

So, quantum mechanics does not define the path that the electron follows; rather, quantum mechanics works by determining the energy of the electron. Once the energy of an electron is known, the probability of finding an electron in a given volume of space can be determined.

Results of Quantum Mechanics

To describe the energy of an electron quantum mechanics tells us we need to know four things about the electron. We need to use four quantum numbers to describe the electron.

Quantum numbers and electrons

It takes four quantum numbers to describe an electron. Additionally, every electron has a unique set of quantum numbers.

n principle quantum number. The base energy level of the electron.

l angular momentum quantum number is the type of orbital (s,p,d,f)

m_l magnetic quantum number is the direction orbital points, number of m_l's determines the number of orbitals that make up an orbital type (1 s orbital, 3 p's, 5 d's)

m_s electron spin quantum number describes the magnetic moment of the electron. Electrons are charged, and they are moving. Moving charged things create magnetic fields (e.g. electromagnets). Spin can be either $+1/2$ or $-1/2$,

- a. discovered by putting atoms and electrons in magnetic fields the magnetic fielding created two new energy levels. Since the electrons were affected by a magnetic field the electrons must be like little magnets. We know that spinning charges create magnetic fields, so the electrons must have "spin" (this does not necessarily mean the electron are spinning in the traditional sense).

- b. 2 allowed spin states—up and down. Since only two new energy levels are observed then there are two possible spin states for an electron.

n is a counting number; i.e., n starts at 1 and counts upwards.

l is $n-1$ down to zero. The size of the quantum state n determines

- how many orbital types are available
 - $n=1$ low energy quantum level, then $l = 0$ (1 orbital type)
 - $n=3$ (higher energy quantum level), then $l = 2, 1, 0$ (three orbital types)
- and the names of the orbital types.
 - quantum state $l = "0"$ named **s**
 - quantum state $l = "1"$ named **p**
 - quantum state $l = "2"$ named **d**
 - quantum state $l = "3"$ named **f**
 - quantum state $l = "4"$ named **g**
 - and on and on....

m_l the size of the quantum state l (orbital type) determines the number of orbitals m_l varies from l to $-l$.

So, an electron could be described as

$$n = 3, l = 2, m_l = -2, \text{ and } m_s = -1/2$$

$$n = 2, l = 0, m_l = 0, \text{ and } m_s = +1/2$$

Cannot be

$$n = 2, l = 0, m_l = 1, \text{ and } m_s = +1/2$$

$$n = 2, l = 2, m_l = -2, \text{ and } m_s = -1/2$$

Shapes of orbitals

an s orbital

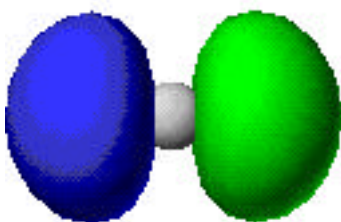


$n = 3, l = 0, m_l = 0$

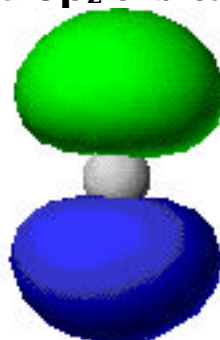
a $3p_x$ orbital



a $3p_y$ orbital

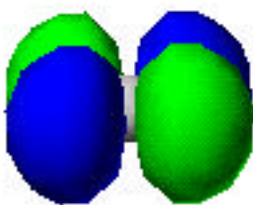


a $3p_z$ orbital



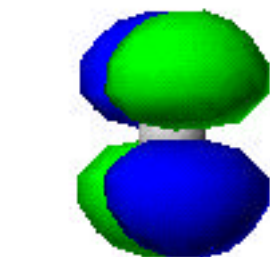
$n = 3, l = 1, m_l = 1$

$3d_{xy}$



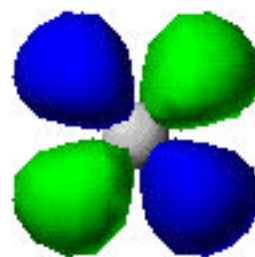
$n = 3, l = 1, m_l = 0$

$3d_{xz}$



$n = 3, l = 1, m_l = -1$

$3d_{yz}$



$n = 3, l = 2, m_l = 2$

$3d_{(x^2+y^2)}$



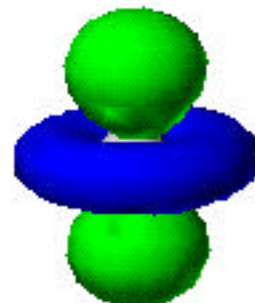
$n = 3, l = 2, m_l = 1$

$3d_{xz}$



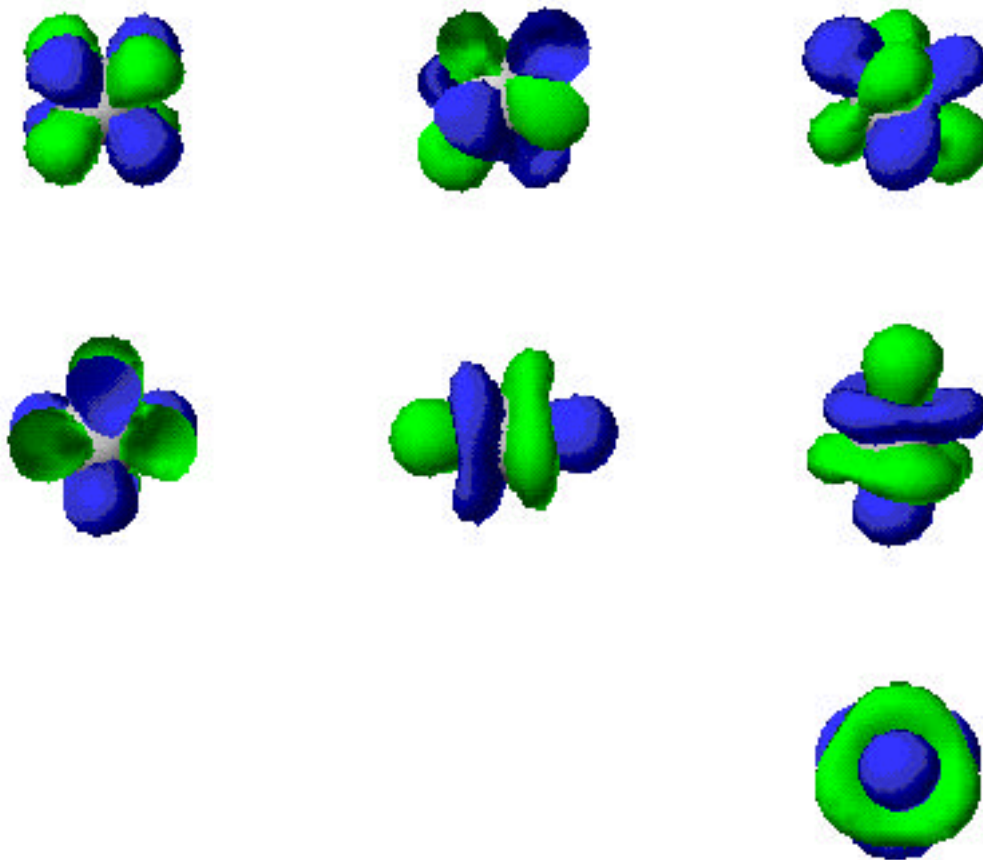
$n = 3, l = 2, m_l = 0$

$3d_{z^2}$



$n = 3, l = 2, m_l = -1$

$n = 3, l = 2, m_l = -2$



$$n = 4, l = 3, m_l = 3 \text{ to } -3$$

f orbitals...these are 4f orbitals. There is no such thing as a 3f orbital!

For an f orbital $l = 3$; therefore, n must be at least 4.

The pictures above are the surfaces within which the electron will be found approximately 90% of the time (actually, I forgot the setting I used when I generated these surfaces).

We can generate a picture of an orbital because quantum mechanics allows us to calculate probability maps, and radial distribution diagrams.

The Energy of an Electron in an Orbital

Above, the 90% probability surfaces are pictured, but more information about the orbital must be known to determine the energy of the electron in an orbital.

Things to consider when determining the energy of an electron in a given orbital.

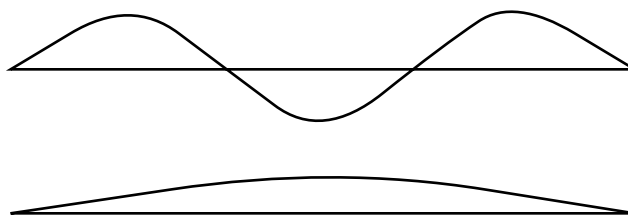
The more attraction between the electron and the nucleus the lower the energy of the electron will be.

When talking about energy, we must consider..

Penetration to the nucleus: the closer the electron can get to the nucleus the lower the energy will be.

Shielding: electrons between the nucleus, and the electron of interest shield the electron from the charge of the nucleus.

Number of nodes: a wave with a lot of nodes has a high energy.



The top wave has more nodes; thus, the wave has a shorter wavelength. The top wave is higher in energy.

Quantum mechanics gives us info about all of these things.

Repulsion between electrons raises the energy of an electron in an orbital. When considering repulsion the only question we must ask is, “Are there two electrons in an orbital.” If there are

two electrons in an orbital, then repulsive forces are present; thus, higher energy.

An additional problem with electrons is the **Electron Correlation Problem**. Since it is impossible for us to know the path of an electron we cannot exactly predict the repulsive forces. Much of the work done in quantum mechanics is the creation of new theories to account for the repulsive forces between the electrons.

Electron Configuration lists all the electrons in the orbitals. The ground state electron configuration is determined by filling in the orbitals from lowest to highest energy.

Draw energy level diagrams.

Energy Level Diagrams

H $1s^1$

The quantum numbers which describe this electron are
 $n = 1, l = 0, m_l = 0, m_s = +1/2$ (or $-1/2$)

↑

He $1s^2$ each orbital can accommodate 2 electrons, one electron
 $m_s = +1/2$ and the other is $m_s = -1/2$.

The quantum numbers which describe the two electrons are
 $n = 1, l = 0, m_l = 0, m_s = +1/2$ and
 $n = 1, l = 0, m_l = 0, m_s = -1/2$

↑↓

Li $1s^2 2s^1$ only two electrons can fit into the same orbital. Every
 electron in an atom must have a unique set of
 quantum number.

The quantum numbers of the first two electrons are
 $n = 1, l = 0, m_l = 0, m_s = +1/2$ and
 $n = 1, l = 0, m_l = 0, m_s = -1/2$

↑

↑↓

The next electron cannot go into the 1s orbital. If the electron did go into the 1s orbital it would have to same set

of quantum numbers as one of the electrons already in the orbital.

So, the third electron goes into a different orbital. Why 2s instead of 2p? Even though the 2s orbital has a node pushing the maximum radial probability out further than a 2p orbital the 2s orbital penetrates to the nucleus better. An electron in the 2s orbital can get closer to the nucleus than an electron in a 2p orbital. So, an electron in the 2s orbital is lower in energy than an electron in a 2p orbital.

The quantum numbers which describe the third electron are
 $n = 2, l = 0, m_l = 0, m_s = +1/2$

Be $1s^2 2s^2$ even though we are pairing electrons, the 2s orbital is lower in energy than the 2p orbital, so it is filled first.	$\uparrow\downarrow$
$n = 1, l = 0, m_l = 0, m_s = +1/2$	
$n = 1, l = 0, m_l = 0, m_s = -1/2$	$\uparrow\downarrow$
$n = 2, l = 0, m_l = 0, m_s = +1/2$	
$n = 2, l = 0, m_l = 0, m_s = -1/2$	

C 6 electrons	$1s^2 2s^2 2p^2$	$\uparrow \uparrow \text{---}$
$n = 1, l = 0, m_l = 0, m_s = +1/2$		$\uparrow\downarrow$
$n = 1, l = 0, m_l = 0, m_s = -1/2$		
$n = 2, l = 0, m_l = 0, m_s = +1/2$		$\uparrow\downarrow$
$n = 2, l = 0, m_l = 0, m_s = -1/2$		
$n = 2, l = 1, m_l = 1, m_s = +1/2$	(We do not know if the electrons	
$n = 2, l = 1, m_l = 0, m_s = +1/2$	are in $m_l = 1, 0, \text{ or } -1$; we just	
	know that they are in different orbitals. Additionally, we do not	
	know what m_s is; by convention we write $+1/2$.)	

Why are the electrons in different p orbitals? Keeping the electrons in separate degenerate (degenerate means the energy is the same) orbitals is lower in energy than pairing the electrons. Electron repulsion raises the energy if you try to put 2 electrons in 1 orbital.

When unpaired electrons are in energy levels with the same energy either spin is possible, but by convention they are up, and parallel.



electrons pair, but when they pair they must have opposite spins



$n = 1, l = 0, m_l = 0, m_s = +1/2$

$n = 1, l = 0, m_l = 0, m_s = -1/2$

$n = 2, l = 0, m_l = 0, m_s = +1/2$

$n = 2, l = 0, m_l = 0, m_s = -1/2$

$n = 2, l = 1, m_l = 1, m_s = +1/2$

$n = 2, l = 1, m_l = 1, m_s = -1/2$

$n = 2, l = 1, m_l = 0, m_s = +1/2$

$n = 2, l = 1, m_l = 0, m_s = -1/2$

$n = 2, l = 1, m_l = -1, m_s = +1/2$

$n = 2, l = 1, m_l = -1, m_s = -1/2$

$n = 3, l = 0, m_l = 0, m_s = +1/2$

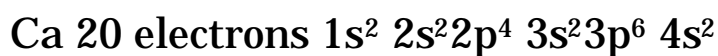
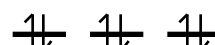
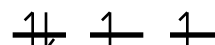
$n = 3, l = 0, m_l = 0, m_s = -1/2$

$n = 3, l = 1, m_l = 1, m_s = +1/2$

$n = 3, l = 1, m_l = 1, m_s = -1/2$

$n = 3, l = 1, m_l = 0, m_s = +1/2$

$n = 3, l = 1, m_l = -1, m_s = +1/2$



$n = 1, l = 0, m_l = 0, m_s = +1/2$

$n = 1, l = 0, m_l = 0, m_s = -1/2$

$n = 2, l = 0, m_l = 0, m_s = +1/2$

$n = 2, l = 0, m_l = 0, m_s = -1/2$

$n = 2, l = 1, m_l = 1, m_s = +1/2$

$n = 2, l = 1, m_l = 1, m_s = -1/2$

$n = 2, l = 1, m_l = 0, m_s = +1/2$

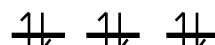
$n = 2, l = 1, m_l = 0, m_s = -1/2$

$n = 2, l = 1, m_l = -1, m_s = +1/2$

$n = 2, l = 1, m_l = -1, m_s = -1/2$

$n = 3, l = 0, m_l = 0, m_s = +1/2$

$n = 3, l = 0, m_l = 0, m_s = -1/2$



$$n = 3, l = 1, m_l = 1, m_s = +1/2$$

$$n = 3, l = 1, m_l = 1, m_s = -1/2$$

$$n = 3, l = 1, m_l = 0, m_s = +1/2$$

$$n = 3, l = 1, m_l = 0, m_s = -1/2$$

$$n = 3, l = 1, m_l = -1, m_s = +1/2$$

$$n = 3, l = 1, m_l = -1, m_s = -1/2$$

There is a shorthand for electron configuration

	longhand	shorthand
O 8 electrons	$1s^2 2s^2 2p^4$	$[\text{He}] 2s^2 2p^4$
S 16 electrons	$1s^2 2s^2 2p^4 3s^2 3p^4$	$[\text{Ne}] 3s^2 3p^4$
Se 34 electrons	$1s^2 2s^2 2p^4 3s^2 3p^4 4s^2 3d^{10} 4p^4$	$[\text{Ar}] 4s^2 3d^{10} 4p^4$
Te 52 electrons	$1s^2 2s^2 2p^4 3s^2 3p^4 4s^2 3d^{10} 4p^4 5s^2 4d^{10} 5p^4$	$[\text{Kr}] 5s^2 4d^{10} 5p^4$

Notice that all 6A end in xs^2xp^4 these are the valence electrons.

The periodic table is set up by valence orbitals. All the elements in a family have the same valence electron configuration.

What are valence electrons? Valence electrons are the electrons in the outermost shell.

Look at ionization energy (energy required to remove an electron from an orbital), huge jump when you go into the core electrons.

Element	I_1	I_2	I_3	I_4	I_5	I_6	I_7
Na	495	4,560					
Mg	735	1,445	7,730				
Al	580	1,815	2,740	11,600			
Si	780	1,575	3,220	4,350	16,100		
P	1,060	1,890	2,905	4,950	6,270	21,200	
S	1,005	2,260	3,375	4,656	6,950	8,490	27,000
Cl	1,255	2,295	3,850	5,160	6,560	9,360	11,000
Ar	1,527	2,665	3,945	5,770	7,230	8,780	12,000

valence electrons

Since the core electrons are held so tightly they do not participate in chemical reactivity. Reactivity of an element is determined by the valence electrons; furthermore, chemical reactions are rearrangements of valence electrons.

Certain trends are observed in the periodic table. Since the periodic table is arranged by valence electron configuration, we should be able to rationalize the trends we observe by applying what we have learned about the energies of the orbitals.

In general the ionization energy increases as one goes across a period. Why?

As we go across the table what changes?

The number of protons in the nucleus increases.

The number of electrons increases too.

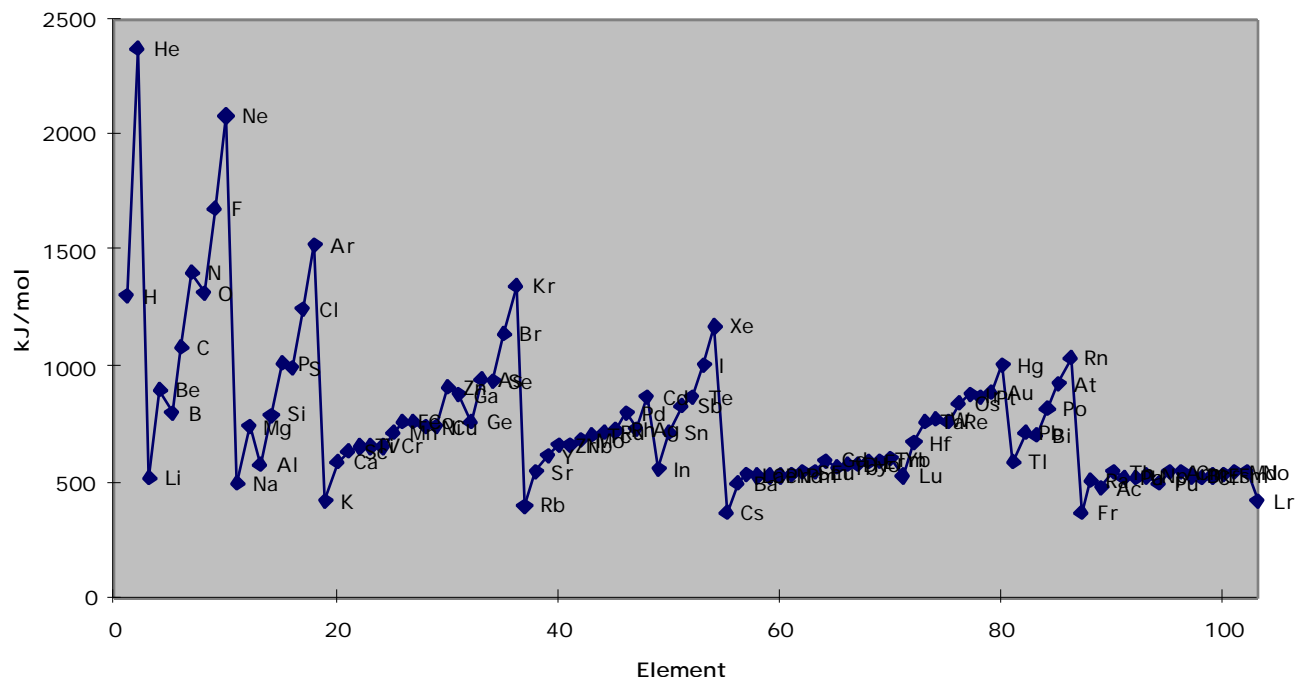
What doesn't change?

The distance between the electrons and the nucleus.

The shielding. All the electrons are going into the same n level, thus you are not putting more electrons between the electron to be removed and the nucleus.

Hey, but there are glitches!

1st Molar Ionization Energy (kJ/mol)



notice drop from Be to B and notice drop in ionization energy from N to O

These cases obviously do not fit into our generalization!

Analyze change from Be to B...

Be 4 protons 4 electrons

electron to be removed is a 2s electron

electron to be removed is shielded from the nucleus by two 1s electrons.

B 5 protons 5 electrons

electron to be removed is a 2p electron

a 2p electron is farther away from the nucleus than a 2s electron

electron to be removed is shielded from the nucleus by two 1s electrons and two 2s electrons.

Boron's electron must be easier to remove because (1) a p electron is farther from the nucleus than an s electron, and (2) a p electron is more effectively shielded from the nuclear charge than an s electron.

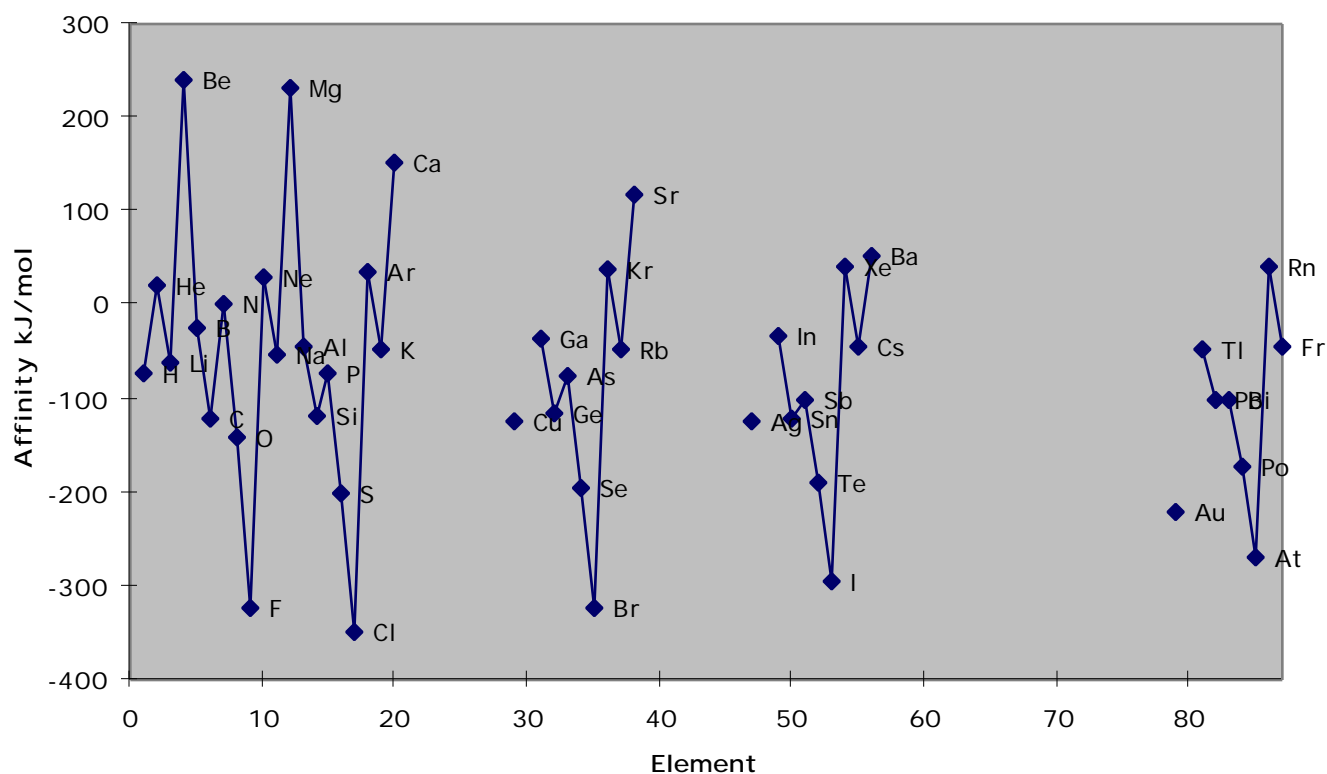
Analyze change from N to O...increased repulsion.

The number of protons increases so the attraction should go up, but it obviously does not.

Cannot explain the difference by considering shielding; shielding is NOT increased.

In N an unpaired electron is removed. In O an electron which is paired is removed. Paired electrons repel each other. The repulsion must overcome the increased nuclear charge.

Electron affinities



Electron affinity is the amount of energy associated with adding 1 electron to an element. As you can see, electron affinity varies with valence configuration.

Adding an electron to H releases energy, whereas adding an electron to He requires energy.

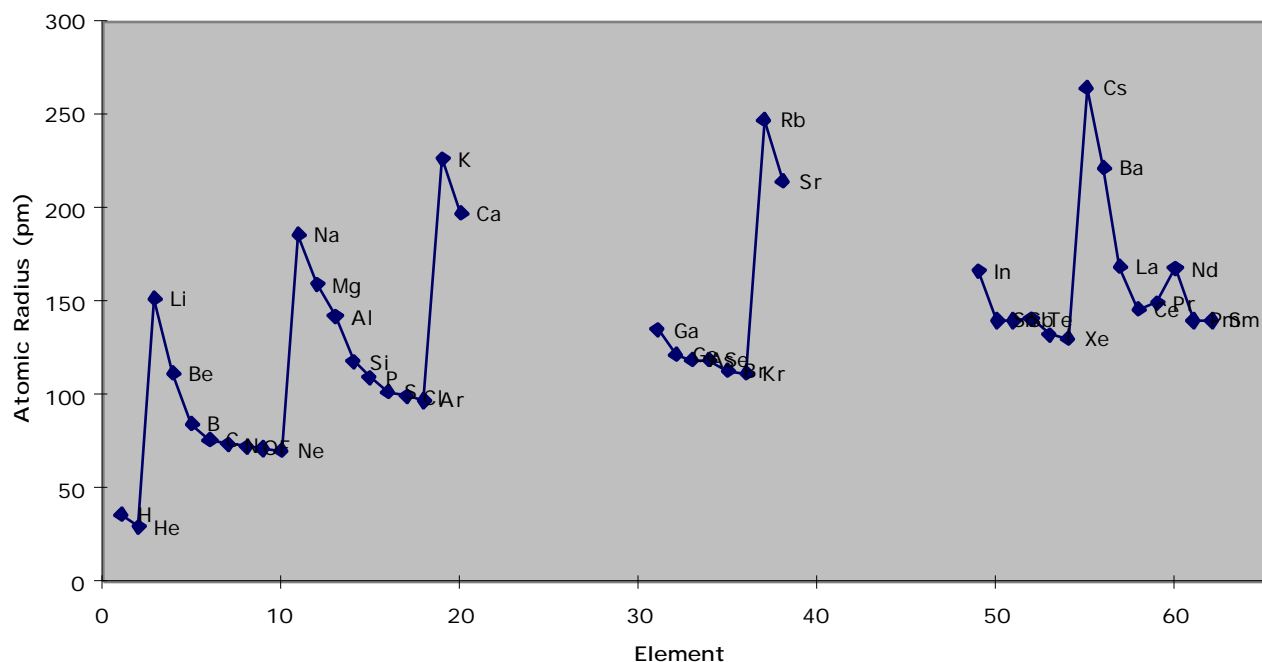
When an electron is added to hydrogen the electron goes into the 1s shell. Thus the electron is close to the nucleus and is attracted to the proton.

When an electron is added to helium the electron goes into the 2s orbital.

The electron which is being added is much farther away, and is very well

shielded from the nucleus-by the 1s electrons-so there is no attraction between the nucleus and the electron.

Atomic Radii



Atomic radii are determined by examining diatomic molecules. Thus, the atomic radius is not exactly an atomic property. However, the general trend is that as nuclear charge increases the electrons are held closer to the nucleus.

Pauling Electronegativity

