**Chem 120 Track**

# Quantum Chemistry

**Chem 108**

*Electron Configurations*

*&*

*The Periodic Table*

*Dr. Ron Rusay*



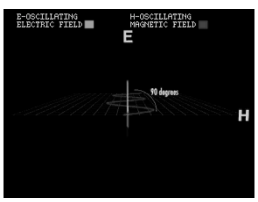
# Quantum Theory

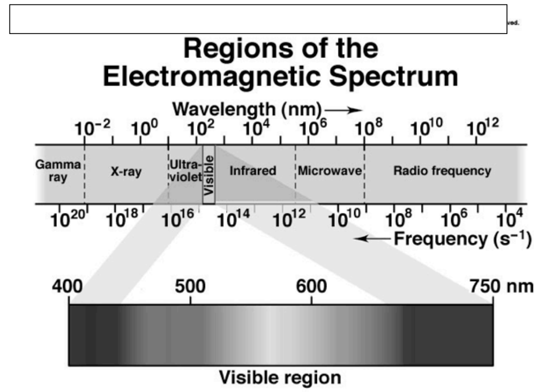
- *Based on experimental observations of light and particles*
- *Developed through rigorous mathematical computations*
- *Bridges physics and chemistry*
- *Generally described as quantum mechanics aka quantum chemistry*

# Electromagnetic Radiation

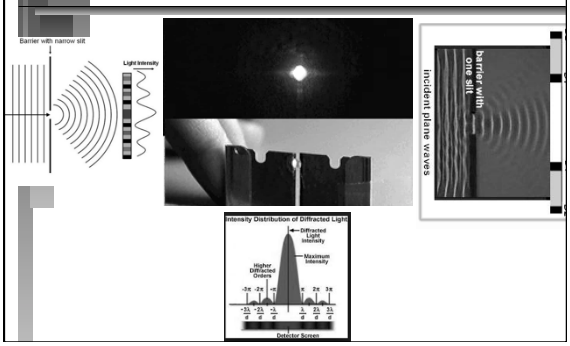
*("Light")*

- *Energy that exhibits wave-like behavior that travels through space at 186,000 mi/s; 3 x $10^8$ m/s*
- *Described by the Electromagnetic Spectrum.*

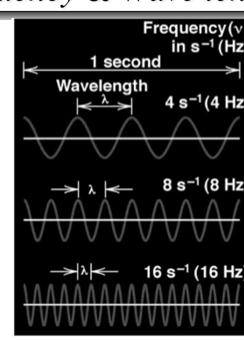


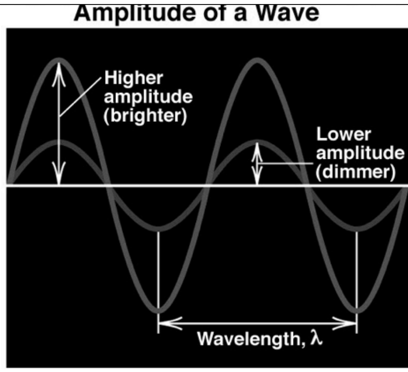

# Demonstrating Light's Wave Nature




# Frequency & Wave length



## Amplitude of a Wave




## *Waves*

*http://chemistry.beloit.edu/BlueLight/waves/index.html*

- *Waves have 4 primary characteristics:*
- *1. Wavelength: distance between two peaks in a wave.*
- *2. Frequency: number of waves per second that pass a given point in space.*
- *3. Amplitude: the height of the wave.*
- *4. Speed: speed of light is $2.9979 \times 10^8$ m/s.*

## *Waves*

*http://chemistry.beloit.edu/BlueLight/waves/index.html*

- *Focus on 2 of the primary characteristics:*
- *1. **Wavelength:** distance between two peaks in a wave.*
- *2. **Frequency:** number of waves per second that pass a given point in space.*
- *3. Amplitude: the height of the wave.*
- *4. Speed: speed of light is $2.9979 \times 10^8$ m/s.*

## *Wavelength and frequency*

$$\nu = c / \lambda$$

- *$\nu$ = frequency ($s^{-1}$)*
- *$\lambda$ = wavelength (m)*
- *c = speed of light (m $s^{-1}$)*

## *QUESTION*

Which of the following frequencies corresponds to light with the longest wavelength?

A. $3.00 \times 10^{13}\ s^{-1}$
B. $4.12 \times 10^{5}\ s^{-1}$
C. $8.50 \times 10^{20}\ s^{-1}$
D. $9.12 \times 10^{12}\ s^{-1}$
E. $3.20 \times 10^{9}\ s^{-1}$

## *Planck's Constant*

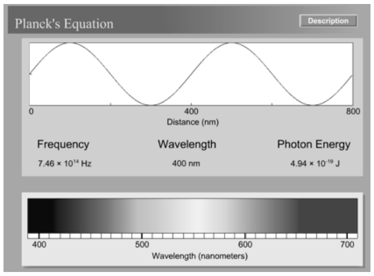
*Transfer of energy is quantized, and can only occur in discrete units, called quanta.*

$$\Delta E = h\nu = \frac{hc}{\lambda}$$

- *$\Delta E$ = change in energy, in J*
- *h = Planck's constant, $6.626 \times 10^{-34}$ J s*
- *$\nu$ = frequency, in $s^{-1}$*
- *$\lambda$ = wavelength, in m*
- *c = speed of light*

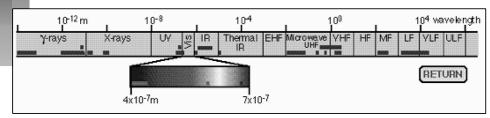
*Planck's Equation (Interactive)*

$$\Delta E = h\nu = \frac{hc}{\lambda}$$




http://chemconnections.org/general/chem120/Flash/plancks_equation_s.html

## *Electromagnetic Energy*




- *EM Spectrum : Chem Connections*
  *http://chemistry.beloit.edu/Stars/EMSpectrum/index.html*

## *Energy and Mass*

- *Energy has mass*
  - $E = mc^2$
- *E = energy*
- *m = mass*
- *c = speed of light*

## *Energy and Mass*

**"Duality"**

$$E_{\text{photon}} = \frac{hc}{\lambda}$$

$$m_{\text{photon}} = \frac{h}{\lambda c}$$

(Hence the dual nature of light.)

## *Wavelength and Mass*

de Broglie's Equation

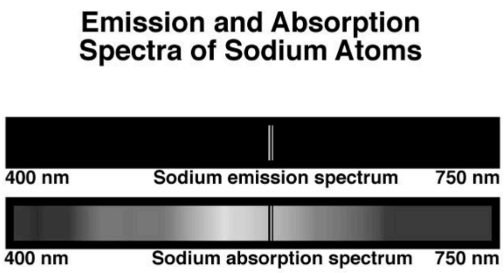
$$\lambda = \frac{h}{m\nu}$$

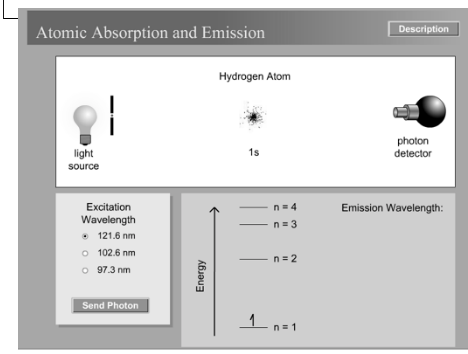
- *$\lambda$ = wavelength, in m*
- *h = Planck's constant, $6.626 \times 10^{-34}$ $J \cdot s$ = $kg\ m^2\ s^{-1}$*
- *m = mass, in kg*
- *$\nu$ = frequency, in $s^{-1}$*

## *Atomic Spectrum of Hydrogen*

*http://chemistry.beloit.edu/BlueLight/pages/color.html*

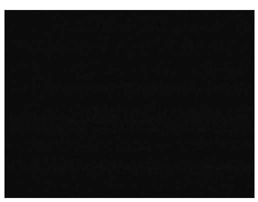
- *Continuous spectrum: Contains all the wavelengths of light.*
- *Absorbtion vs.Emission*
- *http://chemistry.beloit.edu/BlueLight/pages/elements.html*
- *Line (discrete) spectrum: Contains only some of the wavelengths of light.*

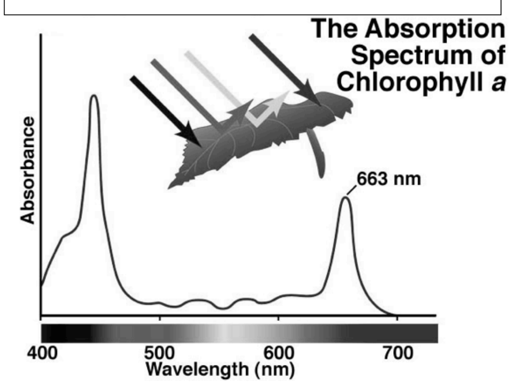



*http://chemconnections.org/general/chem120/Flash/atomic_absorption_s.html*

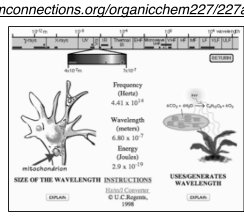
## *Emissions: Flame Tests*



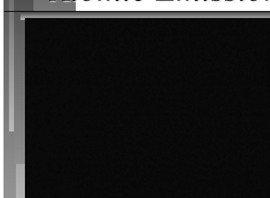


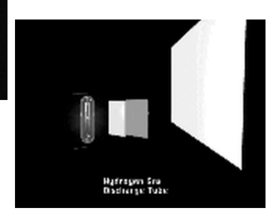

## *Electromagnetic Energy*

- *Visible Light / Color : ChemConnections*
  - *http://chemistry.beloit.edu/Stars/applets/emission/index.html*
- *The Perception of Colors*
  - *http://chemconnections.org/organicchem227/227assign-06.html#vision*

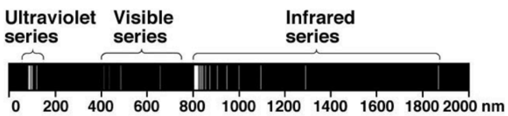


## *Atomic Emission Spectrum of $H_2$*



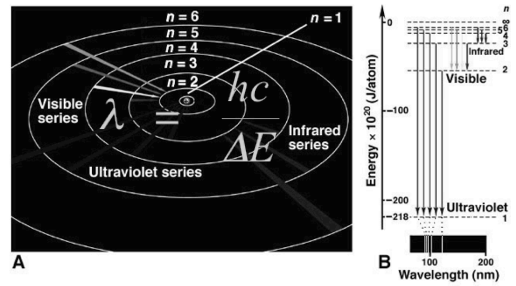


## Three Series of Spectral Lines

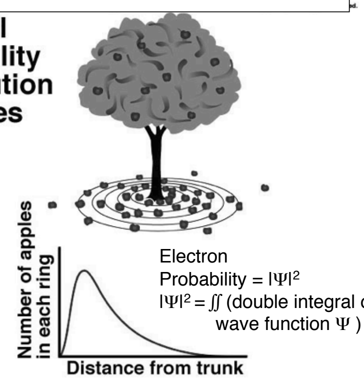



ð $\Delta E = E_{final\ state} - E_{initial\ state}$

## The Bohr Model Explanation of the Three Series of Spectral Lines

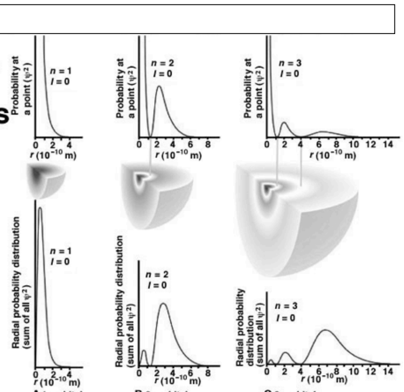



## A Radial Probability Distribution of Apples

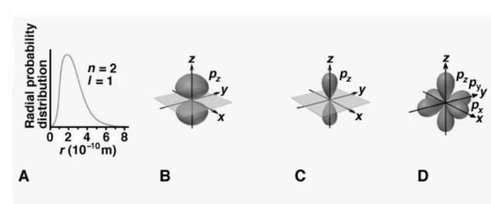


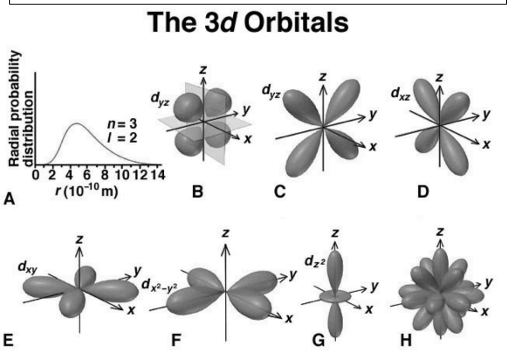

Electron
Probability = $|\Psi|^2$
$|\Psi|^2 = \iint$ (double integral of wave function $\Psi$ )

## The 1s, 2s, 3s Orbitals

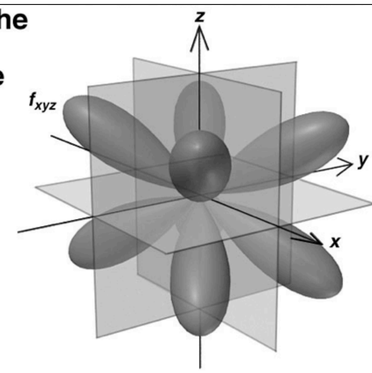



## The 2p Orbitals






One of the Seven Possible 4*f* Orbitals




## *Aufbau Principle*

- *As protons are added one by one to the nucleus to build up the elements, electrons are similarly added to these hydrogen-like orbitals.*


## *Pauli Exclusion Principle*

- *In a given atom, no two electrons can have the same set of four quantum numbers ( **n, l,** $m_l$**,** $m_s$ ).*
- *Therefore, an orbital can hold only two electrons, and they must have opposite spins.*

# *QUESTION*

If *l* = 3, how many electrons can be contained in all the possible orbitals?

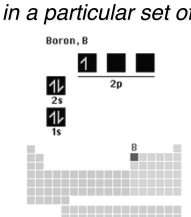
A) 7
B) 6
C) 14
D) 10
E) 5

## *Hund's Rule*

*orbital diagrams*

- *The lowest energy configuration for an atom is the one having the maximum number of unpaired electrons allowed by the Pauli principle in a particular set of degenerate orbitals.*

*Orbital Diagram ->*



# Quantum Chemistry

**Chem 108**

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# Quantum Theory

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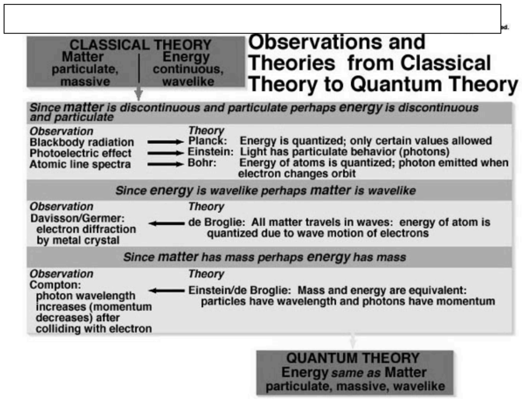



*https://www.youtube.com/watch?v=4QlcKuxDGrs*

# Heisenberg Uncertainty Principle

- *The more accurately we know a particle's position, the less accurately we can know its momentum or vice versa.*

***Quantum Entanglement/Superposition***

*Schrödinger's Cat: Alive or Dead?*

*Can something be in two places at the same time?*


***In quantum microstates, YES.***

*Science, 272, 1132 (1996)*

# Quantum Numbers (QN) for Electrons

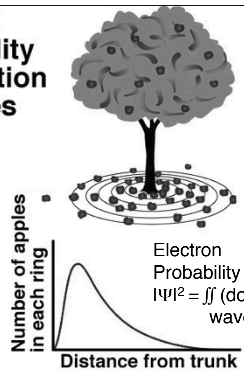
*(Solutions for the Schrödinger Equation: $H\Psi = E\Psi$ )*

*Where: $\Psi$ = Wave function*

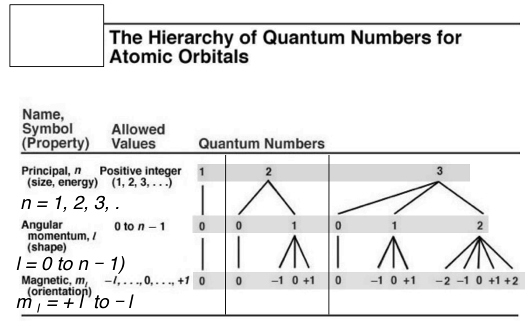
- *1. Principal QN ( integer n = 1, 2, 3, . . .) : relates to size and energy of the orbital.*
- *2. Angular Momentum QN ( integer $l$ or $\lambda$)= 0 to n − 1) : relates to shape of the orbital.*
- *3. Magnetic QN (integer $m_l$ or $m_\lambda$ = + $l$ to − $l$) : relates to orientation of the orbital in space relative to other orbitals.*
- *4. Electron Spin QN : ($m_s = +1/2, -1/2$) : relates to the spin state of the electron.*

*"ORBITAL":*

**A Radial Probability Distribution of Apples**




Electron Probability = $|\Psi|^2$
$|\Psi|^2 = \iint$ (double integral of wave function $\Psi$ )




*n = 1, 2, 3, .*

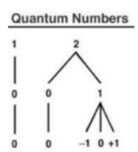
*l = 0 to n − 1)*

*$m_l$ = + l to − l*

# *QUESTION*

If *n* = 2, how many orbitals ($m_l$ values) are possible?

A) 3
B) 4
C) 2
D) 8
E) 6




# *QUESTION*

How many *f* orbitals have the value *n* = 3?

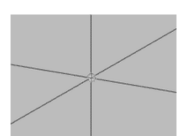
A) 0
B) 3
C) 5
D) 7
E) 1

# *QUESTION*

How many *f* orbitals have the value *n* = 4?

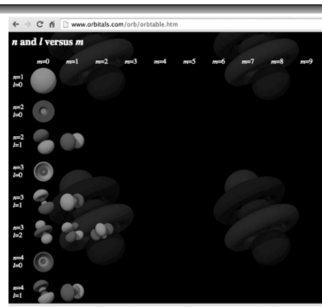
A) 0
B) 3
C) 5
D) 7
E) 1

## *Quantum Numbers : l, $m_l$*
## *Orbital Shape & Orientation*



http://chemconnections.org/general/chem120/atomic-orbitals/orbitals.html

## *Atomic Orbitals*



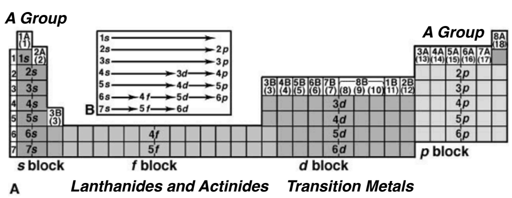
http://www.orbitals.com/orb/orbtable.htm

## *Periodic Table Classifications*

*Electron Configurations & Quantum Numbers*

- *Representative Elements (A Groups): s (l=0) and p (l=1) (N, C, Al, Ne, F, O)*
- *Transition Elements: d (l=2) orbitals (Fe, Co, Ni, etc.)*
- *Lanthanide and Actinide Series (inner transition elements): f (l=3) orbitals (Eu, Am, Es)*

## Relation Between Orbital Filling and the Periodic Table




## *Valence Electrons (A Group)*

Valence electrons are the outermost electrons in the highest principal quantum level of an atom. They are found in the s- and p- orbitals and are the bonding electrons. Examples:

| Atom | Valence Electrons |
|---|---|
| Ca | 2 |
| N | 5 |
| Br | 7 |

Inner electrons are called core electrons.

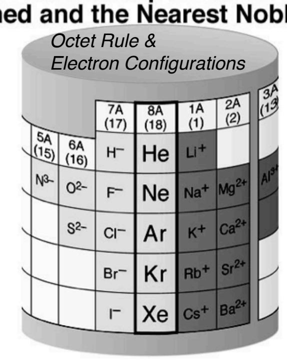
## *Valence Electrons (A Group)*

The A Groups' outer s- and p- orbitals contain the bonding electrons; the A group number equals the total s- and p- electrons, which are the "valence electrons"

| Atom | Valence Electrons |
|---|---|
| Ca | 2 |
| N | 5 |
| Br | 7 |

Inner electrons are called core electrons.

## The Relationship Between Ions Formed and the Nearest Noble Gas




Valence Electrons

# QUESTION

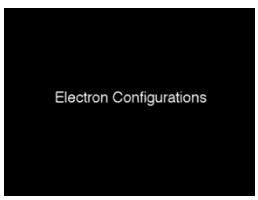
In which groups do all the elements have the same number of valence electrons?

A) K, Ca, Ar, S
B) Na, Mg, S, Cl
C) Na, K, Rb, Cs
D) Li, Be, B, C
E) None of these

## Periodic Table Classifications
### Electron Configurations

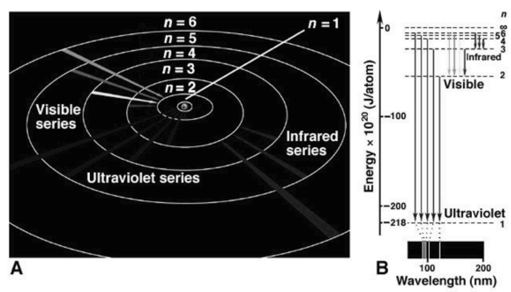
- *Representative Elements (A Groups): fill s and p orbitals (Na, Al, Ne, O)*
- *Transition Elements: fill d orbitals (Fe, Co, Ni)*
- *Lanthanide and Actinide Series (inner transition elements): fill 4f and 5f orbitals (Eu, Am, Es)*

## Multi-electron Atoms
### Electron Configuration

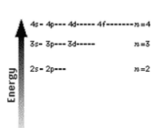


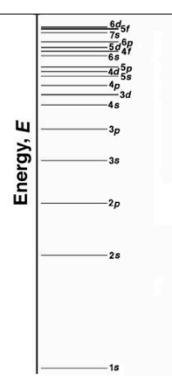

*http://chemconnections.org/general/movies/Quantum-Periodicity/electron-config.MOV*

## The Bohr Model Explanation of the Three Series of Spectral Lines



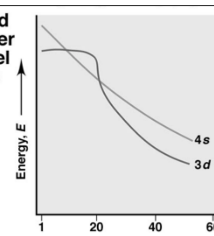

## Order for Filling Energy Sublevels with Electrons

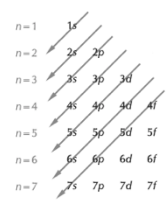


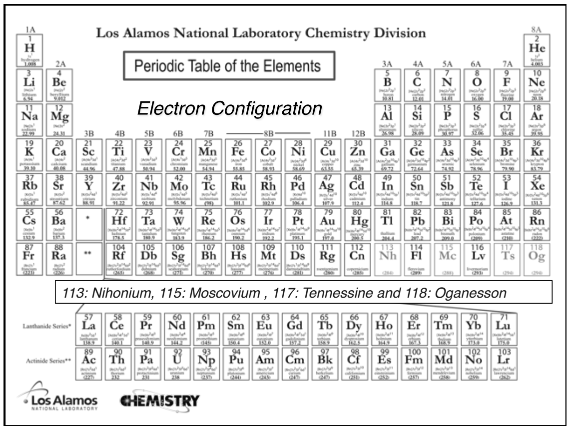




## Multi-electron
### Electron Configuration

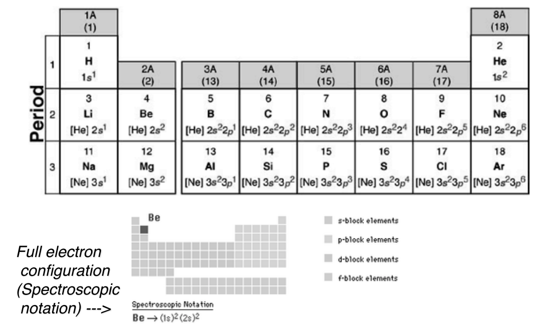
The Period 4 Crossover in Sublevel Energies






## Condensed Ground-State Electron Configurations

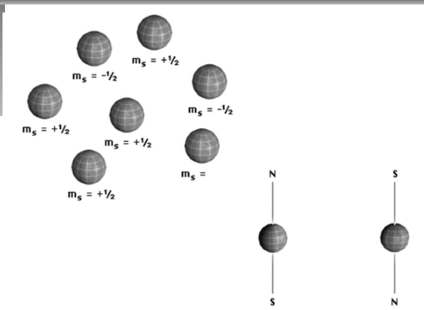



# QUESTION

The electron configuration for the barium atom is:

A) $1s^22s^22p^63s^23p^63d^{10}4s^2$
B) [Xe] $6s^2$
C) $1s^22s^22p^63s^23p^64s^1$
D) $1s^22s^22p^63s^23p^64s^2$
E) none of these

## *Magnetic Spin $m_s$*




**Partial Orbital Diagrams and Electron Configurations***

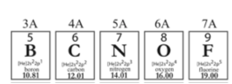
| Atomic Number | Element | Partial Orbital Diagram (4s, 3d, and 4p Sublevels Only): 4s | 3d | 4p | Full Electron Configuration | Condensed Electron Configuration |
|---|---|---|---|---|---|---|
| 19 | K | ↑ | | | $[1s^2 2s^2 2p^6 3s^2 3p^6]\ 4s^1$ | [Ar] $4s^1$ |
| 20 | Ca | ↑↓ | | | $[1s^2 2s^2 2p^6 3s^2 3p^6]\ 4s^2$ | [Ar] $4s^2$ |
| 21 | Sc | ↑↓ | ↑ | | $[1s^2 2s^2 2p^6 3s^2 3p^6]\ 4s^2 3d^1$ | [Ar] $4s^2 3d^1$ |
| 22 | Ti | ↑↓ | ↑ ↑ | | $[1s^2 2s^2 2p^6 3s^2 3p^6]\ 4s^2 3d^2$ | [Ar] $4s^2 3d^2$ |
| 23 | V | ↑↓ | ↑ ↑ ↑ | | $[1s^2 2s^2 2p^6 3s^2 3p^6]\ 4s^2 3d^3$ | [Ar] $4s^2 3d^3$ |
| 24 | Cr | ↑ | ↑ ↑ ↑ ↑ ↑ | | $[1s^2 2s^2 2p^6 3s^2 3p^6]\ 4s^1 3d^5$ | [Ar] $4s^1 3d^5$ |
| 25 | Mn | ↑↓ | ↑ ↑ ↑ ↑ ↑ | | $[1s^2 2s^2 2p^6 3s^2 3p^6]\ 4s^2 3d^5$ | [Ar] $4s^2 3d^5$ |
| 26 | Fe | ↑↓ | ↑↓ ↑ ↑ ↑ ↑ | | $[1s^2 2s^2 2p^6 3s^2 3p^6]\ 4s^2 3d^6$ | [Ar] $4s^2 3d^6$ |
| 27 | Co | ↑↓ | ↑↓ ↑↓ ↑ ↑ ↑ | | $[1s^2 2s^2 2p^6 3s^2 3p^6]\ 4s^2 3d^7$ | [Ar] $4s^2 3d^7$ |
| 28 | Ni | ↑↓ | ↑↓ ↑↓ ↑↓ ↑ ↑ | | $[1s^2 2s^2 2p^6 3s^2 3p^6]\ 4s^2 3d^8$ | [Ar] $4s^2 3d^8$ |
| 29 | Cu | ↑ | ↑↓ ↑↓ ↑↓ ↑↓ ↑↓ | | $[1s^2 2s^2 2p^6 3s^2 3p^6]\ 4s^1 3d^{10}$ | [Ar] $4s^1 3d^{10}$ |
| 30 | Zn | ↑↓ | ↑↓ ↑↓ ↑↓ ↑↓ ↑↓ | | $[1s^2 2s^2 2p^6 3s^2 3p^6]\ 4s^2 3d^{10}$ | [Ar] $4s^2 3d^{10}$ |
| 31 | Ga | ↑↓ | ↑↓ ↑↓ ↑↓ ↑↓ ↑↓ | ↑ | $[1s^2 2s^2 2p^6 3s^2 3p^6]\ 4s^2 3d^{10} 4p^1$ | [Ar]$4s^2 3d^{10} 4p^1$ |
| 32 | Ge | ↑↓ | ↑↓ ↑↓ ↑↓ ↑↓ ↑↓ | ↑ ↑ | $[1s^2 2s^2 2p^6 3s^2 3p^6]\ 4s^2 3d^{10} 4p^2$ | [Ar]$4s^2 3d^{10} 4p^2$ |
| 33 | As | ↑↓ | ↑↓ ↑↓ ↑↓ ↑↓ ↑↓ | ↑ ↑ ↑ | $[1s^2 2s^2 2p^6 3s^2 3p^6]\ 4s^2 3d^{10} 4p^3$ | [Ar]$4s^2 3d^{10} 4p^3$ |
| 34 | Se | ↑↓ | ↑↓ ↑↓ ↑↓ ↑↓ ↑↓ | ↑↓ ↑ ↑ | $[1s^2 2s^2 2p^6 3s^2 3p^6]\ 4s^2 3d^{10} 4p^4$ | [Ar]$4s^2 3d^{10} 4p^4$ |
| 35 | Br | ↑↓ | ↑↓ ↑↓ ↑↓ ↑↓ ↑↓ | ↑↓ ↑↓ ↑ | $[1s^2 2s^2 2p^6 3s^2 3p^6]\ 4s^2 3d^{10} 4p^5$ | [Ar]$4s^2 3d^{10} 4p^5$ |
| 36 | Kr | ↑↓ | ↑↓ ↑↓ ↑↓ ↑↓ ↑↓ | ↑↓ ↑↓ ↑↓ | $[1s^2 2s^2 2p^6 3s^2 3p^6]\ 4s^2 3d^{10} 4p^6$ | [Ar]$4s^2 3d^{10} 4p^6$ |

*Colored type indicates sublevel(s) whose occupancy changes when last electron is added.

# QUESTION

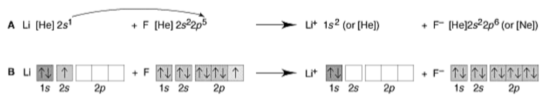
Nitrogen has 5 valence electrons. Consider the following electron arrangements.

| | 2s | 2p | | |
|---|---|---|---|---|
| A) | ↑↓ | ↑ | ↑ | ↑ |
| B) | ↑ | ↑↓ | ↑ | ↑ |
| C) | ↑ | ↑↑ | ↑ | ↑ |
| D) | ↑↓ | ↑ | ↑ | |
| E) | ↑↓ | ↑↓ | ↑ | ↑ |



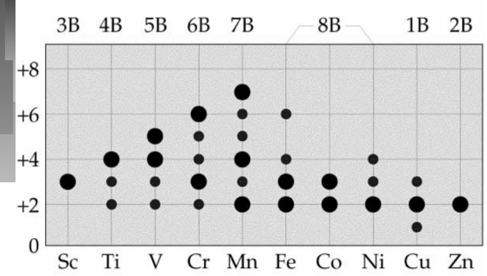

Which represents the ground state for the Nitrogen atom?

*Two ways of showing the formation of lithium fluoride: LiF; [$Li^+$ and $F^-$] using electron configurations & diagrams*




## Transition Metal Ions (B Groups)

### Oxidation Numbers (States): Ion Charge




## Summary: Information from the Periodic Table

- *1. Can obtain Group A valence electron configurations*
- *2. Can determine individual electron configurations.*

  *This information can be used to:*
- *a. Predict the physical properties and general chemical behavior of the elements.*
- *b. Identify metals and nonmetals.*
- *c. Predict ions & formulas of compounds*