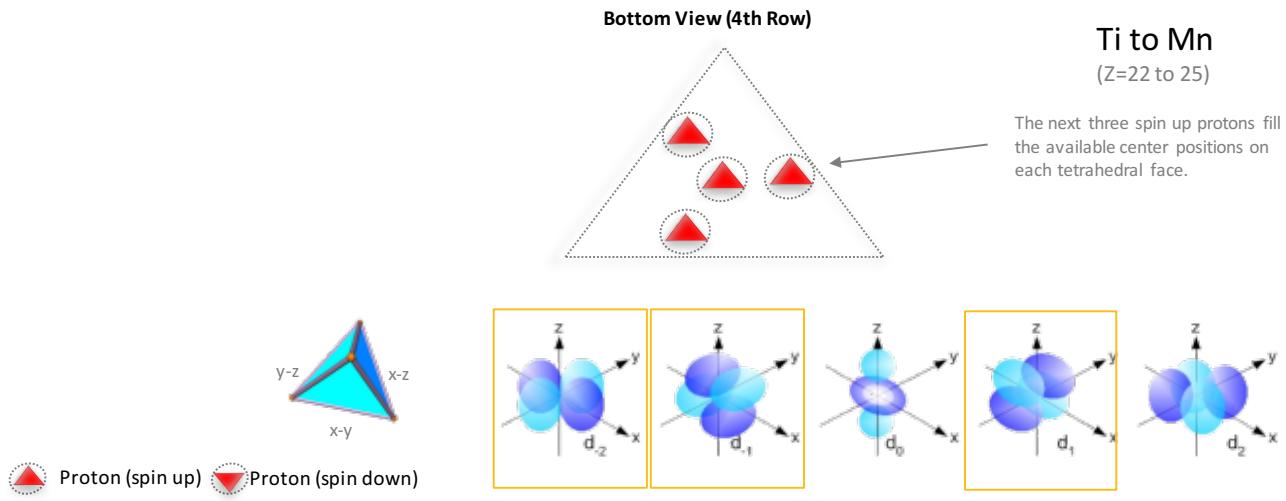


Fig. 3.2.11 – Fill order of the 2nd to 4th d orbital electrons (bottom view shown)

The final spin up proton must be placed on one of the existing three sides. This is manganese (Mn). Since it shares a tetrahedral face with another spin up proton (x-y), its orbital will also be in this plane but will be shifted slightly based on the protons location as shown in Fig. 3.2.12. This is also highlighted in yellow below.

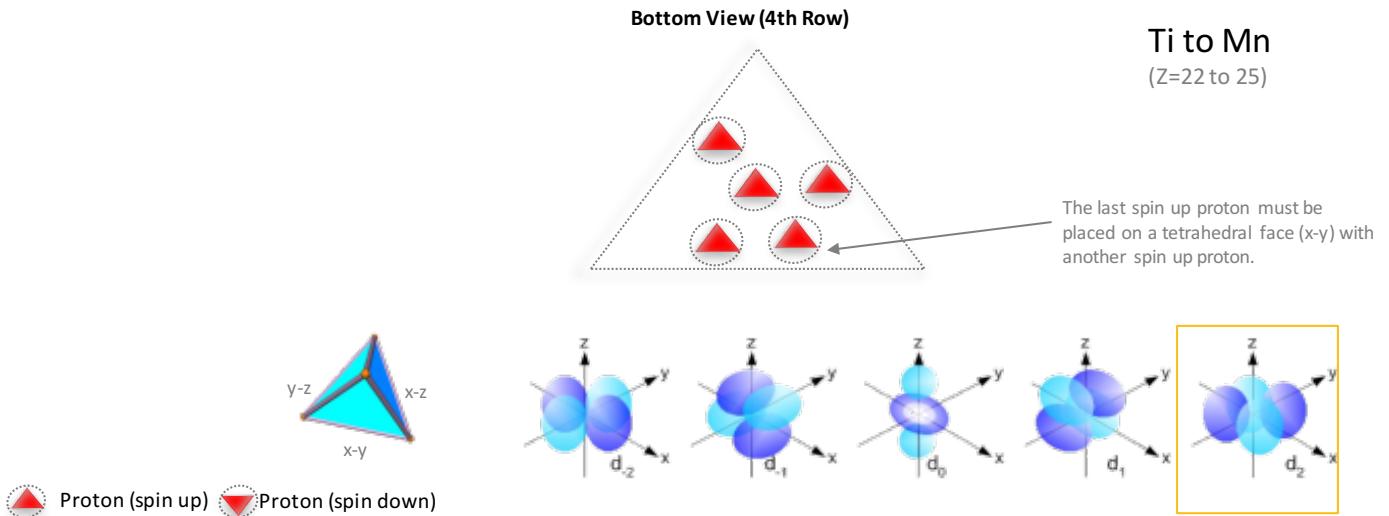


Fig. 3.2.12 – Fill order of the 5th d orbital electron (bottom view shown)

Finally, all of the five spin down protons complete the 4th row of a tetrahedron to complete the orbitals.

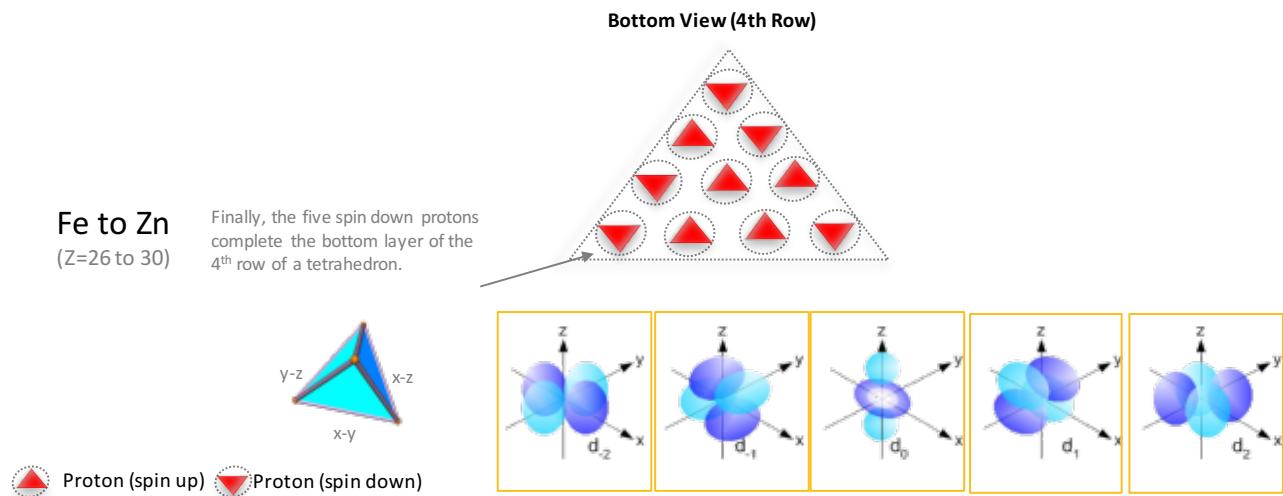


Fig. 3.2.13 – Fill order of the spin down orbital electrons (bottom view shown)

3.5. F Orbital

The sequence for the f block is unique. Beginning with lanthanum (Z=57) it starts a block that contains 15 elements. Again, refer to Fig. 3.1. The 5th level of a tetrahedron has 15 units. There are 15 elements for the f block (Z=57 to 71), although an odd number affects the number of orbitals (14 / 2 = 7). It converts a proton to neutron in the next d block to compensate, beginning with the 5d block.

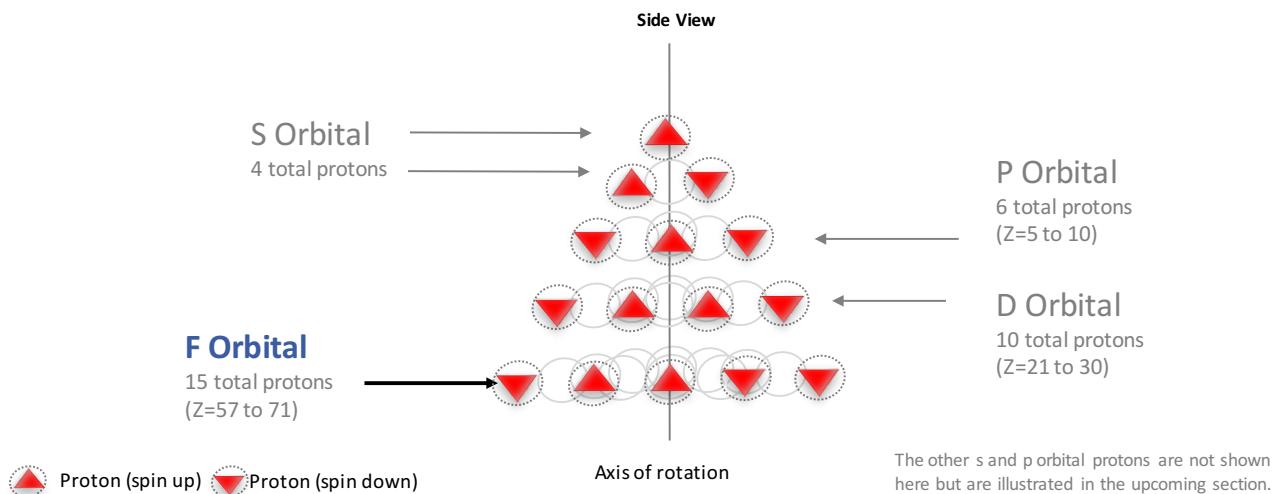


Fig. 3.2.14 – Protons forming in nucleus. The f orbital has 15 protons to complete a fifth level of a tetrahedral structure.

Shape

The f orbital is more complex, but follows the same rules based on proton alignment as the p and d orbitals. When completely full it is similar to the d orbital, but cut in half (eight lobes instead of four). It is based on the points in the nucleus rotation where the gluons of opposite spin protons align.

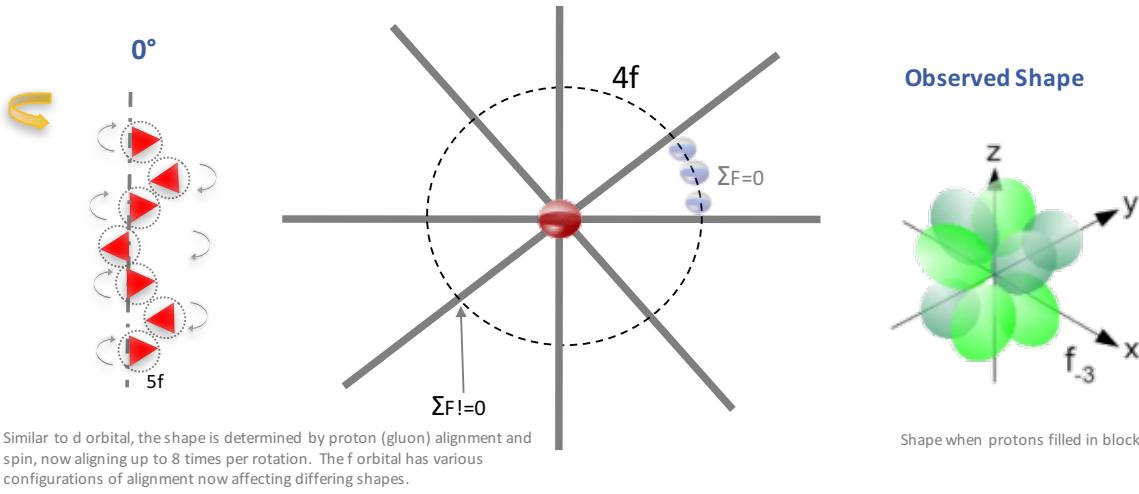


Fig. 3.2.15 – Shape of the f orbital due to eight points in rotation where sum of forces is not at 4f distance

Proton Fill Order

Similar to the d orbital, the first proton has a unique shape because it is in the center and does not have multiple protons in alignment on the tetrahedral edge. The 5th row of a tetrahedron has three center protons now ($Z=57$ to 59). As a result, these three elements have different shapes than the remaining spin up protons which will be placed on the triangle's edge (tetrahedral face). These shapes are highlighted in yellow in Fig. 3.2.16.

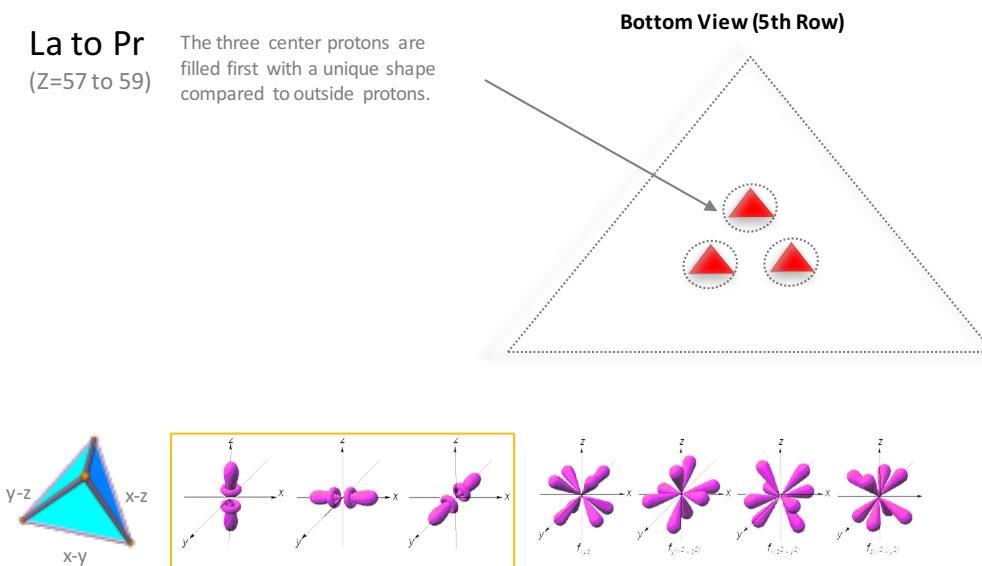


Fig. 3.2.16 – Fill order of the 1st to 3rd f orbital electrons (bottom view shown)

Also, similar to the d orbital, protons continue to build outwards from the center. The next three protons ($Z=60$ to 63) occupy the space at the edge of the triangle and tetrahedral face. Now, with many protons in alignment on this face, it has the lobe shapes seen in the p and d orbitals, but they are cut in half due to an extra proton now matching spin during the nucleus rotation. These shapes are highlighted in yellow below.

Nd to Eu (Z=60 to 63)

The next three spin up protons fill the available center positions on each tetrahedral face.

Bottom View (5th Row)

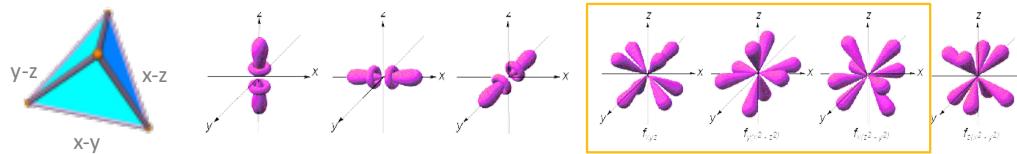
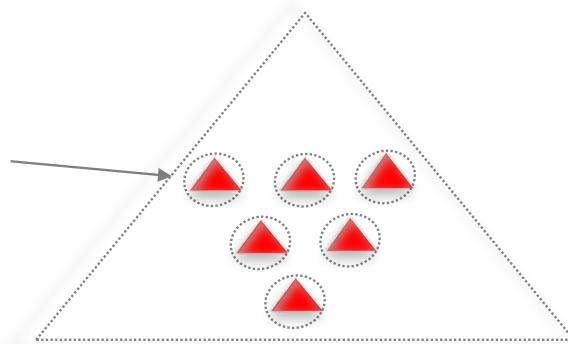


Fig. 3.2.17 – Fill order of the 4th to 6th f orbital electrons (bottom view shown)

Once again, similar to the d orbital, the last spin up proton must be placed on one of the three triangular edges. It will share an edge with an existing x-y spin up proton, but the orbital is shifted on this plane because of the location of the proton.

Nd to Eu (Z=60 to 63)

The last spin up proton must be placed on a tetrahedral face with another spin up proton.

Bottom View (5th Row)

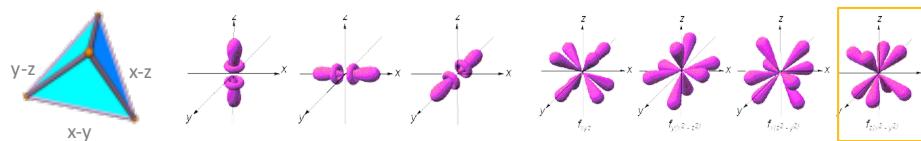
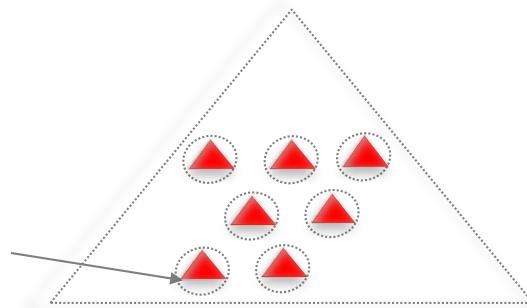


Fig. 3.2.18 – Fill order of the 7th f orbital electron (bottom view shown)

Finally, seven spin down protons are added to the 5th row of a tetrahedral structure to complete the orbitals. There are now 7 spin up and 7 spin down protons. This matches the orbitals seen in the f series. However, there is one more space in the 5th row of a tetrahedron because it has 15 units. One last proton completes this row and it causes the next d block series to have 9 elements. This is confirmed in the Periodic Table of Elements as the 5d block (Z=72 to 80) contains 9 elements. In addition, the transition from 4f to 5d and again from 5f to 6d shows a mass increase that includes at least three neutrons before the next element. This means that the d block has a neutron take the

position of a proton so that it can have 9 protons in a row, otherwise it requires 10 units to complete a row (two of the three neutrons are separation neutrons and the third occupies the proton's position).

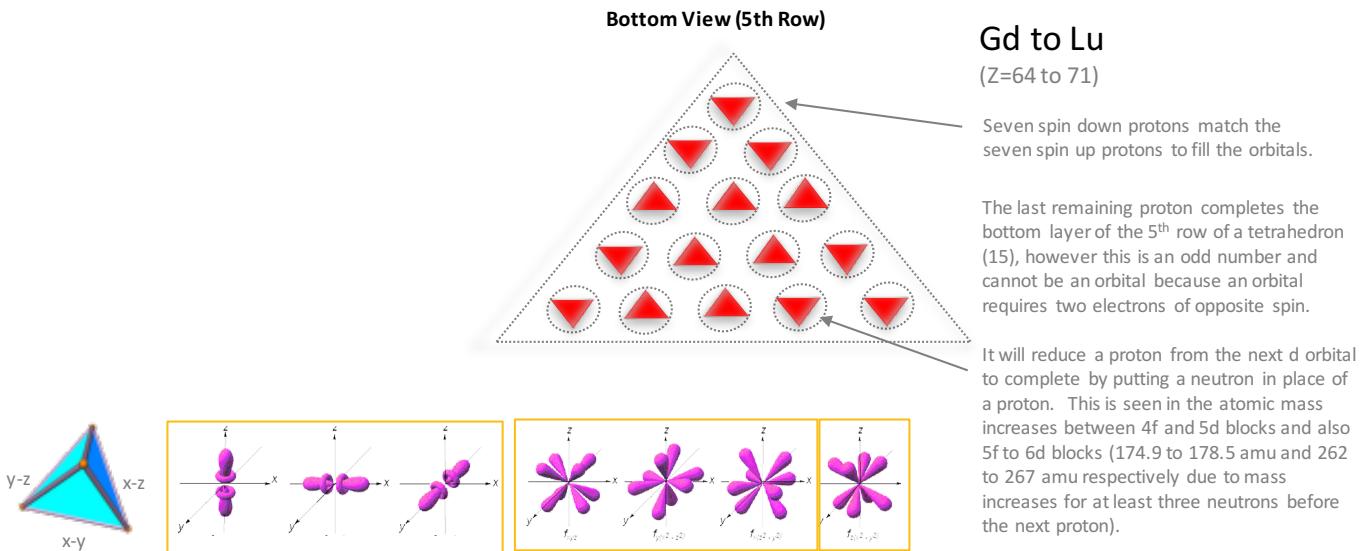


Fig. 3.2.19 – Fill order of the remaining f orbital electrons (bottom view shown)

Using the same rules that enabled the calculations of orbital distances in Section 2, specifically that the proton is a pentaquark with gluons that align to cause a repelling force, the probability nature and shape of orbitals can be logically explained. The shapes match a nucleus structure that is based on a tetrahedral sequence. This nucleus structure is then further validated by the atomic element sequence seen in the Periodic Table of Elements, described in more detail in the next section.

4. Atomic Element Sequence

In the previous section, tetrahedral structures were proposed for the nucleus structure due to the geometric stability in three-dimensional space for particles that are constantly moving to minimize wave amplitude.

In this section, this tetrahedral structure is further explained and related to the atomic element sequence from the Periodic Table of Elements.¹⁶ In addition to orbital shapes, this structure also explains the transitions of s, p, d and f blocks. The rules of nucleon stacking explain the sequence in the periodic table: 1s, 2s, 2p, 3s, 3p, 4s, 3d, 4p, 5s, 4d, 5p, 6s, 4f, 5d, 6p, 7s, 5f, 6d, 7p which are circled in red in Fig. 4.1.

○ Completion of a tetrahedral row

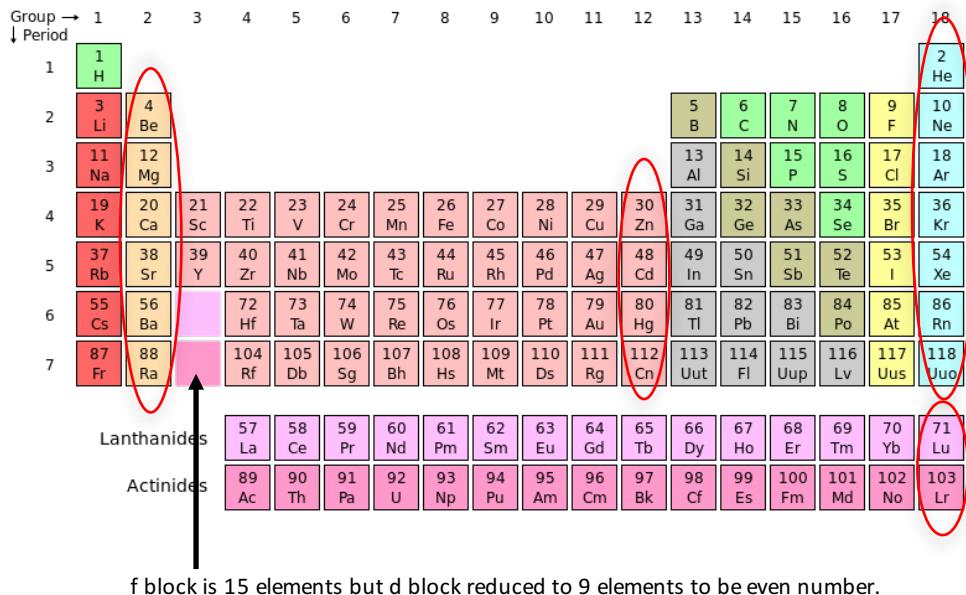


Fig. 4.1 – Periodic Table of Elements – Annotated marking sequence completion

Nucleon Stacking Rules

A set of rules was established for nucleons (protons and neutrons) stacking in an atomic nucleus to match the sequence of the Periodic Table of Elements and also meeting the proton fill order for orbital shapes as shown in Section 3. Each of these rules are ultimately a result of the fundamental rule that subatomic particles that form these composite particles (nucleons) move to minimize wave amplitude.

1. Nucleons **arrange from the center** first, then outward.
2. A **neutron may replace a proton** (in the proton's position), but not vice versa, due to proton separation rules.
3. **Each level fills the easiest proton spin first**, which is the same spin direction as the atom (it takes less energy/wave amplitude). Then, the opposite spin direction is filled.
4. Protons first form a linear structure (1s), then planar structure (2s), **before building in three dimensions in a tetrahedral structure** (2p).

- After the first complete tetrahedron (2p), **the nucleons build symmetrically - a second tetrahedron.**
- Nucleons maintain a required proton to neutron ($p \rightarrow n$) and proton to proton ($p \rightarrow p$) separation rule.

Legend

Fig. 4.2 shows a legend of nucleon stacking in the upcoming models that will be presented. A proton is represented in red and neutron in blue color. To reduce complexity viewing the models, only neutrons that replace a proton are shown. In the atomic nucleus, neutrons separate protons at required distances. These separation neutrons are not shown in the models to simplify the diagrams, although an example is provided in Fig. 4.2. A neutron can also take a proton's position. These protons will be shown in the models because they are required to complete a tetrahedral row.

Only the side view of the atomic nucleus is shown in the models. Using the tetrahedron numbers from Fig. 3.1, it is easy to decipher how many total nucleons are in each row despite what is shown in the side view. For example, a second-level tetrahedron shows two nucleons in a side view, yet there is a total of three nucleons (the third is positioned behind the first two). This is also illustrated in the legend in Fig. 4.2.

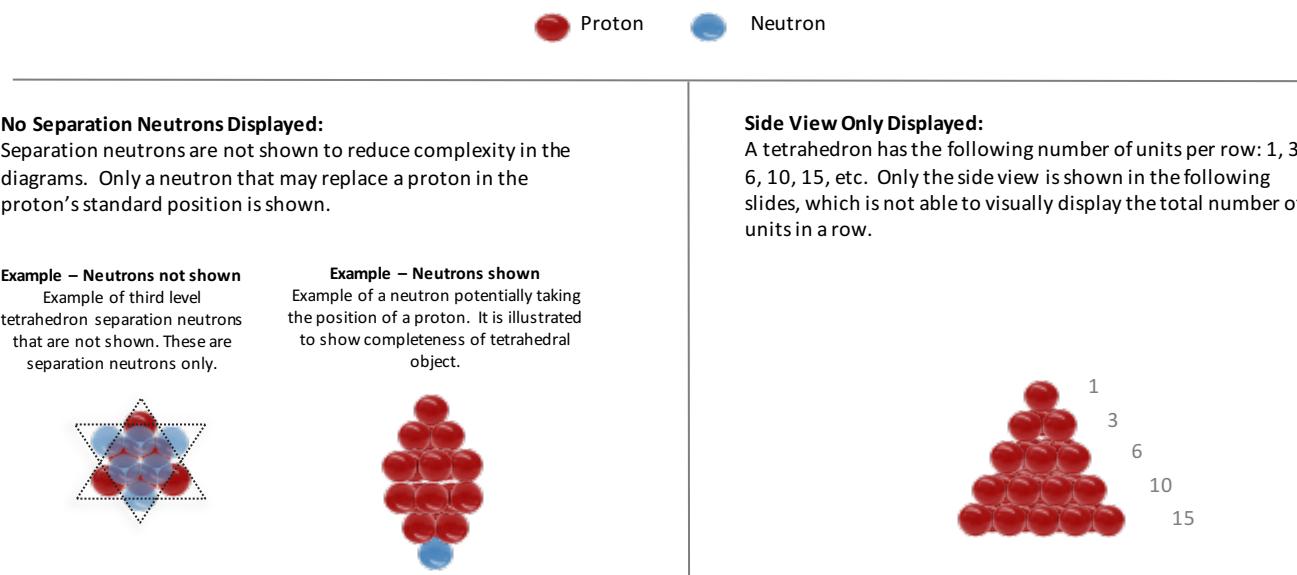


Fig. 4.2 – Nucleon stacking legend

Nucleon Stacking – to d Orbital

Using the aforementioned nucleon stacking rules and legend, a model of the atomic nucleus from 1s to 3d was established. The periodic table sequence corresponds to a completion of a row in the tetrahedral-based structure. Argon (Ar) shows an example of completing a stable tetrahedral structure, but using a neutron in the place of a proton. This is validated by the fact that argon ($Z=18$) has the same nucleon count as calcium ($Z=20$) as noted by the atomic mass units (amu).¹⁷

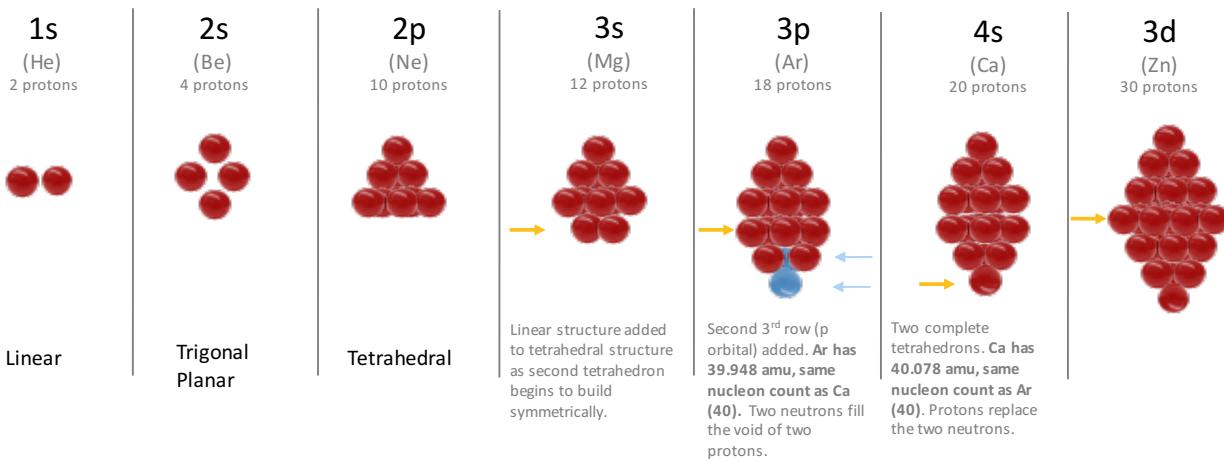


Fig. 4.3 – Nucleon stacking from 1s to 3d atomic elements (He to Zn)

Nucleon Stacking – to f Orbital (*potential arrangement*)

The nucleon stacking model was continued through the first f orbital (Hg), although the variations and possibilities for symmetry become more complex. Thus, these models are potential arrangements that match the nucleon stacking rules to keep symmetry and stability in the nucleus when it corresponds to the end of a block sequence.

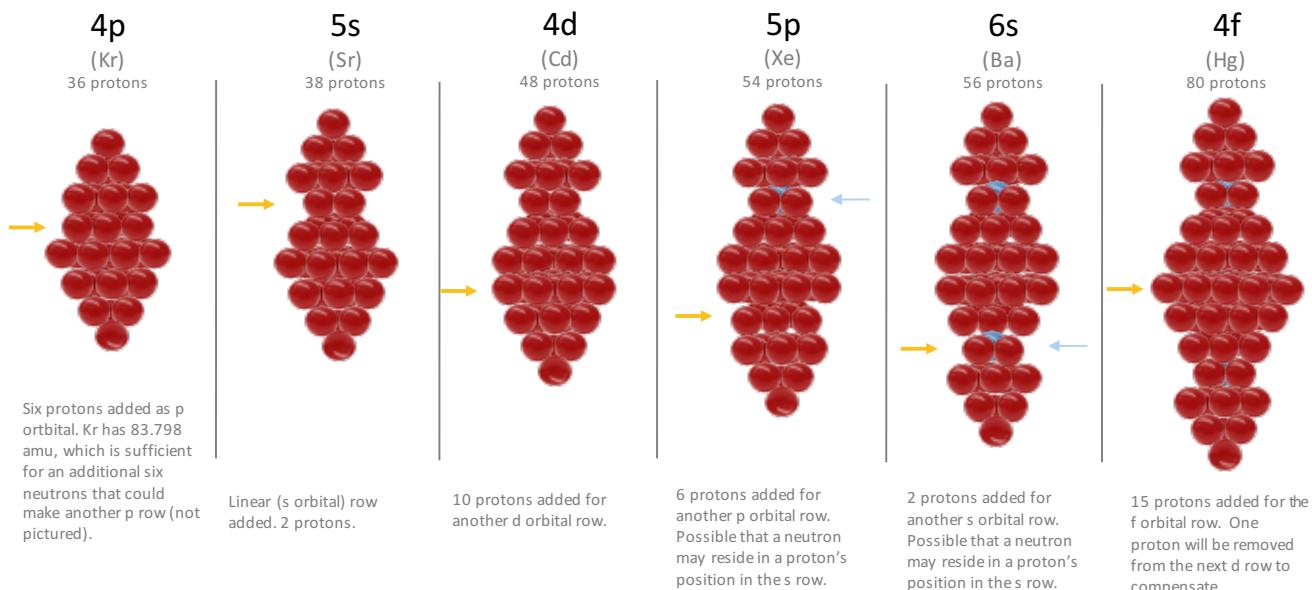


Fig. 4.4 – Nucleon stacking from 4p to 4f atomic elements (Kr to Hg)

5. Conclusion

Atomic orbitals and the behavior of the electron in the presence of an atomic nuclei consisting of one or more protons can be calculated and explained using classical mechanics equations for forces. Specifically, the resting position of the electron is based on the point where the attractive and repulsive forces are equal – known as the point where the sum of the forces is zero.

This required a different model of the proton – using the recently discovered pentaquark structure. The repulsive force is the effect of two quarks in alignment, which produces a strong, axial attraction when within standing wave distance, but is a repelling force beyond these standing waves. This repulsive force is what causes the electron to stay at a distance from the nucleus that becomes the orbital. It also has an attractive force due to the anti-quark in the center of the proton. Because there are distinct points in the proton's spin where the electron experiences this outward, axial force, the electron is constantly being pushed and pulled by the nucleus. This four-quark and one anti-quark configuration of the proton has recently been observed in pentaquark experiments.

After manually calculating the distances for hydrogen and helium and establishing a set of rules and equations, elements beyond lithium required greater computational power to simultaneously solve multiple equations and unknowns as electrons reside in two or more orbital distances. Using Mathcad, orbital distances were solved for elements up to the 4s subshell (calcium), which required computing six equations and six unknowns simultaneously. Elements greater than calcium may be computed in the future with enhanced computer modeling, which will also require better methods for determining specific electron angles.

The orbital distances were compared to measured results of atomic distances and were within reasonable accuracy (exact measurements of atomic orbitals are difficult due to the constantly changing electron's position). Twenty comparisons were charted in Fig. 1.1 for orbital distances. A second method was selected to validate orbital distance that allowed a greater number of comparisons. More than 150 comparisons of calculated ionization energies versus measured energies were provided in Figs. 1.2 to 1.6. This method was chosen as a second validation because orbital distance is required in the calculation of ionization energy.

A classical explanation of the electron's orbit and a pentaquark model of the proton also provides an explanation for the probability cloud of the electron and the shape of the orbital, including quantum leaps. These shapes and leaps are based on the arrangement of the axial force from proton alignment. This led to modeling of the atomic nucleus to explain the exact shape of each orbital and the sequence of the Periodic Table of Elements.

There are several ways to further prove this model:

- Most proton collision experiments produce three quarks. Only recently, pentaquarks (four quarks and one anti-quark) have been discovered in proton collisions. Higher energy proton collisions should yield more observations of the pentaquark if there is sufficient energy to keep the anti-quark from immediately annihilating with one of the quarks. This is the likely reason that most experiments observe three quarks.
- The accuracy of the ionization energies of heavily ionized elements begins to decline as the electron is closer to the nucleus. This is due to electron angles being set to known values based on 0 or 60 degrees, so that the only unknowns in the equations are distances. More precise modeling will require these angles to be also calculated in the solutions instead of estimated. It is expected that the accuracy of the heavily ionized elements calculated in Appendix C would improve with this precise modeling of electron angles.
- Elements greater than calcium can be solved and proven using these equations with computer modeling that is sufficient to handle the required number of unknowns and equations for elements beginning with the 3d subshell.

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Appendix

A. Mathcad Solutions for Orbital Distances

The atomic orbital distances for elements from helium (He) to calcium (Ca) are provided in this section for each of the orbitals (1s, 2s, 2p, 3s, 3p, 4p) using Mathcad to simultaneously solve multiple equations. Hydrogen is provided earlier in this paper as a manual calculation and does not need a complex solver, such as Mathcad.

Due to the complexity of the solution to solve multiple equations, a common constant in each of the equations is removed (Bohr radius), so that the solution provides a ratio of the Bohr radius. **To find the distance in meters, multiply the result by the Bohr radius.**

Helium

Helium

Solve

Guess Values

$$r_{1s} := .05 \quad Z := 2$$

Constraints

$$\frac{Z}{r_{1s}^2} = \frac{1}{(r_{1s} + r_{1s})^2} + \frac{1}{r_{1s}^3}$$

Solver

$$\text{find } (r_{1s}) = 0.571$$

Lithium

Guess Values

$$r_{1s} := .03 \quad r_{2s} := .2 \quad Z := 3$$

Constraints

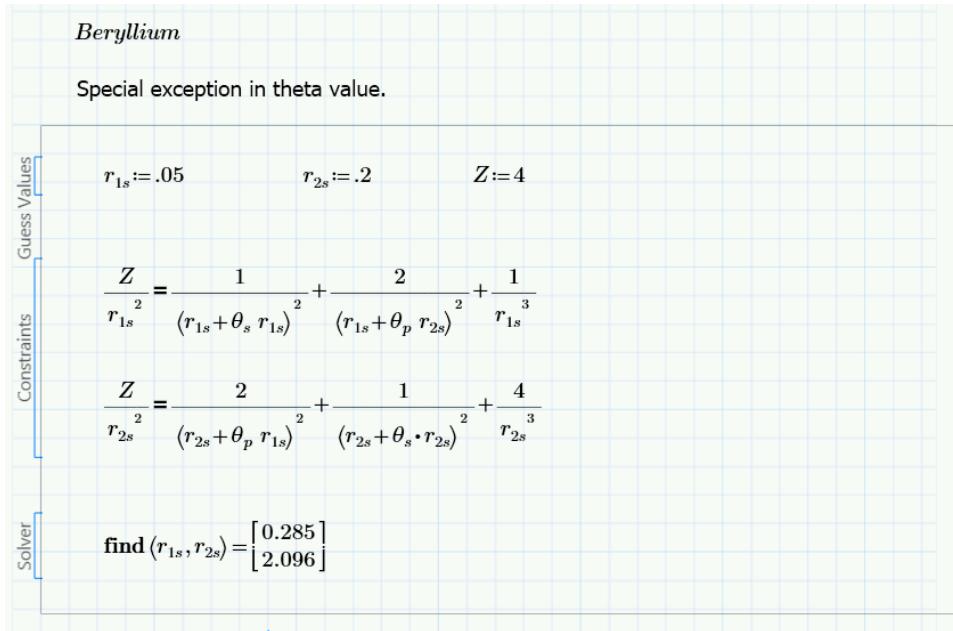
$$\frac{Z}{r_{1s}^2} = \frac{1}{(r_{1s} + \theta_s \cdot r_{1s})^2} + \frac{1}{(r_{1s} + \theta_s \cdot r_{2s})^2} + \frac{1}{r_{1s}^3}$$
$$\frac{Z}{r_{2s}^2} = \frac{2}{(r_{2s} + \theta_s \cdot r_{1s})^2} + \frac{0}{(r_{2s} + \theta_s \cdot r_{2s})^2} + \frac{4}{r_{2s}^3}$$

Solver

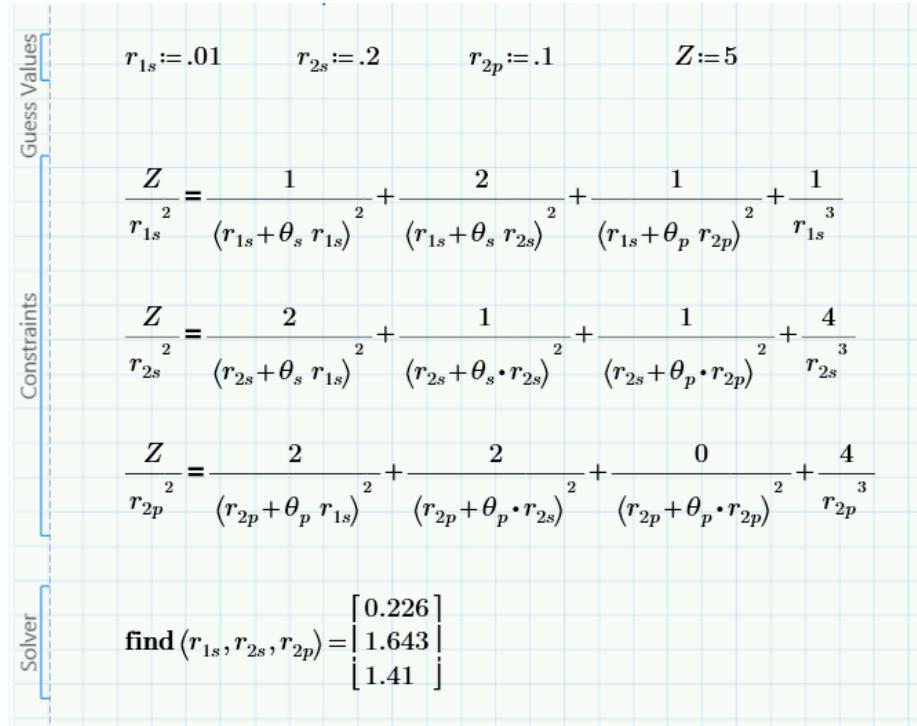
$$\text{find } (r_{1s}, r_{2s}) = \begin{bmatrix} 0.397 \\ 3.272 \end{bmatrix}$$

Beryllium

Beryllium has a special exception in the theta value as it begins to build the 2s configuration.



Boron



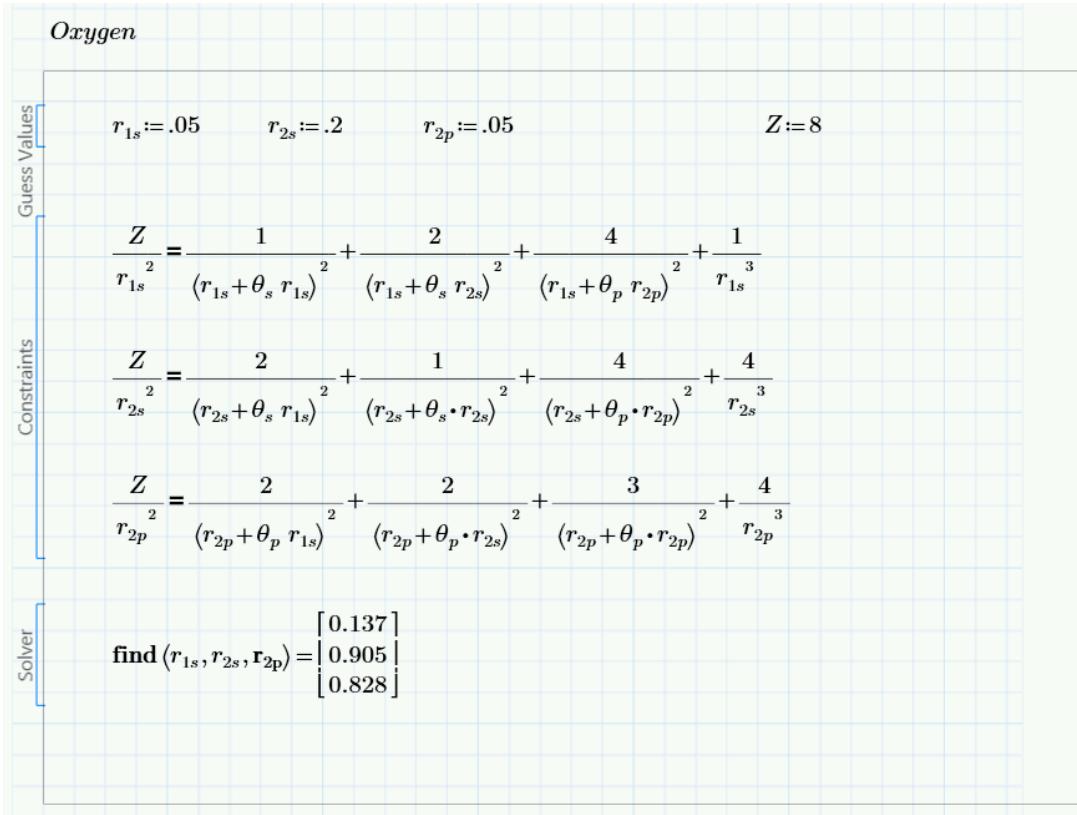
Carbon

Carbon				
Guess Values	$r_{1s} := .01$	$r_{2s} := .2$	$r_{2p} := .2$	
Constraints	$\frac{Z}{r_{1s}^2} = \frac{1}{(r_{1s} + \theta_s r_{1s})^2} + \frac{2}{(r_{1s} + \theta_s r_{2s})^2} + \frac{2}{(r_{1s} + \theta_p r_{2p})^2} + \frac{1}{r_{1s}^3}$ $\frac{Z}{r_{2s}^2} = \frac{2}{(r_{2s} + \theta_s r_{1s})^2} + \frac{1}{(r_{2s} + \theta_s \cdot r_{2s})^2} + \frac{2}{(r_{2s} + \theta_p \cdot r_{2p})^2} + \frac{4}{r_{2s}^3}$ $\frac{Z}{r_{2p}^2} = \frac{2}{(r_{2p} + \theta_p r_{1s})^2} + \frac{2}{(r_{2p} + \theta_p \cdot r_{2s})^2} + \frac{1}{(r_{2p} + \theta_p \cdot r_{2p})^2} + \frac{4}{r_{2p}^3}$			
Solver	$\text{find } (r_{1s}, r_{2s}, r_{2p}) = \begin{bmatrix} 0.185 \\ 1.294 \\ 1.143 \end{bmatrix}$			

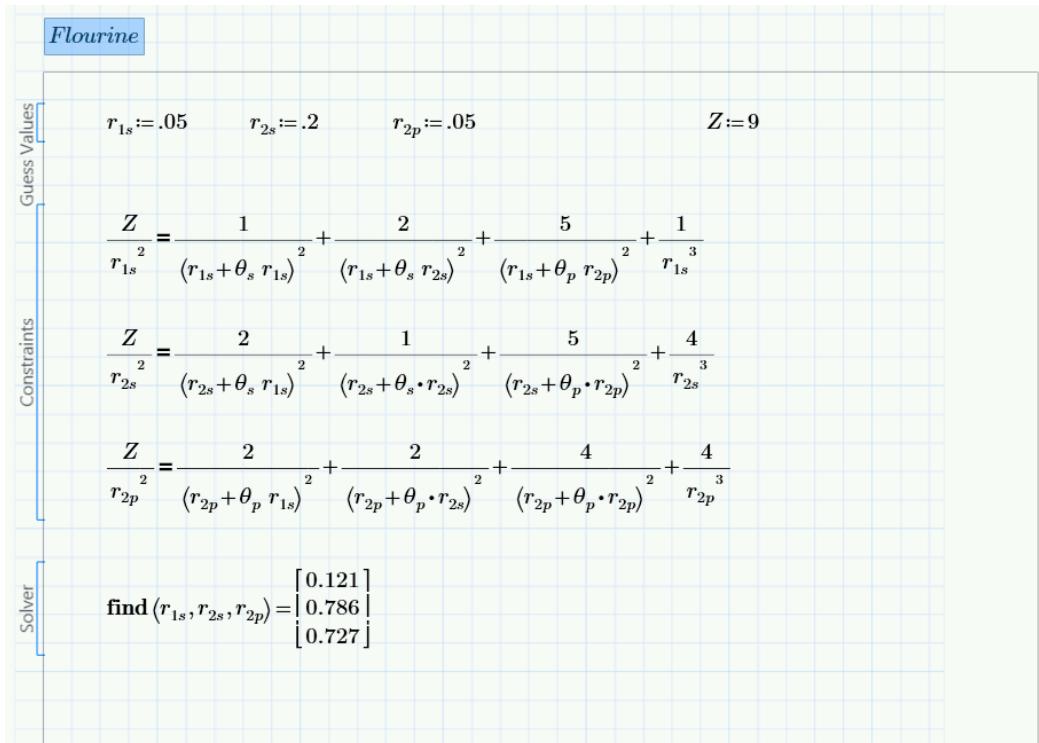
Nitrogen

Nitrogen				
Guess Values	$r_{1s} := .05$	$r_{2s} := .3$	$r_{2p} := .05$	
Constraints	$\frac{Z}{r_{1s}^2} = \frac{1}{(r_{1s} + \theta_s r_{1s})^2} + \frac{2}{(r_{1s} + \theta_s r_{2s})^2} + \frac{3}{(r_{1s} + \theta_p r_{2p})^2} + \frac{1}{r_{1s}^3}$ $\frac{Z}{r_{2s}^2} = \frac{2}{(r_{2s} + \theta_s r_{1s})^2} + \frac{1}{(r_{2s} + \theta_s \cdot r_{2s})^2} + \frac{3}{(r_{2s} + \theta_p \cdot r_{2p})^2} + \frac{4}{r_{2s}^3}$ $\frac{Z}{r_{2p}^2} = \frac{2}{(r_{2p} + \theta_p r_{1s})^2} + \frac{2}{(r_{2p} + \theta_p \cdot r_{2s})^2} + \frac{2}{(r_{2p} + \theta_p \cdot r_{2p})^2} + \frac{4}{r_{2p}^3}$			
Solver	$\text{find } (r_{1s}, r_{2s}, r_{2p}) = \begin{bmatrix} 0.157 \\ 1.066 \\ 0.96 \end{bmatrix}$			

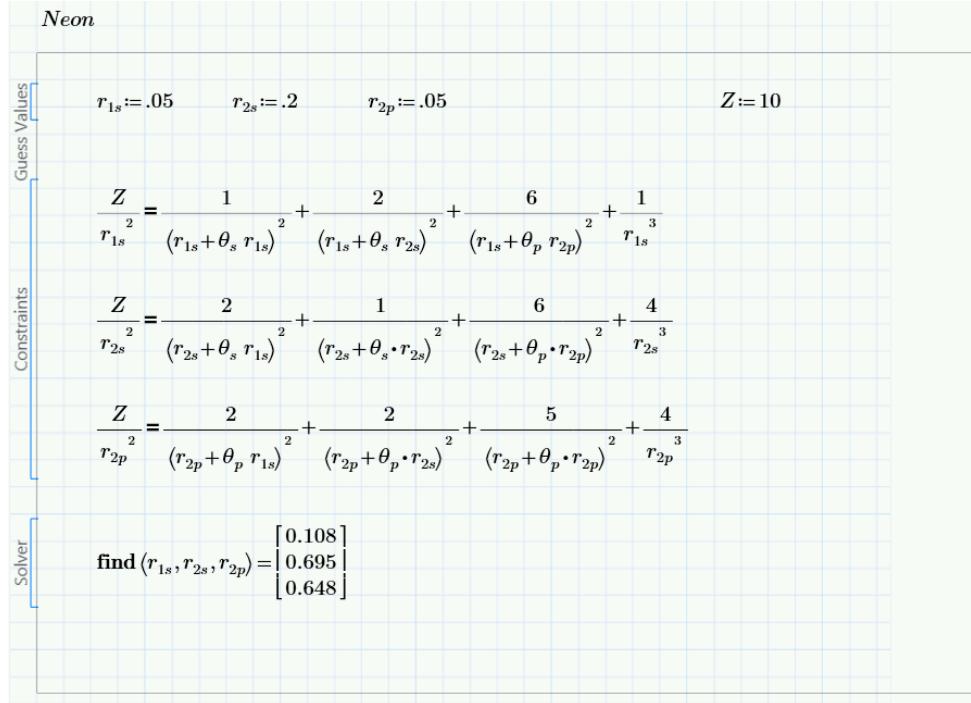
Oxygen



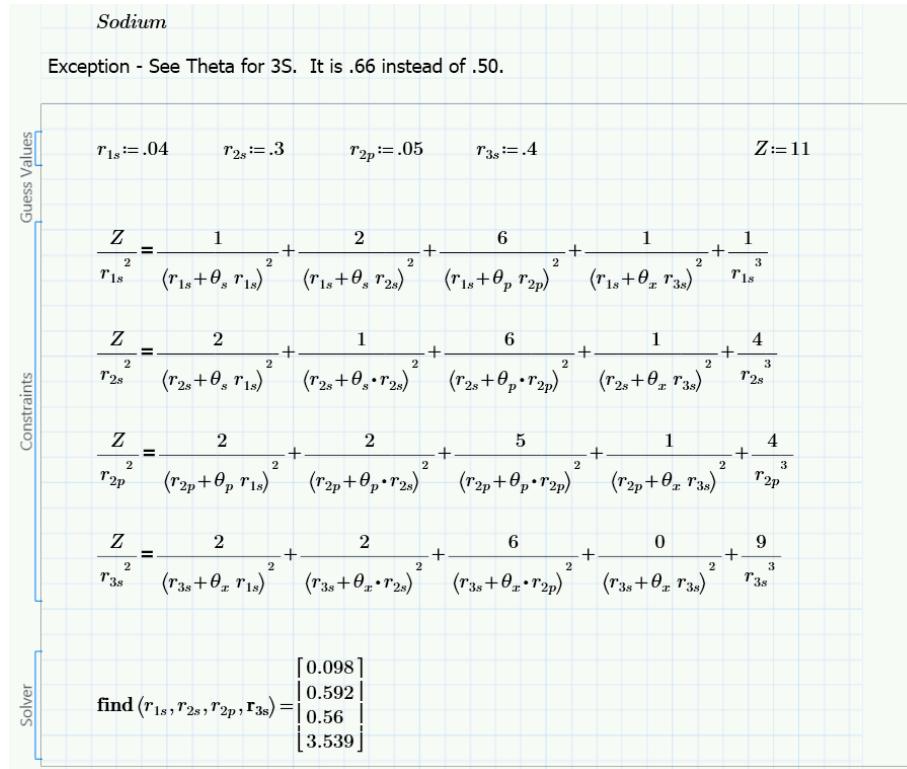
Flourine



Neon



Sodium



Magnesium

Magnesium

Exception - see Theta in 3S. Same exception as Sodium.

$$r_{1s} := .03 \quad r_{2s} := .2 \quad r_{2p} := .05 \quad r_{3s} := .4 \quad Z := 12$$

$$\frac{Z}{r_{1s}^2} = \frac{1}{(r_{1s} + \theta_s r_{1s})^2} + \frac{2}{(r_{1s} + \theta_s r_{2s})^2} + \frac{6}{(r_{1s} + \theta_p r_{2p})^2} + \frac{2}{(r_{1s} + \theta_x r_{3s})^2} + \frac{1}{r_{1s}^3}$$

$$\frac{Z}{r_{2s}^2} = \frac{2}{(r_{2s} + \theta_s r_{1s})^2} + \frac{1}{(r_{2s} + \theta_s r_{2s})^2} + \frac{6}{(r_{2s} + \theta_p r_{2p})^2} + \frac{2}{(r_{2s} + \theta_x r_{3s})^2} + \frac{4}{r_{2s}^3}$$

$$\frac{Z}{r_{2p}^2} = \frac{2}{(r_{2p} + \theta_p r_{1s})^2} + \frac{2}{(r_{2p} + \theta_p r_{2s})^2} + \frac{5}{(r_{2p} + \theta_p r_{2p})^2} + \frac{2}{(r_{2p} + \theta_x r_{3s})^2} + \frac{4}{r_{2p}^3}$$

$$\frac{Z}{r_{3s}^2} = \frac{2}{(r_{3s} + \theta_x r_{1s})^2} + \frac{2}{(r_{3s} + \theta_x r_{2s})^2} + \frac{6}{(r_{3s} + \theta_x r_{2p})^2} + \frac{1}{(r_{3s} + \theta_x r_{3s})^2} + \frac{9}{r_{3s}^3}$$

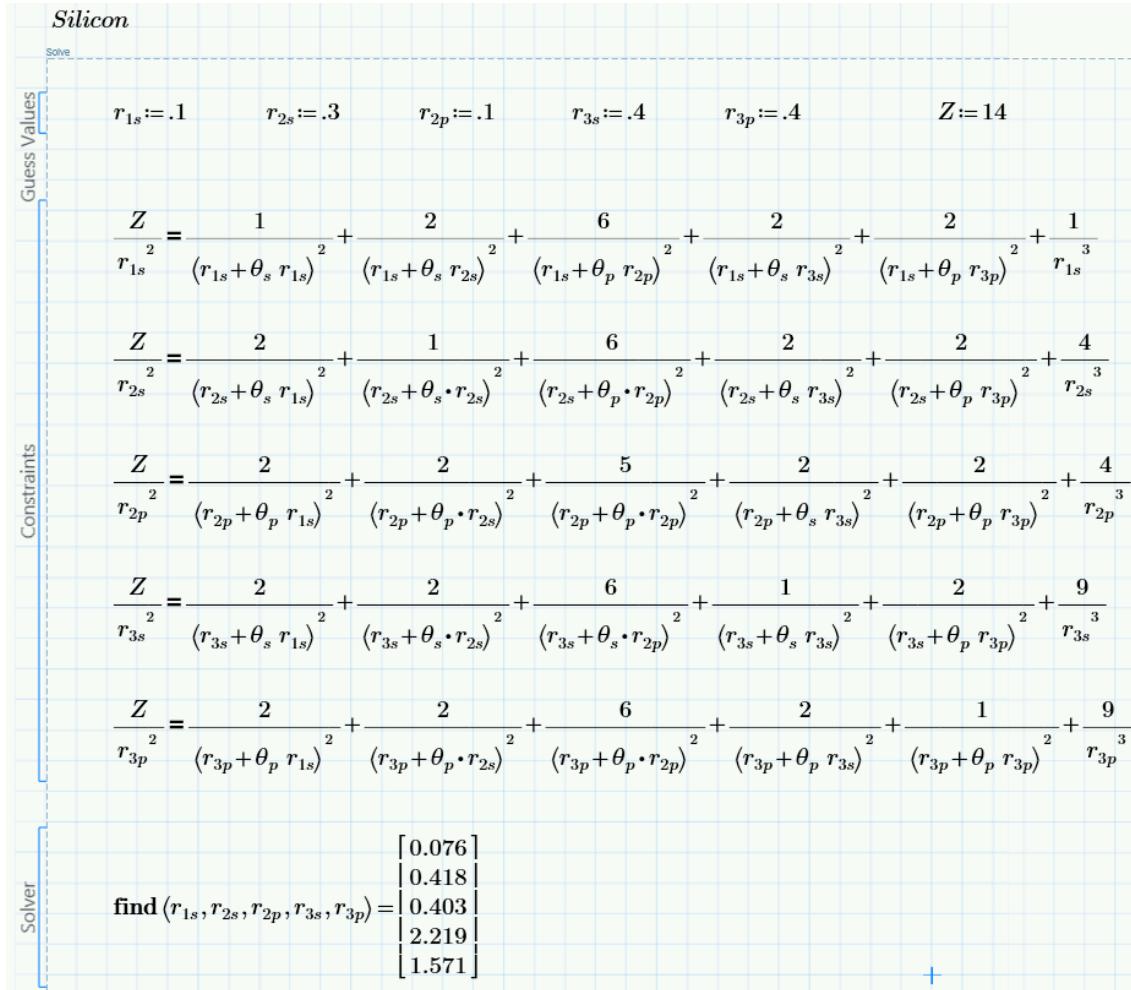
$$\text{find } (r_{1s}, r_{2s}, r_{2p}, r_{3s}) = \begin{bmatrix} 0.089 \\ 0.518 \\ 0.494 \\ 2.623 \end{bmatrix}$$

Aluminum

Aluminum

Guess Values	$r_{1s} := .1$	$r_{2s} := .3$	$r_{2p} := .1$	$r_{3s} := .4$	$r_{3p} := .4$	$Z := 13$
Constraints	$\frac{Z}{r_{1s}^2} = \frac{1}{(r_{1s} + \theta_s r_{1s})^2} + \frac{2}{(r_{1s} + \theta_s r_{2s})^2} + \frac{6}{(r_{1s} + \theta_p r_{2p})^2} + \frac{2}{(r_{1s} + \theta_s r_{3s})^2} + \frac{1}{(r_{1s} + \theta_p r_{3p})^2} + \frac{1}{r_{1s}^3}$					
	$\frac{Z}{r_{2s}^2} = \frac{2}{(r_{2s} + \theta_s r_{1s})^2} + \frac{1}{(r_{2s} + \theta_s r_{2s})^2} + \frac{6}{(r_{2s} + \theta_p r_{2p})^2} + \frac{2}{(r_{2s} + \theta_s r_{3s})^2} + \frac{1}{(r_{2s} + \theta_p r_{3p})^2} + \frac{4}{r_{2s}^3}$					
	$\frac{Z}{r_{2p}^2} = \frac{2}{(r_{2p} + \theta_p r_{1s})^2} + \frac{2}{(r_{2p} + \theta_p r_{2s})^2} + \frac{5}{(r_{2p} + \theta_p r_{2p})^2} + \frac{2}{(r_{2p} + \theta_s r_{3s})^2} + \frac{1}{(r_{2p} + \theta_p r_{3p})^2} + \frac{4}{r_{2p}^3}$					
	$\frac{Z}{r_{3s}^2} = \frac{2}{(r_{3s} + \theta_s r_{1s})^2} + \frac{2}{(r_{3s} + \theta_s r_{2s})^2} + \frac{6}{(r_{3s} + \theta_s r_{2p})^2} + \frac{1}{(r_{3s} + \theta_s r_{3s})^2} + \frac{1}{(r_{3s} + \theta_p r_{3p})^2} + \frac{9}{r_{3s}^3}$					
	$\frac{Z}{r_{3p}^2} = \frac{2}{(r_{3p} + \theta_p r_{1s})^2} + \frac{2}{(r_{3p} + \theta_p r_{2s})^2} + \frac{6}{(r_{3p} + \theta_p r_{2p})^2} + \frac{2}{(r_{3p} + \theta_p r_{3s})^2} + \frac{0}{(r_{3p} + \theta_p r_{3p})^2} + \frac{9}{r_{3p}^3}$					
Solver	$\text{find } (r_{1s}, r_{2s}, r_{2p}, r_{3s}, r_{3p}) = \begin{bmatrix} 0.082 \\ 0.463 \\ 0.444 \\ 2.676 \\ 1.797 \end{bmatrix}$					

Silicon



Phosphorus

Phosphorus

Solve

Guess Values	$r_{1s} := .1$	$r_{2s} := .3$	$r_{2p} := .2$	$r_{3s} := .4$	$r_{3p} := .4$	$Z := 15$
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Constraints

$$\frac{Z}{r_{1s}^2} = \frac{1}{(r_{1s} + \theta_s r_{1s})^2} + \frac{2}{(r_{1s} + \theta_s r_{2s})^2} + \frac{6}{(r_{1s} + \theta_p r_{2p})^2} + \frac{2}{(r_{1s} + \theta_s r_{3s})^2} + \frac{3}{(r_{1s} + \theta_p r_{3p})^2} + \frac{1}{r_{1s}^3}$$

$$\frac{Z}{r_{2s}^2} = \frac{2}{(r_{2s} + \theta_s r_{1s})^2} + \frac{1}{(r_{2s} + \theta_s r_{2s})^2} + \frac{6}{(r_{2s} + \theta_p r_{2p})^2} + \frac{2}{(r_{2s} + \theta_s r_{3s})^2} + \frac{3}{(r_{2s} + \theta_p r_{3p})^2} + \frac{4}{r_{2s}^3}$$

$$\frac{Z}{r_{2p}^2} = \frac{2}{(r_{2p} + \theta_p r_{1s})^2} + \frac{2}{(r_{2p} + \theta_p r_{2s})^2} + \frac{5}{(r_{2p} + \theta_p r_{2p})^2} + \frac{2}{(r_{2p} + \theta_s r_{3s})^2} + \frac{3}{(r_{2p} + \theta_p r_{3p})^2} + \frac{4}{r_{2p}^3}$$

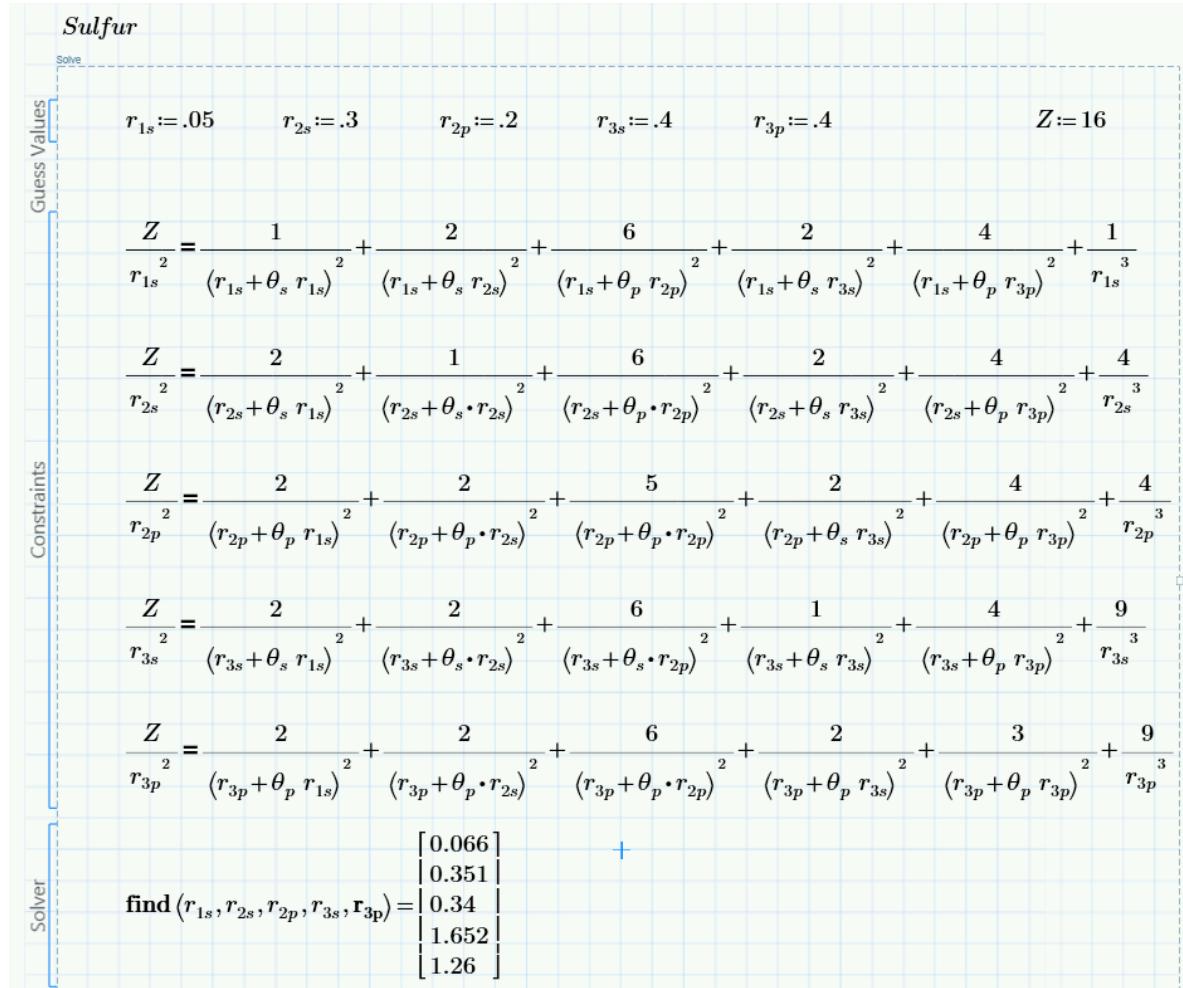
$$\frac{Z}{r_{3s}^2} = \frac{2}{(r_{3s} + \theta_s r_{1s})^2} + \frac{2}{(r_{3s} + \theta_s r_{2s})^2} + \frac{6}{(r_{3s} + \theta_s r_{2p})^2} + \frac{1}{(r_{3s} + \theta_s r_{3s})^2} + \frac{3}{(r_{3s} + \theta_p r_{3p})^2} + \frac{9}{r_{3s}^3}$$

$$\frac{Z}{r_{3p}^2} = \frac{2}{(r_{3p} + \theta_p r_{1s})^2} + \frac{2}{(r_{3p} + \theta_p r_{2s})^2} + \frac{6}{(r_{3p} + \theta_p r_{2p})^2} + \frac{2}{(r_{3p} + \theta_p r_{3s})^2} + \frac{2}{(r_{3p} + \theta_p r_{3p})^2} + \frac{9}{r_{3p}^3}$$

Solver

$$\text{find } (r_{1s}, r_{2s}, r_{2p}, r_{3s}, r_{3p}) = \begin{bmatrix} 0.071 \\ 0.381 \\ 0.369 \\ 1.894 \\ 1.398 \end{bmatrix} +$$

Sulfur



Chlorine

Chlorine

	$r_{1s} := .05$	$r_{2s} := .3$	$r_{2p} := .2$	$r_{3s} := .4$	$r_{3p} := .4$	$Z := 17$
Guess Values						
	$\frac{Z}{r_{1s}^2} = \frac{1}{(r_{1s} + \theta_s r_{1s})^2} + \frac{2}{(r_{1s} + \theta_s r_{2s})^2} + \frac{6}{(r_{1s} + \theta_p r_{2p})^2} + \frac{2}{(r_{1s} + \theta_s r_{3s})^2} + \frac{5}{(r_{1s} + \theta_p r_{3p})^2} + \frac{1}{r_{1s}^3}$					
	$\frac{Z}{r_{2s}^2} = \frac{2}{(r_{2s} + \theta_s r_{1s})^2} + \frac{1}{(r_{2s} + \theta_s r_{2s})^2} + \frac{6}{(r_{2s} + \theta_p r_{2p})^2} + \frac{2}{(r_{2s} + \theta_s r_{3s})^2} + \frac{5}{(r_{2s} + \theta_p r_{3p})^2} + \frac{4}{r_{2s}^3}$					
Constraints	$\frac{Z}{r_{2p}^2} = \frac{2}{(r_{2p} + \theta_p r_{1s})^2} + \frac{2}{(r_{2p} + \theta_p r_{2s})^2} + \frac{5}{(r_{2p} + \theta_p r_{2p})^2} + \frac{2}{(r_{2p} + \theta_s r_{3s})^2} + \frac{5}{(r_{2p} + \theta_p r_{3p})^2} + \frac{4}{r_{2p}^3}$					
	$\frac{Z}{r_{3s}^2} = \frac{2}{(r_{3s} + \theta_s r_{1s})^2} + \frac{2}{(r_{3s} + \theta_s r_{2s})^2} + \frac{6}{(r_{3s} + \theta_s r_{2p})^2} + \frac{1}{(r_{3s} + \theta_s r_{3s})^2} + \frac{5}{(r_{3s} + \theta_p r_{3p})^2} + \frac{9}{r_{3s}^3}$					
	$\frac{Z}{r_{3p}^2} = \frac{2}{(r_{3p} + \theta_p r_{1s})^2} + \frac{2}{(r_{3p} + \theta_p r_{2s})^2} + \frac{6}{(r_{3p} + \theta_p r_{2p})^2} + \frac{2}{(r_{3p} + \theta_p r_{3s})^2} + \frac{4}{(r_{3p} + \theta_p r_{3p})^2} + \frac{9}{r_{3p}^3}$					
Solver	$\text{find } (r_{1s}, r_{2s}, r_{2p}, r_{3s}, r_{3p}) = \begin{bmatrix} 0.062 \\ 0.325 \\ 0.316 \\ 1.465 \\ 1.148 \end{bmatrix}$					

Argon

Argon

Guess Values	$r_{1s} := .05$ $r_{2s} := .3$ $r_{2p} := .2$ $r_{3s} := .4$ $r_{3p} := .4$ $Z := 18$
Constraints	$\frac{Z}{r_{1s}^2} = \frac{1}{(r_{1s} + \theta_s r_{1s})^2} + \frac{2}{(r_{1s} + \theta_s r_{2s})^2} + \frac{6}{(r_{1s} + \theta_p r_{2p})^2} + \frac{2}{(r_{1s} + \theta_s r_{3s})^2} + \frac{6}{(r_{1s} + \theta_p r_{3p})^2} + \frac{1}{r_{1s}^3}$ $\frac{Z}{r_{2s}^2} = \frac{2}{(r_{2s} + \theta_s r_{1s})^2} + \frac{1}{(r_{2s} + \theta_s r_{2s})^2} + \frac{6}{(r_{2s} + \theta_p r_{2p})^2} + \frac{2}{(r_{2s} + \theta_s r_{3s})^2} + \frac{6}{(r_{2s} + \theta_p r_{3p})^2} + \frac{4}{r_{2s}^3}$ $\frac{Z}{r_{2p}^2} = \frac{2}{(r_{2p} + \theta_p r_{1s})^2} + \frac{2}{(r_{2p} + \theta_p r_{2s})^2} + \frac{5}{(r_{2p} + \theta_p r_{2p})^2} + \frac{2}{(r_{2p} + \theta_s r_{3s})^2} + \frac{6}{(r_{2p} + \theta_p r_{3p})^2} + \frac{4}{r_{2p}^3}$ $\frac{Z}{r_{3s}^2} = \frac{2}{(r_{3s} + \theta_s r_{1s})^2} + \frac{2}{(r_{3s} + \theta_s r_{2s})^2} + \frac{6}{(r_{3s} + \theta_s r_{2p})^2} + \frac{1}{(r_{3s} + \theta_s r_{3s})^2} + \frac{6}{(r_{3s} + \theta_p r_{3p})^2} + \frac{9}{r_{3s}^3}$ $\frac{Z}{r_{3p}^2} = \frac{2}{(r_{3p} + \theta_p r_{1s})^2} + \frac{2}{(r_{3p} + \theta_p r_{2s})^2} + \frac{6}{(r_{3p} + \theta_p r_{2p})^2} + \frac{2}{(r_{3p} + \theta_p r_{3s})^2} + \frac{5}{(r_{3p} + \theta_p r_{3p})^2} + \frac{9}{r_{3p}^3}$
Solver	$\text{find } (r_{1s}, r_{2s}, r_{2p}, r_{3s}, r_{3p}) = \begin{bmatrix} 0.058 \\ 0.302 \\ 0.295 \\ 1.316 \\ 1.055 \end{bmatrix}$

Potassium

Guess Values	$r_{1s} := .05 \quad r_{2s} := .3 \quad r_{2p} := .2 \quad r_{3s} := .4 \quad r_{3p} := .4 \quad r_{4s} := .7 \quad Z := 19$
Constraints	$\frac{Z}{r_{1s}^2} = \frac{1}{(r_{1s} + \theta_s r_{1s})^2} + \frac{2}{(r_{1s} + \theta_s r_{2s})^2} + \frac{6}{(r_{1s} + \theta_p r_{2p})^2} + \frac{2}{(r_{1s} + \theta_s r_{3s})^2} + \frac{6}{(r_{1s} + \theta_p r_{3p})^2} + \frac{1}{(r_{1s} + \theta_s r_{4s})^2} + \frac{1}{r_{1s}^3}$ $\frac{Z}{r_{2s}^2} = \frac{2}{(r_{2s} + \theta_s r_{1s})^2} + \frac{1}{(r_{2s} + \theta_s r_{2s})^2} + \frac{6}{(r_{2s} + \theta_p r_{2p})^2} + \frac{2}{(r_{2s} + \theta_s r_{3s})^2} + \frac{6}{(r_{2s} + \theta_p r_{3p})^2} + \frac{1}{(r_{2s} + \theta_s r_{4s})^2} + \frac{4}{r_{2s}^3}$ $\frac{Z}{r_{2p}^2} = \frac{2}{(r_{2p} + \theta_p r_{1s})^2} + \frac{2}{(r_{2p} + \theta_p r_{2s})^2} + \frac{5}{(r_{2p} + \theta_p r_{2p})^2} + \frac{2}{(r_{2p} + \theta_s r_{3s})^2} + \frac{6}{(r_{2p} + \theta_p r_{3p})^2} + \frac{1}{(r_{2p} + \theta_s r_{4s})^2} + \frac{4}{r_{2p}^3}$ $\frac{Z}{r_{3s}^2} = \frac{2}{(r_{3s} + \theta_s r_{1s})^2} + \frac{2}{(r_{3s} + \theta_s r_{2s})^2} + \frac{6}{(r_{3s} + \theta_s r_{2p})^2} + \frac{1}{(r_{3s} + \theta_s r_{3s})^2} + \frac{6}{(r_{3s} + \theta_p r_{3p})^2} + \frac{1}{(r_{3s} + \theta_s r_{4s})^2} + \frac{9}{r_{3s}^3}$ $\frac{Z}{r_{3p}^2} = \frac{2}{(r_{3p} + \theta_p r_{1s})^2} + \frac{2}{(r_{3p} + \theta_p r_{2s})^2} + \frac{6}{(r_{3p} + \theta_p r_{2p})^2} + \frac{2}{(r_{3p} + \theta_p r_{3s})^2} + \frac{5}{(r_{3p} + \theta_p r_{3p})^2} + \frac{1}{(r_{3p} + \theta_s r_{4s})^2} + \frac{9}{r_{3p}^3}$ $\frac{Z}{r_{4s}^2} = \frac{2}{(r_{4s} + \theta_p r_{1s})^2} + \frac{2}{(r_{4s} + \theta_p r_{2s})^2} + \frac{6}{(r_{4s} + \theta_p r_{2p})^2} + \frac{2}{(r_{4s} + \theta_p r_{3s})^2} + \frac{6}{(r_{4s} + \theta_p r_{3p})^2} + \frac{0}{(r_{4s} + \theta_s r_{4s})^2} + \frac{16}{r_{4s}^3}$
Solver	$\text{find } (r_{1s}, r_{2s}, r_{2p}, r_{3s}, r_{3p}, r_{4s}) = \begin{bmatrix} 0.055 \\ 0.282 \\ 0.275 \\ 1.147 \\ 0.949 \\ 3.674 \end{bmatrix}$ +

Calcium

Guess Values	$r_{1s} := .05$ $r_{2s} := .3$ $r_{2p} := .2$ $r_{3s} := .4$ $r_{3p} := .4$ $r_{4s} := .7$	$Z := 20$
Constraints	$\frac{Z}{r_{1s}^2} = \frac{1}{(r_{1s} + \theta_s r_{1s})^2} + \frac{2}{(r_{1s} + \theta_s r_{2s})^2} + \frac{6}{(r_{1s} + \theta_p r_{2p})^2} + \frac{2}{(r_{1s} + \theta_s r_{3s})^2} + \frac{6}{(r_{1s} + \theta_p r_{3p})^2} + \frac{2}{(r_{1s} + \theta_s r_{4s})^2} + \frac{1}{r_{1s}^3}$	
	$\frac{Z}{r_{2s}^2} = \frac{2}{(r_{2s} + \theta_s r_{1s})^2} + \frac{1}{(r_{2s} + \theta_s r_{2s})^2} + \frac{6}{(r_{2s} + \theta_p r_{2p})^2} + \frac{2}{(r_{2s} + \theta_s r_{3s})^2} + \frac{6}{(r_{2s} + \theta_p r_{3p})^2} + \frac{2}{(r_{2s} + \theta_s r_{4s})^2} + \frac{4}{r_{2s}^3}$	
	$\frac{Z}{r_{2p}^2} = \frac{2}{(r_{2p} + \theta_p r_{1s})^2} + \frac{2}{(r_{2p} + \theta_p r_{2s})^2} + \frac{5}{(r_{2p} + \theta_p r_{2p})^2} + \frac{2}{(r_{2p} + \theta_s r_{3s})^2} + \frac{6}{(r_{2p} + \theta_p r_{3p})^2} + \frac{2}{(r_{2p} + \theta_s r_{4s})^2} + \frac{4}{r_{2p}^3}$	
	$\frac{Z}{r_{3s}^2} = \frac{2}{(r_{3s} + \theta_s r_{1s})^2} + \frac{2}{(r_{3s} + \theta_s r_{2s})^2} + \frac{6}{(r_{3s} + \theta_s r_{2p})^2} + \frac{1}{(r_{3s} + \theta_s r_{3s})^2} + \frac{6}{(r_{3s} + \theta_p r_{3p})^2} + \frac{2}{(r_{3s} + \theta_s r_{4s})^2} + \frac{9}{r_{3s}^3}$	
	$\frac{Z}{r_{3p}^2} = \frac{2}{(r_{3p} + \theta_p r_{1s})^2} + \frac{2}{(r_{3p} + \theta_p r_{2s})^2} + \frac{6}{(r_{3p} + \theta_p r_{2p})^2} + \frac{2}{(r_{3p} + \theta_p r_{3s})^2} + \frac{5}{(r_{3p} + \theta_p r_{3p})^2} + \frac{2}{(r_{3p} + \theta_s r_{4s})^2} + \frac{9}{r_{3p}^3}$	
	$\frac{Z}{r_{4s}^2} = \frac{2}{(r_{4s} + \theta_p r_{1s})^2} + \frac{2}{(r_{4s} + \theta_p r_{2s})^2} + \frac{6}{(r_{4s} + \theta_p r_{2p})^2} + \frac{2}{(r_{4s} + \theta_p r_{3s})^2} + \frac{6}{(r_{4s} + \theta_p r_{3p})^2} + \frac{1}{(r_{4s} + \theta_s r_{4s})^2} + \frac{16}{r_{4s}^3}$	
Solver	$\text{find } (r_{1s}, r_{2s}, r_{2p}, r_{3s}, r_{3p}, r_{4s}) = \begin{bmatrix} 0.052 \\ 0.264 \\ 0.259 \\ 1.023 \\ 0.866 \\ 3.131 \end{bmatrix}$	

B. Orbital Distance Tables

The distances from Appendix A, which is the calculations of the orbital distances using Mathcad and the classical equations found in this paper, are summarized for neutral atoms and for ionized atoms containing one to ten electrons, for each of the orbitals (1s, 2s, 2p, 3s, 4p and 4s). Calculations are provided from hydrogen (H) to calcium (Ca).

The results are a **ratio of the Bohr radius**. E.g. Hydrogen 1s orbital distance is $1.00 * a_0 = 52.92 \text{ pm}$

Neutral Atoms

	H	He	Li	Be	B	C	N	O	F	Ne	Na	Mg	Al	Si	P	S	Cl	Ar	K	Ca						
1s	1.00	0.57	0.40	0.29	0.23	0.19	0.16	0.14	0.12	0.11	0.10	0.09	0.08	0.08	0.07	0.07	0.06	0.06	0.06	0.05						
2s						3.27	2.10	1.64	1.29	1.07	0.91	0.79	0.70	0.59	0.52	0.46	0.42	0.38	0.35	0.33	0.30	0.28	0.26			
2p											1.41	1.14	0.96	0.83	0.73	0.65	0.56	0.49	0.44	0.40	0.37	0.34	0.32	0.30	0.28	0.26
3s															3.54	2.62	2.68	2.22	1.89	1.65	1.47	1.32	1.15	1.02		
3p																	1.80	1.57	1.40	1.26	1.15	1.06	0.95	0.87		
4s																					3.67	3.13				

Ionized Atoms – 1 to 6 Electrons

Ionized atoms are calculated in a similar method using the Mathcad solutions from Appendix B, but changing the number of protons (Z) in the solution. For example, Ca18+ is calcium with 2 electrons. This is the same electron configuration as helium, so the helium Mathcad solution is used, but the Z value is changed to Z=20 instead of Z=2.

		Ionized Atom Distance - 1 Electron Atoms																			
Electrons	1s	1	He1+	Li2+	Be3+	B4+	C5+	N6+	O7+	F8+	Ne9+	Na10+	Mg11+	Al12+	Si13+	P14+	S15+	Cl16+	Ar17+	K18+	Ca19+
Ionized Atom Distance - 2 Electron Atoms																					
Electrons	1s	2	He	Li1+	Be2+	B3+	C4+	N5+	O6+	F7+	Ne8+	Na9+	Mg10+	Al11+	Si12+	P13+	S14+	Cl15+	Ar16+	K17+	Ca18+
Ionized Atom Distance - 3 Electron Atoms																					
Electrons	1s	3	Li	Be1+	B2+	C3+	N4+	O5+	F6+	Ne7+	Na8+	Mg9+	Al10+	Si11+	P12+	S13+	Cl14+	Ar15+	K16+	Ca17+	
	1s			0.397	0.286	0.223	0.183	0.155	0.134	0.118	0.106	0.096	0.087	0.080	0.074	0.069	0.065	0.061	0.057	0.054	0.051
	2s			3.272	1.746	1.203	0.921	0.747	0.628	0.542	0.477	0.426	0.385	0.351	0.323	0.299	0.278	0.26	0.244	0.23	0.217
Ionized Atom Distance - 4 Electron Atoms																					
Electrons	1s	4	Be	B1+	C2+	N3+	O4+	F5+	Ne6+	Na7+	Mg8+	Al9+	Si10+	P11+	S12+	Cl13+	Ar14+	K15+	Ca16+		
	1s			0.285	0.223	0.183	0.155	0.134	0.118	0.106	0.096	0.087	0.080	0.074	0.069	0.065	0.061	0.057	0.054	0.051	
	2s			2.096	1.345	0.998	0.795	0.661	0.567	0.496	0.441	0.397	0.361	0.331	0.305	0.284	0.265	0.248	0.234	0.221	
Ionized Atom Distance - 5 Electron Atoms																					
Electrons	1s	5	B	C1+	N2+	O3+	F4+	Ne5+	Na6+	Mg7+	Al8+	Si9+	P10+	S11+	Cl12+	Ar13+	K14+	Ca15+			
	1s			0.226	0.185	0.157	0.136	0.120	0.107	0.097	0.088	0.081	0.075	0.070	0.065	0.061	0.058	0.055	0.052		
	2s			1.643	1.146	0.885	0.722	0.61	0.528	0.466	0.417	0.378	0.345	0.317	0.294	0.274	0.256	0.241	0.227		
	2p			1.41	1.041	0.824	0.682	0.582	0.508	0.45	0.405	0.367	0.336	0.31	0.288	0.268	0.252	0.237	0.223		
Ionized Atom Distance - 6 Electron Atoms																					
Electrons	1s	6	C	N1+	O2+	F3+	Ne4+	Na5+	Mg6+	Al7+	Si8+	P9+	S10+	Cl11+	Ar12+	K13+	Ca14+				
	1s			0.185	0.157	0.136	0.120	0.107	0.097	0.089	0.081	0.075	0.070	0.065	0.061	0.058	0.055	0.052			
	2s			1.294	0.965	0.773	0.645	0.554	0.486	0.433	0.39	0.355	0.326	0.302	0.28	0.262	0.246	0.232			
	2p			1.143	0.887	0.725	0.613	0.531	0.468	0.419	0.379	0.346	0.318	0.295	0.275	0.257	0.241	0.228			

Ionized Atoms – 7 to 12 Electrons

		Ionized Atom Distance - 7 Electron Atoms													
Electrons	7	N	O1+	F2+	Ne3+	Na4+	Mg5+	Al6+	Si7+	P8+	S9+	Cl10+	Ar11+	K12+	Ca13+
1s		0.157	0.137	0.120	0.108	0.097	0.089	0.082	0.076	0.070	0.066	0.062	0.058	0.055	0.052
2s		1.066	0.833	0.685	0.583	0.508	0.45	0.404	0.367	0.336	0.31	0.287	0.268	0.251	0.236
2p		0.96	0.773	0.647	0.556	0.488	0.434	0.392	0.356	0.327	0.302	0.281	0.263	0.246	0.232
		Ionized Atom Distance - 8 Electron Atoms													
Electrons	8	O	F1+	Ne2+	Na3+	Mg4+	Al5+	Si6+	P7+	S8+	Cl9+	Ar10+	K11+	Ca12+	
1s		0.137	0.121	0.108	0.098	0.089	0.082	0.076	0.070	0.066	0.062	0.058	0.055	0.052	
2s		0.905	0.732	0.615	0.532	0.468	0.419	0.379	0.346	0.318	0.294	0.274	0.256	0.241	
2p		0.828	0.684	0.584	0.509	0.451	0.405	0.368	0.336	0.31	0.288	0.268	0.252	0.237	
		Ionized Atom Distance - 9 Electron Atoms													
Electrons	9	F	Ne1+	Na2+	Mg3+	Al4+	Si5+	P6+	S7+	Cl8+	Ar9+	K10+	Ca11+		
1s		0.121	0.108	0.098	0.089	0.082	0.076	0.071	0.066	0.062	0.058	0.055	0.052		
2s		0.786	0.652	0.558	0.489	0.435	0.392	0.356	0.327	0.302	0.281	0.262	0.246		
2p		0.727	0.614	0.532	0.469	0.419	0.379	0.346	0.319	0.295	0.275	0.257	0.241		
		Ionized Atom Distance - 10 Electron Atoms													
Electrons	10	Ne	Na1+	Mg2+	Al3+	Si4+	P5+	S6+	Cl7+	Ar8+	K9+	Ca10+			
1s		0.108	0.098	0.089	0.082	0.076	0.071	0.066	0.062	0.058	0.055	0.052			
2s		0.695	0.588	0.511	0.452	0.405	0.368	0.336	0.31	0.288	0.268	0.251			
2p		0.648	0.557	0.488	0.435	0.392	0.357	0.327	0.302	0.281	0.263	0.246			
		Ionized Atom Distance - 11 Electron Atoms													
Electrons	11	Na	Mg1+	Al2+	Si3+	P4+	S5+	Cl6+	Ar7+	K8+	Ca9+				
1s		0.098	0.089	0.082	0.076	0.071	0.066	0.062	0.058	0.055	0.052				
2s		0.592	0.516	0.457	0.41	0.371	0.34	0.313	0.29	0.27	0.253				
2p		0.56	0.492	0.439	0.395	0.3	0.33	0.305	0.283	0.265	0.248				
3s		3.539	2.225	1.689	1.38	1.177	1.029	0.916	0.827	0.754	0.693				
		Ionized Atom Distance - 12 Electron Atoms													
Electrons	12	Mg	Al1+	Si2+	P3+	S4+	Cl5+	Ar6+	K7+	Ca8+					
1s		0.089	0.082	0.076	0.071	0.066	0.062	0.058	0.055	0.052					
2s		0.518	0.46	0.413	0.374	0.343	0.316	0.292	0.273	0.255					
2p		0.494	0.441	0.398	0.363	0.333	0.307	0.286	0.267	0.25					
3s		2.623	1.88	1.496	1.255	1.085	0.959	0.861	0.781	0.716					

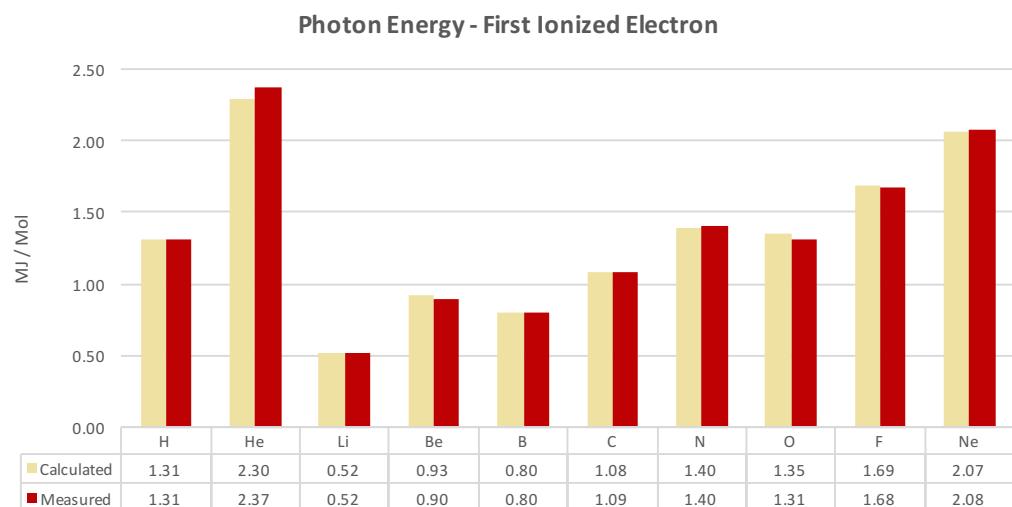
C. Ionization Energies of Atomic Elements

The ionization energies of atomic elements are calculated and compared against measured values for neutral atoms and ionized atoms containing one to ten electrons.

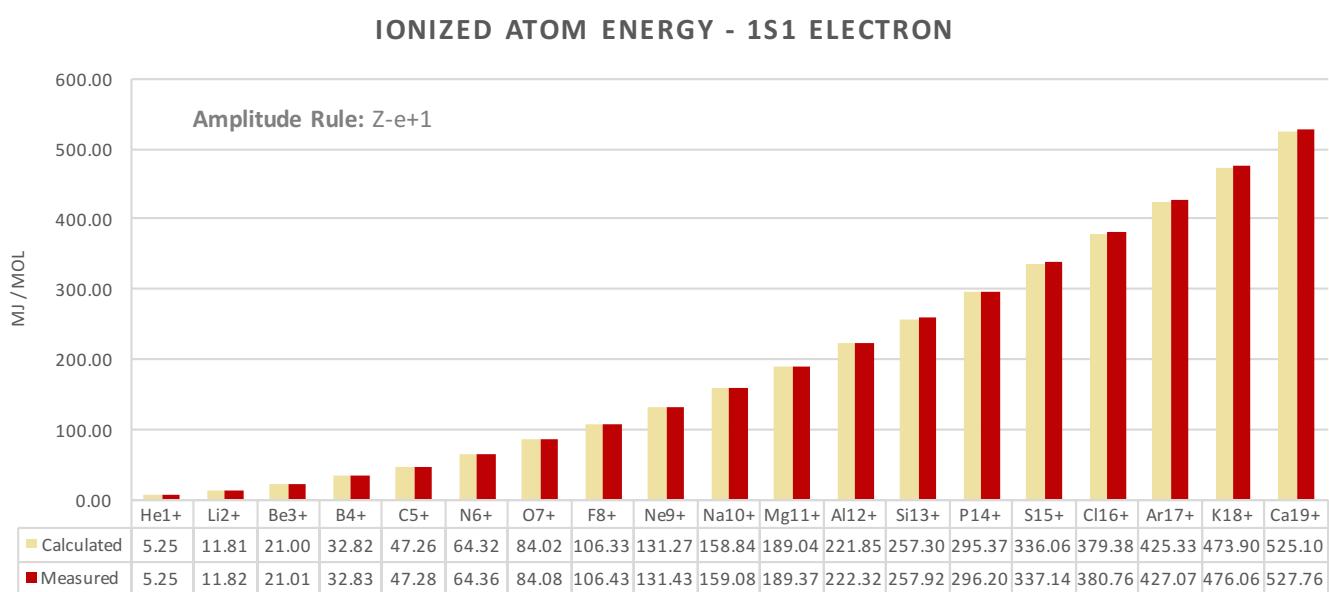
Each of the graphs in this section contains:

- Calculated (column):** Using the Ionization Energy Equation - amplitude factor as shown on graph and orbital distance from tables for ionized electrons in Appendix B.
- Measured (column):** Data values from NIST Atomic Spectra Database (ver. 5.2), [Online]. Available: <http://physics.nist.gov/asd>.

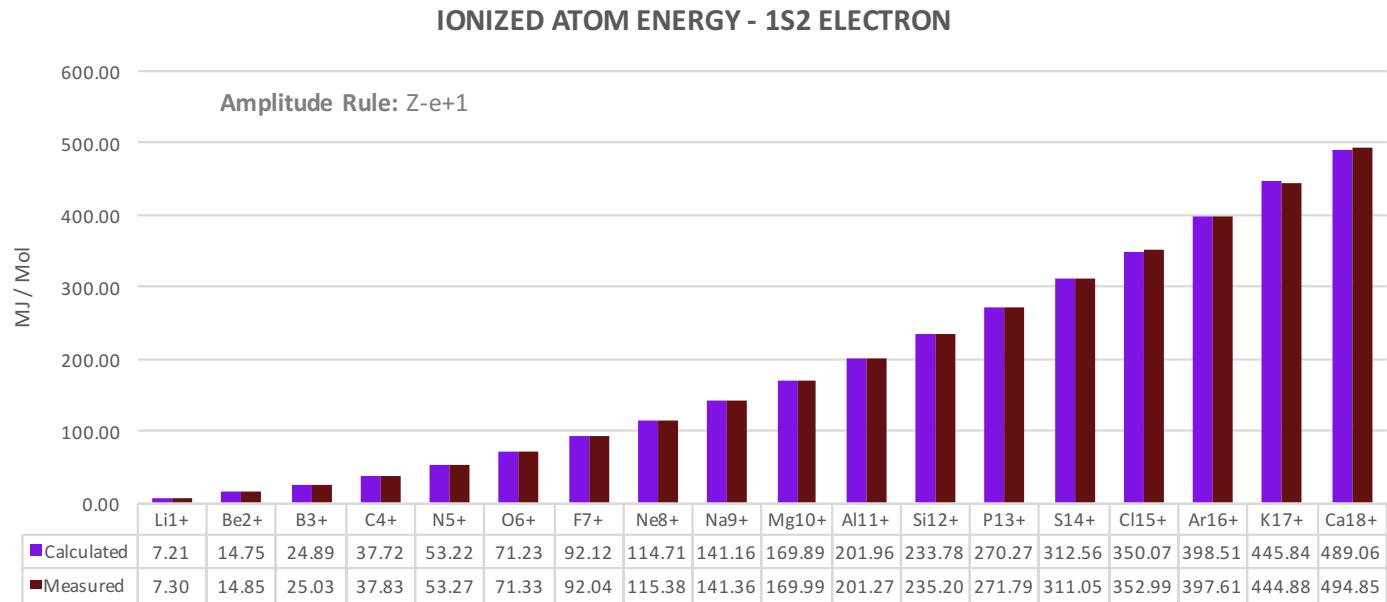
Ionization Energy - Neutral Elements



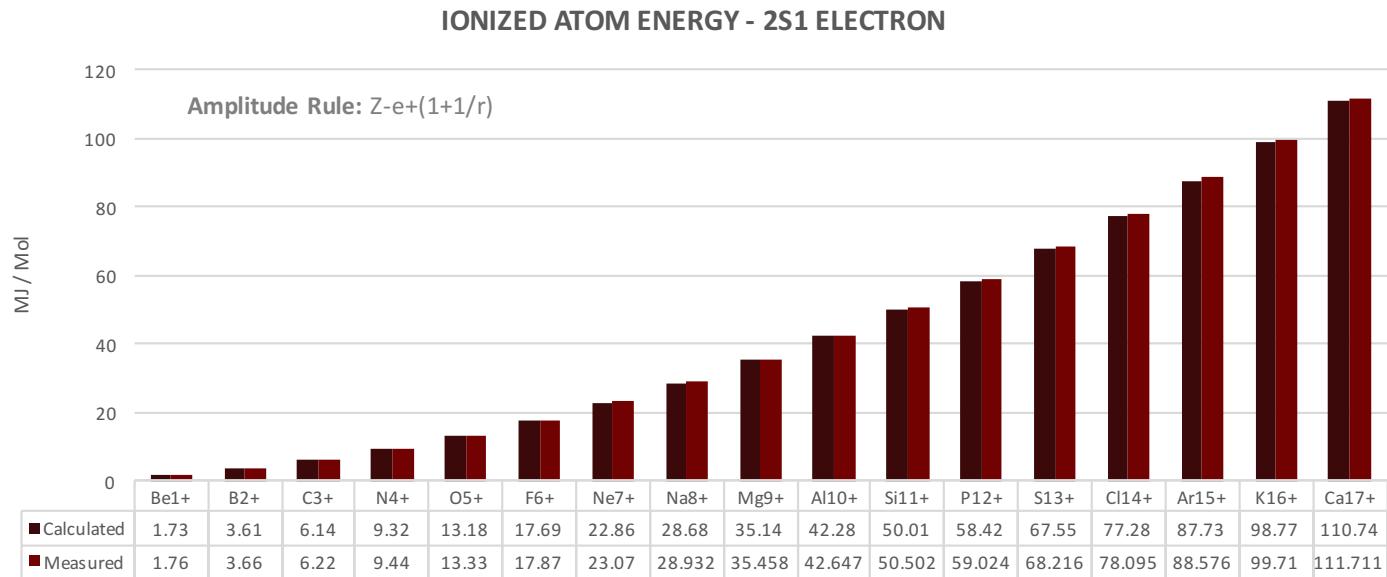
Ionization Energy - Ionized Elements with 1 Electron



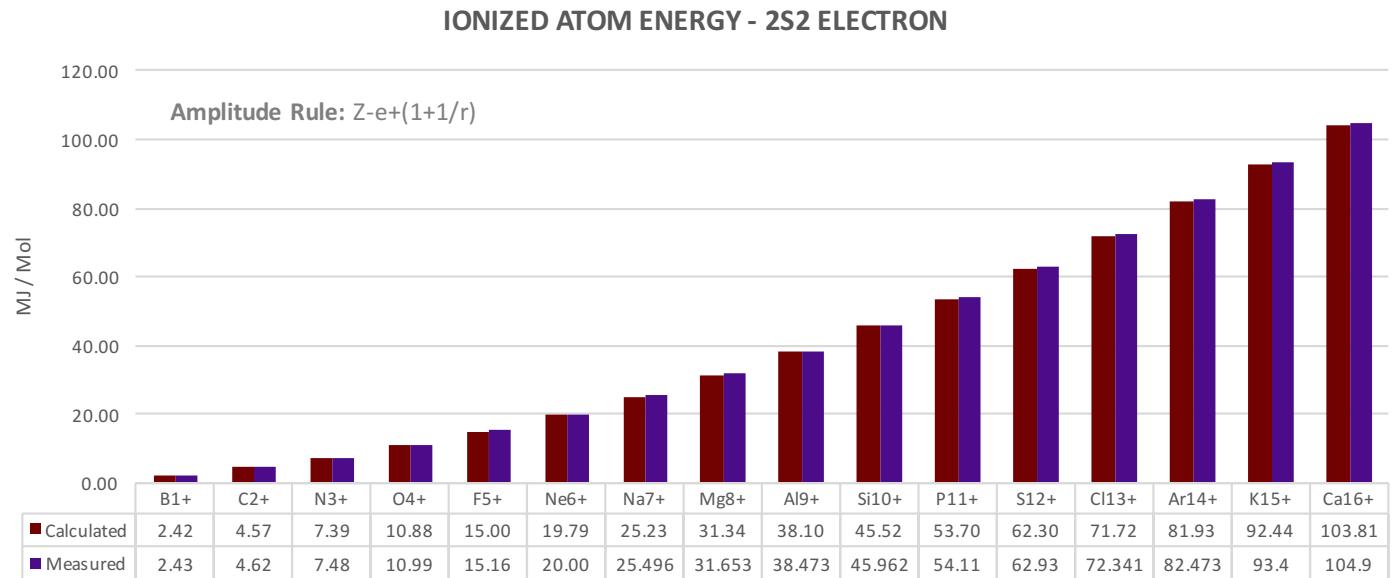
Ionization Energy - Ionized Elements with 2 Electrons



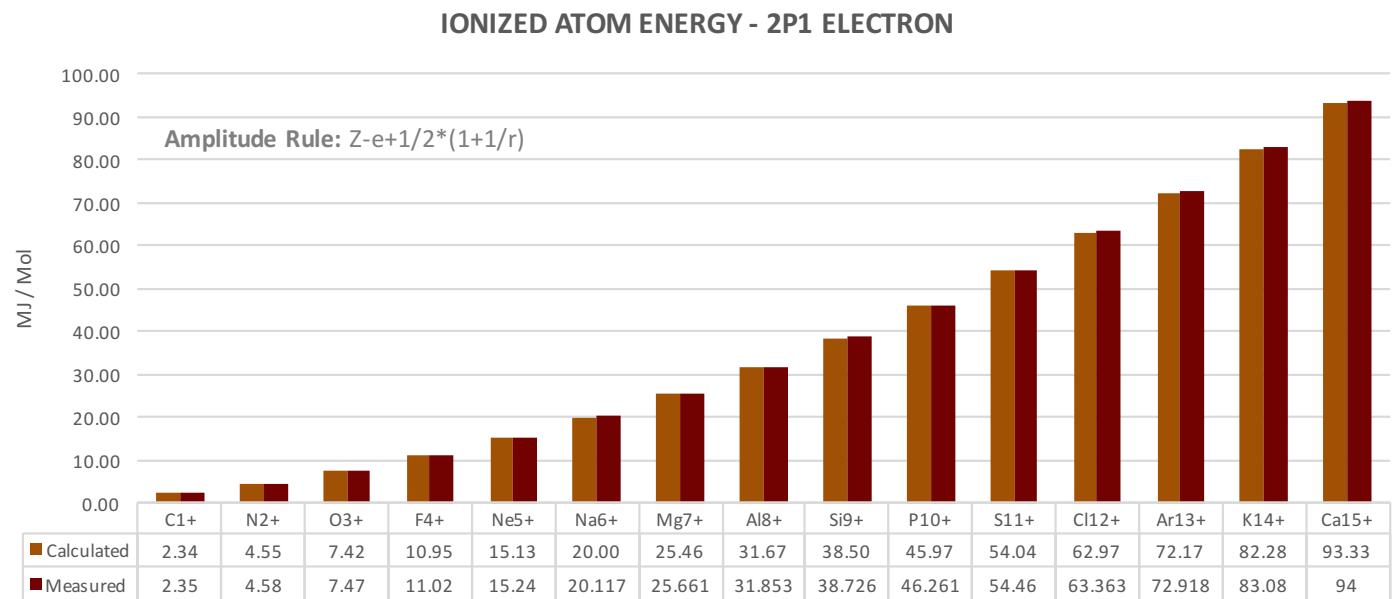
Ionization Energy - Ionized Elements with 3 Electrons



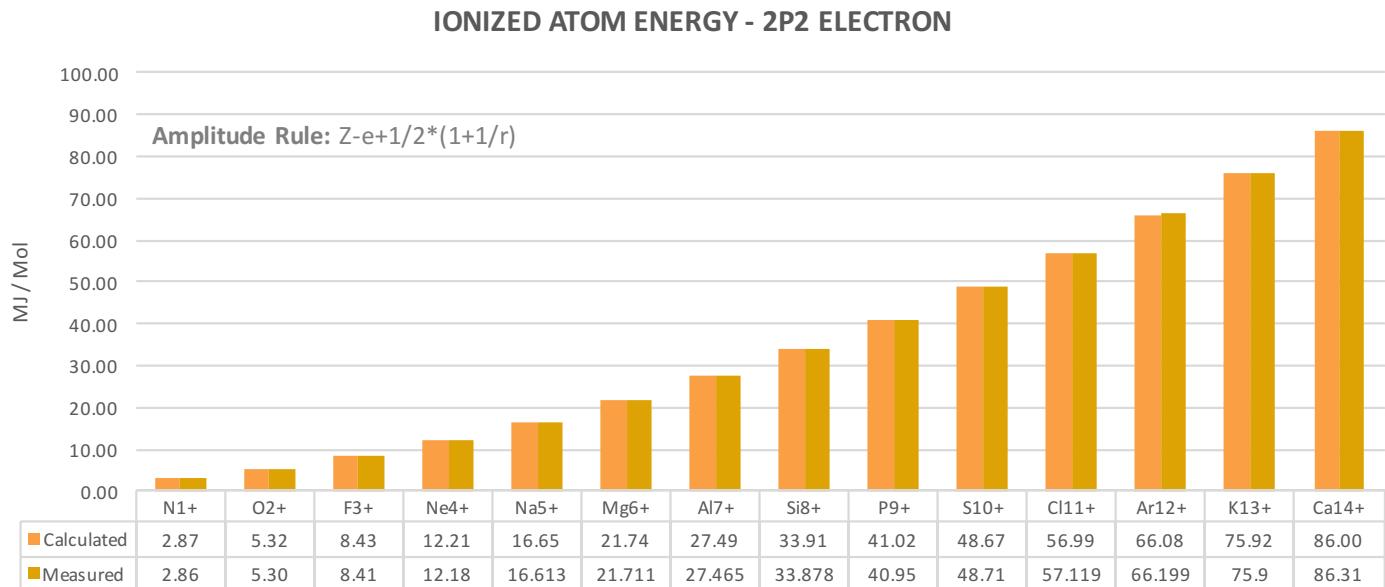
Ionization Energy - Ionized Elements with 4 Electrons



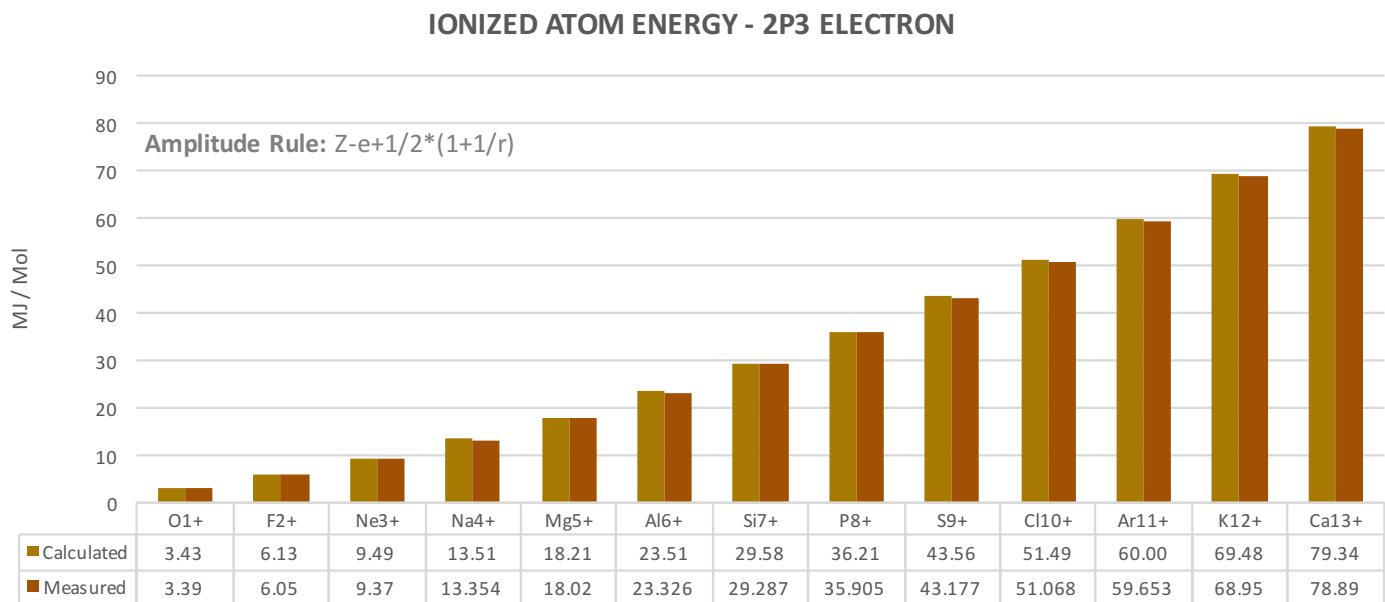
Ionization Energy - Ionized Elements with 5 Electrons



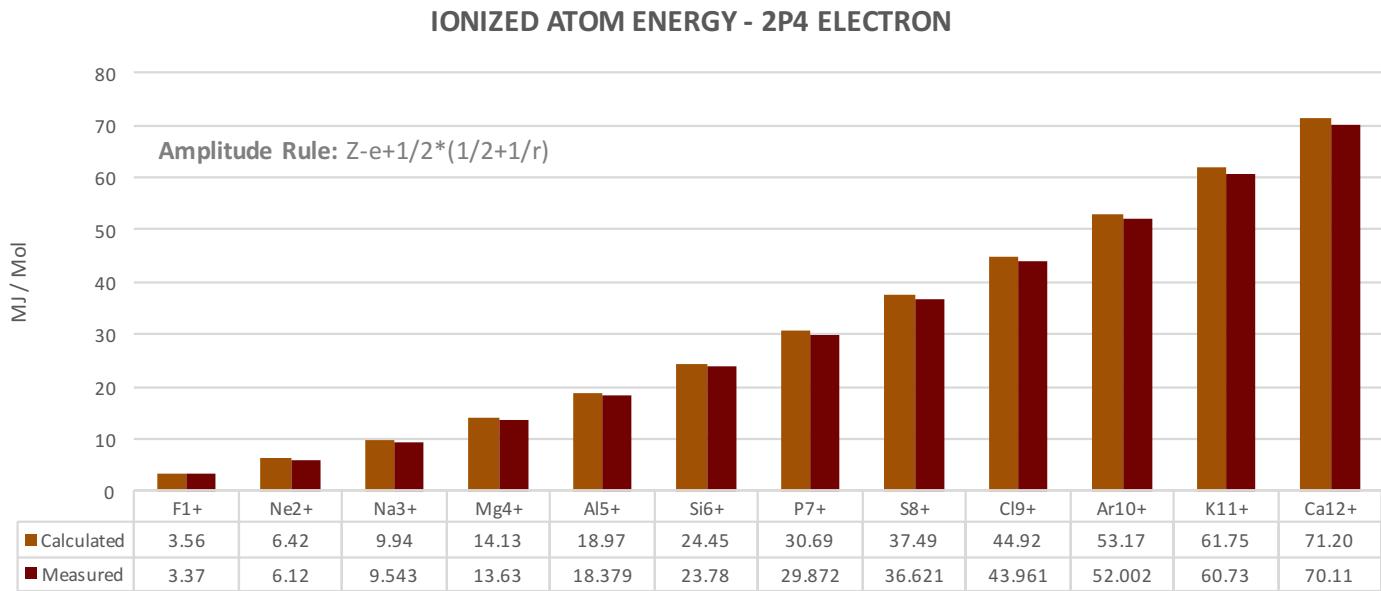
Ionization Energy - Ionized Elements with 6 Electrons



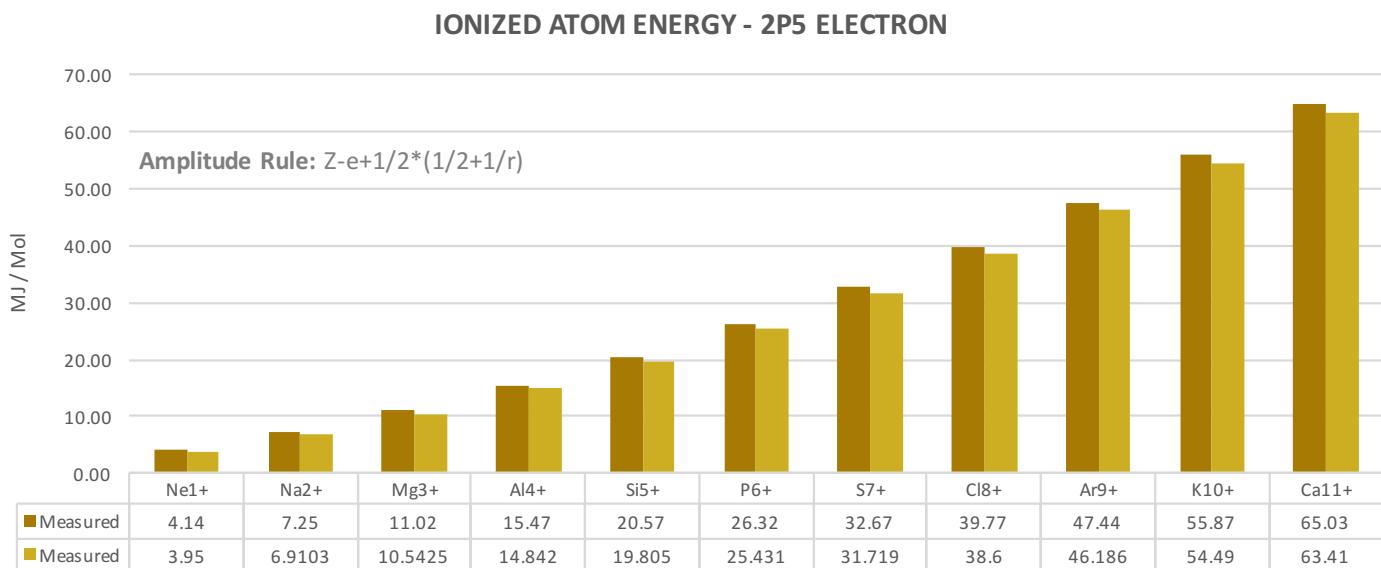
Ionization Energy - Ionized Elements with 7 Electrons



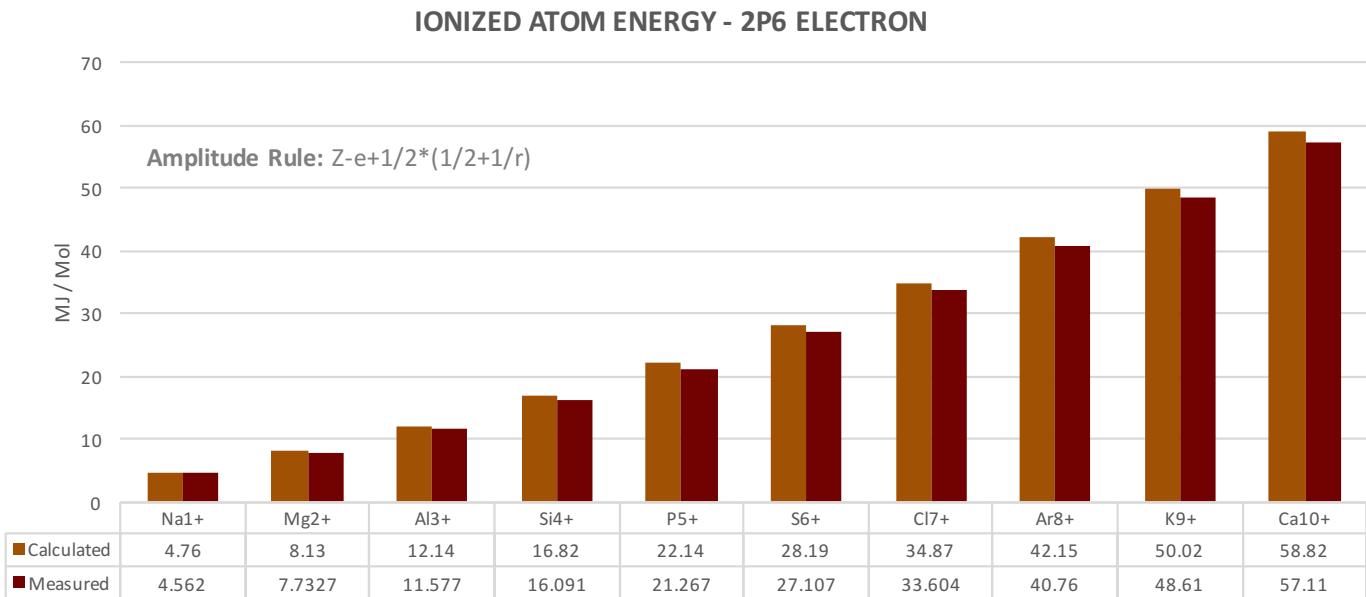
Ionization Energy - Ionized Elements with 8 Electrons



Ionization Energy - Ionized Elements with 9 Electrons



Ionization Energy - Ionized Elements with 10 Electrons



The $2p^6$ configuration is the last atomic element configuration calculated using the estimation method because the accuracy begins to decline.

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- ¹ Yee, J., Atomic Orbitals: Explained and Derived by Energy Wave Equations, Vixra.org [1708.0146](https://vixra.org/pdf/1708.0146.pdf) (2019).
- ² Webelements, Orbital Distances, [Online]. Available: <https://www.webelements.com>
- ³ Data values from NIST Atomic Spectra Database (ver. 5.2), [Online]. Available: <http://physics.nist.gov/asd>
- ⁴ Bohr, N., On the Constitution of Atoms and Molecules - Part II Systems Containing Only a Single Nucleus, Philosophical Magazine **26**, 153, (1913).
- ⁵ Liboff, R., *Introductory Quantum Mechanics*, (Addison-Wesley, Reading, 2002).
- ⁶ BBC, Large Hadron Collider discovers new pentaquark particle, [Online]. Available: <https://www.bbc.com/news/science-environment-33517492>
- ⁷ NIST, CODATA Value of Bohr Radius, [Online]. Available: <https://physics.nist.gov/cgi-bin/cuu/Value?bohrada0>
- ⁸ Mohr, P., Newell, D. and Taylor, B., CODATA Recommended Values of the Fundamental Physical Constants 2014 Rev. Mod. Phys. 88, 035009 (2016).
- ⁹ Zeeman, P., On the influence of Magnetism on the Nature of the Light emitted by a Substance, Phil. Mag. **43**: 226 (1897).
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