

# **Shielding and Such**

## Shielding

- In a multielectron system, electrons are simultaneously attracted to the nucleus and repelled by each other.
- Outer electrons are *shielded* from the nucleus by the core electrons.
  - ✓ Shielding effect
  - ✓ Outer electrons do not effectively screen for each other.
- The shielding causes the outer electrons to not experience the full strength of the nuclear charge.

### **Effective Nuclear Charge**

- The effective nuclear charge is a net positive charge that is attracting a particular electron.
- Z is the nuclear charge, and S is the number of electrons in lower energy levels.
  - Electrons in the same energy level contribute to screening but since their contribution is so small they are not part of the calculation.
  - Trend is s > p > d > f.

 $Z_{effective} = Z - S$ 

### **Shielding and Penetration**



#### **Shielding and Effective Nuclear Charge**



An orbital is a region within an atom where there is a probability of finding an electron. This is a probability diagram for the s orbital in the <u>first</u> <u>energy level...</u>



Orbital shapes are defined as the surface that contains 90% of the total electron probability.

#### Sizes of s orbitals

Orbitals of the same shape (s, for instance) grow larger as n increases...



Nodes are regions of low probability within an orbital.





### **Penetration and Shielding**

- The radial distribution function shows that the 2s orbital penetrates more deeply into the 1s orbital than does the 2p.
- The weaker penetration of the 2p sublevel means that electrons in the 2p sublevel experience more repulsive force; they are more shielded from the attractive force of the nucleus.
- The deeper penetration of the 2s electrons means electrons in the 2s sublevel experience a greater attractive force to the nucleus and are not shielded as effectively.



### Penetration

- The closer an electron is to the nucleus, the more attraction it experiences.
- The better an outer electron is at penetrating through the electron cloud of inner electrons, the more attraction it will have for the nucleus.
- The degree of penetration is related to the orbital's radial distribution function.
  - In particular, the distance the maxima of the function are from the nucleus

#### Orbitals in outer energy levels DO penetrate into lower energy levels. Penetration #1



This is a probability Distribution for a 3s orbital.

What parts of the diagram correspond to "nodes" – regions of zero probability?

#### **Probability distribution**



#### **Probability distribution**

