## Quantum theory predicts that an atom's electrons are found in:

- Shells (principle quantum number, n)
- Subshells (angular momentum, $\ell$)
- Orbitals (magnetic quantum number, $m_\ell$)
- We will examine those predictions

## To account that orbitals hold two electrons, we need:

- Spin quantum number, $m_s$= +½ or −½)
- $m_s$= +½ represents one electron, and $m_s$= −½ represents the other.
- Scientists verified electron spin experimentally

## Electron spin affects magnetic properties

- Diamagnetic: not attracted to magnetic field
- Paramagnetic: attracted to magnetic field
- Substances with unpaired electrons are paramagnetic

## Four quantum numbers account for all electrons in atoms:

- n= 1, 2, 3, 4, ... (integers)
- $\ell$= 0 to n-1 (integers)
- $m_\ell$= $-\ell$ to $\ell$ (integers)
- $m_s$ = +½, −½

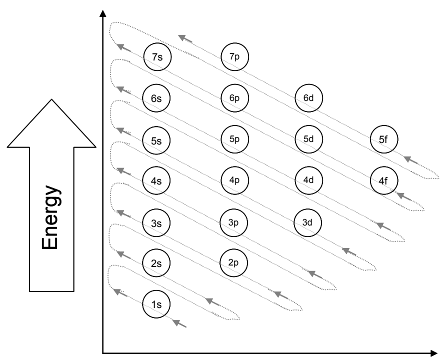
## Pauli Exclusion Principle

- No two electrons can have the same quantum numbers.
- For a 1s orbital with 2 electrons, if 1 electron has quantum numbers of n=0, $\ell$=0, $m_\ell$=0 and $m_s$= +½, the other electron has n=0, $\ell$=0, $m_\ell$=0 and $m_s$= −½.
- Electrons have unique addresses.

## Electron placement in atoms

- The n=1 shell has 2 electrons, both in a 1s orbital.
- The n=2 shell has 8 electrons, 2 in a 2s orbital, and 6 in three 2p orbitals.
- The n=3 shell has 18 electrons, 2 in a 3s orbital, 6 in three 3p orbitals, and 10 in five 3d orbitals.
- The n=4 shell has 32 electrons, 2 in a 4s orbital, 6 in three 4p orbitals, 10 in five 4d orbitals, and 14 in seven 4f orbitals.

Aufbau Principle gives filling order for electrons in orbitals in atoms




...or use the periodic table

# Write electron configurations using spdf notation

- Example: an electron configuration (EC) of $1s^2$ means 2 electrons in the 1s orbital. It would refer to helium in the ground state.
- Example: an EC of $1s^1$ means 1 electron in the 1s orbital. It refers to hydrogen in the ground state.
- For the ground state EC, fill one type of orbital before starting the next.

# More EC Examples

- Write the EC of Li. Answer: $1s^2\ 2s^1$.
- Write the EC of B. Answer: $1s^2\ 2s^2\ 2p^1$.
- Write the EC of C. Answer: $1s^2\ 2s^2\ 2p^2$.
- Write the EC of Na. $1s^2\ 2s^2\ 2p^6\ 3s^1$.
- Write the EC of Ar. $1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^6$.
- Write the EC of Fe. $1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^6\ 4s^2\ 3d^6$.

Write EC using spdf and orbital box notation

| spdf | Orbital box notation | Element |
|---|---|---|
| $1s^1$ | [↑] 1s | H |
| $1s^2$ | [↑↓] 1s | He |
| $1s^2\ 2s^2$ | [↑↓] 1s [↑↓] 2s | Be |
| $1s^2\ 2s^2\ 2p^1$ | [↑↓] 1s [↑↓] 2s [↑][ ][ ] 2p | B |

Which would be paramagnetic and diamagnetic

# Hund's Rule

- Place electrons singly and with spins aligned within orbitals of the same energy.
- Write the orbital box notation for carbon, nitrogen, oxygen, fluorine, and neon

| | 1s | 2s | 2p |
|---|---|---|---|
| C | [↑↓] | [↑↓] | [↑][↑][ ] |
| N | [↑↓] | [↑↓] | [↑][↑][↑] |
| O | [↑↓] | [↑↓] | [↑↓][↑][↑] |
| F | [↑↓] | [↑↓] | [↑↓][↑↓][↑] |
| Ne | [↑↓] | [↑↓] | [↑↓][↑↓][↑↓] |

# Shorthand notation

- The spdf or orbital box shorthand notation starts from the previous noble gas.
- Write the EC for Na and Ca in shorthand orbital box and spdf notation.

| Orbital box | spdf |
|---|---|
| Na [Ne] [↑] 3s | Na $[Ne]3s^1$ |
| Ca [Ar] [↑↓] 4s | Ca $[Ar]4s^2$ |

# Shorthand notation

- Write the EC for P and Fe and Se in shorthand orbital box and spdf notation.

| | Orbital box | spdf |
|---|---|---|
| P | [Ne] [↑↓] (3s) [↑][↑][↑] (3p) | P [Ne]$3s^2$ $3p^3$ |
| Fe | [Ar] [↑↓] (4s) [↑↓][↑][↑][↑][↑] (3d) | Fe [Ar]$4s^2$ $3d^6$ |
| Se | [Ar] [↑↓] (4s) [↑↓][↑↓][↑↓][↑↓][↑↓] (3d) [↑↓][↑][↑] (4p) | Se [Ar]$4s^2$ $3d^{10}$ $4p^4$ |

# Shorthand notation

- Write the EC for La, Ce, Th, and U in shorthand spdf notation (see periodic table).

spdf notation

La [Xe]$6s^2$ $5d^1$

Ce [Xe]$6s^2$ $5d^1$ $4f^1$

Th [Rn]$7s^2$ $6d^1$ $5f^1$

U [Rn]$7s^2$ $6d^1$ $5f^3$

# EC of Ions

- To get the EC of an ion, remove electrons from shell with the highest n first.
- For example, form +1 and +3 ions of Ga [Ar]$4s^2$ $3d^{10}$ $4p^1$
- $Ga^+$ [Ar]$4s^2$ $3d^{10}$
- $Ga^{+3}$ [Ar]$3d^{10}$
- Electrons come from n=4 before n=3, p subshells empty before s subshells.

# EC of Ions

- Form +3, +5, and -3 ions of N [He]$2s^2$ $2p^3$
- $N^{+3}$ [Ne]$2s^2$
- $N^{+5}$ [He]
- $N^{-3}$ [He]$2s^2$ $2p^6$

# EC of Ions

- A half filled subshell has a special stability.
- Form +2 and +4 ions of Co [Ar]$4s^2$ $3d^7$
- $Co^{+2}$ [Ar]$3d^7$
- $Co^{+4}$ [Ar]$3d^5$
- Is $Co^{+4}$ paramagnetic or diamagnetic?

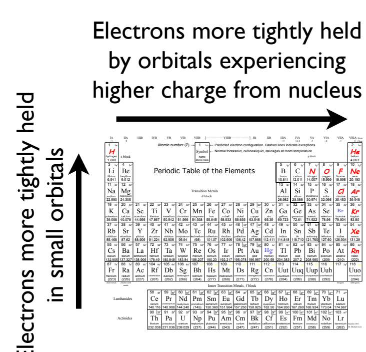
Draw the orbital box diagram. $Co^{+4}$ is paramagnetic with 5 unpaired electrons. The ion has a special stability from a half-filled d subshell.

Co [Ar] [ ] (4s) [↑][↑][↑][↑][↑] (3d)

Predictions about magnetic properties need the orbitals that came from the quantum mechanics model.

# Periodic Trends

- Atomic size
- Ion size
- Ionization energy
- Electron affinity

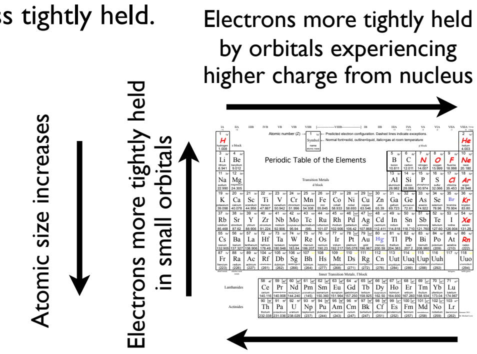


## Shielding of charge from nucleus by electrons

- A noble gas EC is very effective at shielding the charge from the nucleus to outside the atom because all of the orbital space is filled by electrons.
- An incomplete EC is less effective at shielding charge from the nucleus because the orbital space is not filled.
- Nuclear charge experienced outside the atom increases as we move to the right on the periodic table because nuclear charge is poorly shielded by an incomplete EC.

## Atomic Size

- Atomic size increases when electrons are less tightly held.



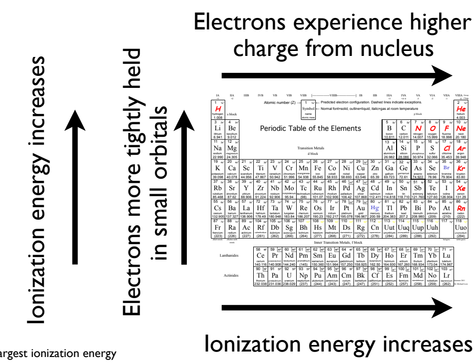

Fr is the largest atom.

## Ion Size

- Cations are smaller than the atoms from which they come because there is an excess of positive nuclear charge that pulls more strongly on the remaining negatively charged electrons, shrinking the cation.
- Anions are larger than the atoms from which they come because the excess of negative charge from the electrons causes repulsion, so the anion grows in size.

## Ionization energy

- Ionization energy is the energy needed to remove an electron from the gas phase atom.



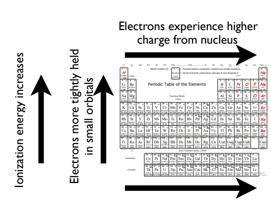

He has the largest ionization energy

## Ionization Energy

- The first ionization energy of Mg is about 740kJ, $Mg \rightarrow Mg^{+} + e^{-}$
- The second ionization energy of Mg is about 1500kJ, $Mg^{+} \rightarrow Mg^{+2} + e^{-}$
- The third ionization energy of Mg is about 7800kJ, $Mg^{+2} \rightarrow Mg^{+3} + e^{-}$
- Breaking a filled subshell requires a large amount of energy 7.8MJ, so this chemistry does not happen unless high energy is used.

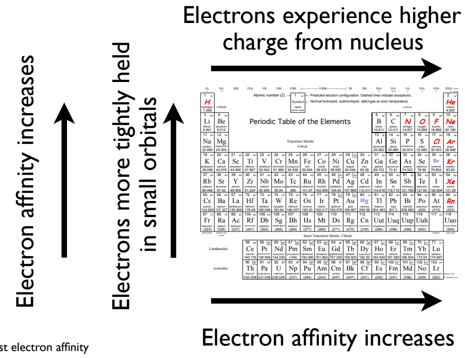
## Ionization energy

- Metals lose electrons (good reducing agents) more easily than nonmetals (good oxidizing agents).
- Metals lower in a group are better reducing agents, while nonmetals (other than noble gases) higher in a group are better oxidizing agents.



# Electron Affinity

- Electron affinity is the energy released when adding an electron to a gas phase atom.




F has the largest electron affinity

# Electron Affinity

- Noble gases have no affinity for electrons.
- Oxygen has an affinity for electrons but nitrogen does not. Use use the orbital box notation to explain why this might be so.

| | 1s | 2s | 2p | | |
|---|---|---|---|---|---|
| N | ↑↓ | ↑↓ | ↑ | ↑ | ↑ |
| O | ↑↓ | ↑↓ | ↑↓ | ↑ | ↑ |

- Nitrogen enjoys the special stability of a half-filled subshell, so it does not easily take another electron (it would require electron pairing). Oxygen takes electrons because electrons experience a strong nuclear charge.