Quantum Chemistry

Chem 108

Electron Configurations

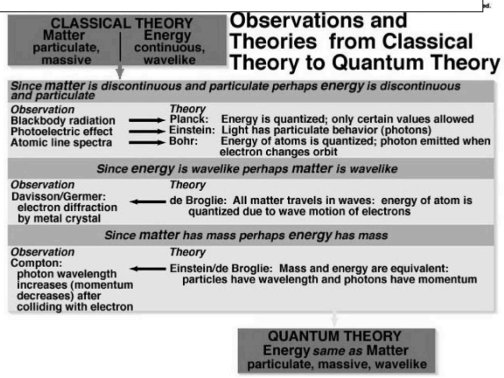
&

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*



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. (NON-intuitive)*

Quantum Entanglement/Superposition

Schrödinger's Cat: Alive or Dead?

Can something be in two places at the same time?

Science, 272, 1132 (1996)

Quantum Numbers (QN) for Electrons

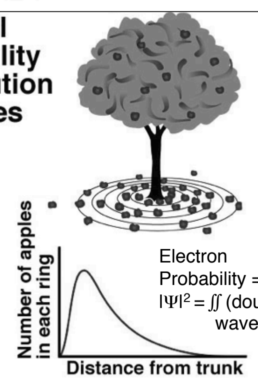
(Solutions for the Schrödinger Equation: $H\Psi = E\Psi$)

Where: Ψ = 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 λ)= 0 to n − 1) : relates to shape of the orbital.*
- *3. Magnetic QN (integer m_l or m_λ = + 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.*

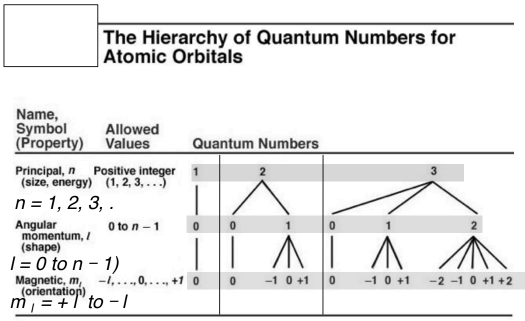
"ORBITAL":

A Radial Probability Distribution of Apples



Electron Probability = $|\Psi|^2$

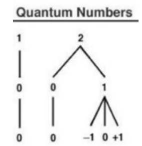
$|\Psi|^2$ = ∬ (double integral of wave function Ψ)



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?

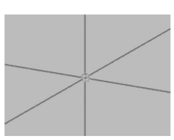
A) 0
B) 3
C) 5
D) 7
E) 1

QUESTION

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

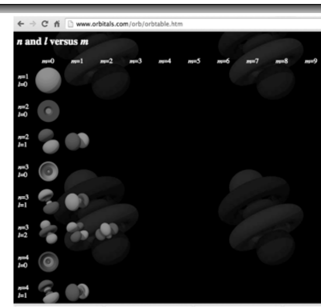
A) 0
B) 3
C) 5
D) 7
E) 1

Quantum Numbers : l, m_l Orbital Shape & Orientation



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

Atomic Orbitals

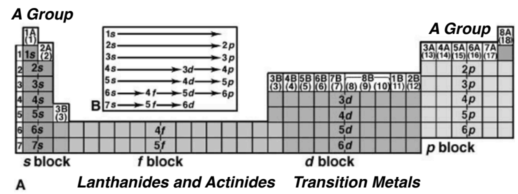


http://www.orbitals.com/orb/orbtable.htm

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.

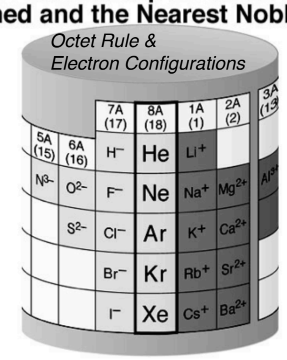
Valence Electrons (A Group)

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

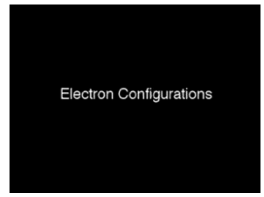
In which groups do all the elements have the same number of valence electrons?

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

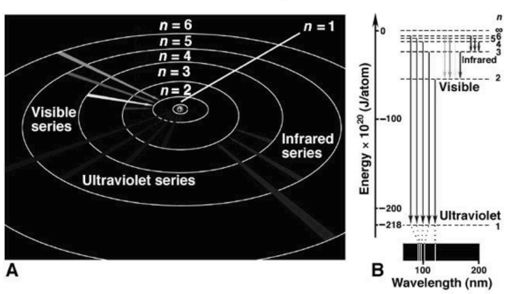
- *Representative Elements (A Groups): fill s and p orbitals (Na, Al, Ne, O)*
- *Transition Elements: fill d orbitals (Fe, Co, Ni)*
- *Lanthanide and Actinide Series (inner transition elements): fill 4f and 5f orbitals (Eu, Am, Es)*

Multi-electron Atoms
Electron Configuration

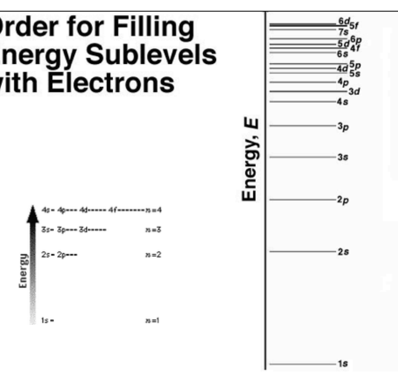


http://chemconnections.org/general/movies/Quantum-Periodicity/electron-config.MOV

The Bohr Model Explanation of the Three Series of Spectral Lines

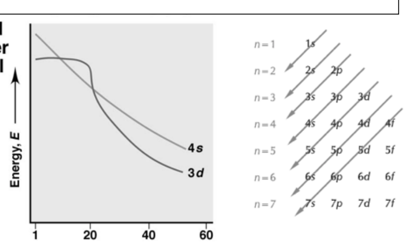


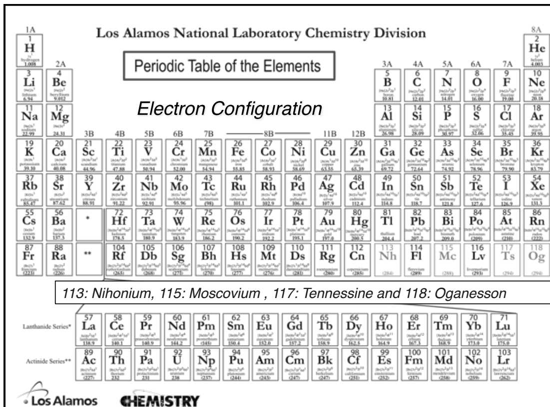
Order for Filling Energy Sublevels with Electrons



Multi-electron
Electron Configuration

The Period 4 Crossover in Sublevel Energies

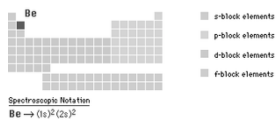




Condensed Ground-State Electron Configurations

Period	1A (1)	2A (2)	3A (13)	4A (14)	5A (15)	6A (16)	7A (17)	8A (18)
1	1 H $1s^1$							2 He $1s^2$
2	3 Li [He] $2s^1$	4 Be [He] $2s^2$	5 B [He] $2s^22p^1$	6 C [He] $2s^22p^2$	7 N [He] $2s^22p^3$	8 O [He] $2s^22p^4$	9 F [He] $2s^22p^5$	10 Ne [He] $2s^22p^6$
3	11 Na [Ne] $3s^1$	12 Mg [Ne] $3s^2$	13 Al [Ne] $3s^23p^1$	14 Si [Ne] $3s^23p^2$	15 P [Ne] $3s^23p^3$	16 S [Ne] $3s^23p^4$	17 Cl [Ne] $3s^23p^5$	18 Ar [Ne] $3s^23p^6$

Full electron configuration (Spectroscopic notation) --->



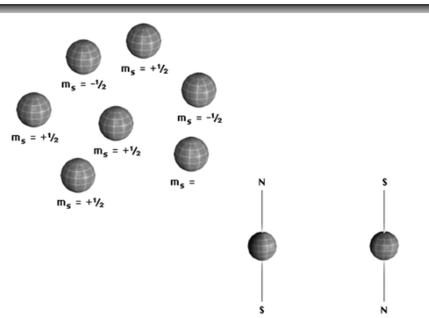
QUESTION

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

(Nuclear Applications in MRI & NMR)



Partial Orbital Diagrams and Electron Configurations*

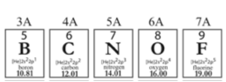
Atomic Number	Element	Partial Orbital Diagram (4s, 3d, and 4p Sublevels Only): 4s	3d	4p	Full Electron Configuration	Condensed Electron Configuration
19	K	↑	[ ][ ][ ][ ][ ]	[ ][ ][ ]	$[1s^22s^22p^63s^23p^6]\,4s^1$	[Ar] $4s^1$
20	Ca	↑↓	[ ][ ][ ][ ][ ]	[ ][ ][ ]	$[1s^22s^22p^63s^23p^6]\,4s^2$	[Ar] $4s^2$
21	Sc	↑↓	[↑][ ][ ][ ][ ]	[ ][ ][ ]	$[1s^22s^22p^63s^23p^6]\,4s^23d^1$	[Ar] $4s^23d^1$
22	Ti	↑↓	[↑][↑][ ][ ][ ]	[ ][ ][ ]	$[1s^22s^22p^63s^23p^6]\,4s^23d^2$	[Ar] $4s^23d^2$
23	V	↑↓	[↑][↑][↑][ ][ ]	[ ][ ][ ]	$[1s^22s^22p^63s^23p^6]\,4s^23d^3$	[Ar] $4s^23d^3$
24	Cr	↑	[↑][↑][↑][↑][↑]	[ ][ ][ ]	$[1s^22s^22p^63s^23p^6]\,4s^13d^5$	[Ar] $4s^13d^5$
25	Mn	↑↓	[↑][↑][↑][↑][↑]	[ ][ ][ ]	$[1s^22s^22p^63s^23p^6]\,4s^23d^5$	[Ar] $4s^23d^5$
26	Fe	↑↓	[↑↓][↑][↑][↑][↑]	[ ][ ][ ]	$[1s^22s^22p^63s^23p^6]\,4s^23d^6$	[Ar] $4s^23d^6$
27	Co	↑↓	[↑↓][↑↓][↑][↑][↑]	[ ][ ][ ]	$[1s^22s^22p^63s^23p^6]\,4s^23d^7$	[Ar] $4s^23d^7$
28	Ni	↑↓	[↑↓][↑↓][↑↓][↑][↑]	[ ][ ][ ]	$[1s^22s^22p^63s^23p^6]\,4s^23d^8$	[Ar] $4s^23d^8$
29	Cu	↑	[↑↓][↑↓][↑↓][↑↓][↑↓]	[ ][ ][ ]	$[1s^22s^22p^63s^23p^6]\,4s^13d^{10}$	[Ar] $4s^13d^{10}$
30	Zn	↑↓	[↑↓][↑↓][↑↓][↑↓][↑↓]	[ ][ ][ ]	$[1s^22s^22p^63s^23p^6]\,4s^23d^{10}$	[Ar] $4s^23d^{10}$
31	Ga	↑↓	[↑↓][↑↓][↑↓][↑↓][↑↓]	[↑][ ][ ]	$[1s^22s^22p^63s^23p^6]\,4s^23d^{10}4p^1$	[Ar] $4s^23d^{10}4p^1$
32	Ge	↑↓	[↑↓][↑↓][↑↓][↑↓][↑↓]	[↑][↑][ ]	$[1s^22s^22p^63s^23p^6]\,4s^23d^{10}4p^2$	[Ar] $4s^23d^{10}4p^2$
33	As	↑↓	[↑↓][↑↓][↑↓][↑↓][↑↓]	[↑][↑][↑]	$[1s^22s^22p^63s^23p^6]\,4s^23d^{10}4p^3$	[Ar] $4s^23d^{10}4p^3$
34	Se	↑↓	[↑↓][↑↓][↑↓][↑↓][↑↓]	[↑↓][↑][↑]	$[1s^22s^22p^63s^23p^6]\,4s^23d^{10}4p^4$	[Ar] $4s^23d^{10}4p^4$
35	Br	↑↓	[↑↓][↑↓][↑↓][↑↓][↑↓]	[↑↓][↑↓][↑]	$[1s^22s^22p^63s^23p^6]\,4s^23d^{10}4p^5$	[Ar] $4s^23d^{10}4p^5$
36	Kr	↑↓	[↑↓][↑↓][↑↓][↑↓][↑↓]	[↑↓][↑↓][↑↓]	$[1s^22s^22p^63s^23p^6]\,4s^23d^{10}4p^6$	[Ar] $4s^23d^{10}4p^6$

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

QUESTION

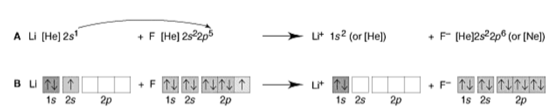
Nitrogen has 5 valence electrons. Consider the following electron arrangements.

	2s	2p
A)	[↑↓]	[↑][↑][↑]
B)	[↑]	[↑↓][↑][↑]
C)	[↑]	[↑↑][↑][↑]
D)	[↑↓]	[↑][↑][ ]
E)	[↑↓]	[↑↓][↑][↑]



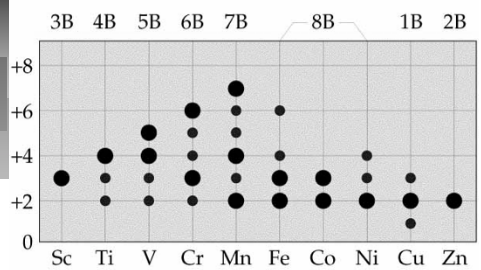
Which represents the ground state for the Nitrogen atom?

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



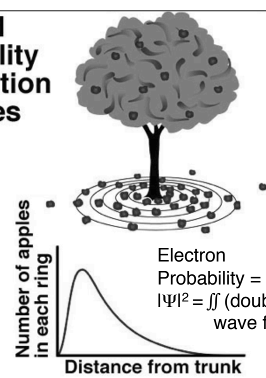
Summary: Information from the Periodic Table

- *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*

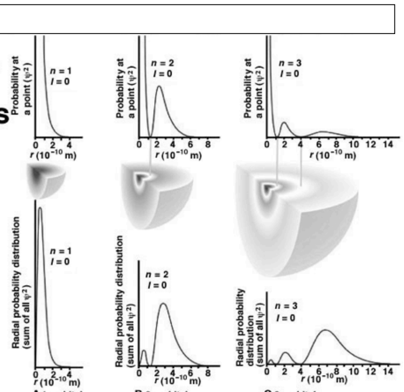
A Radial Probability Distribution of Apples



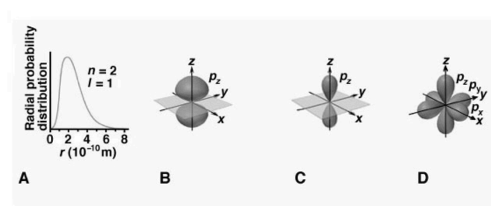
Electron Probability = $|\Psi|^2$

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

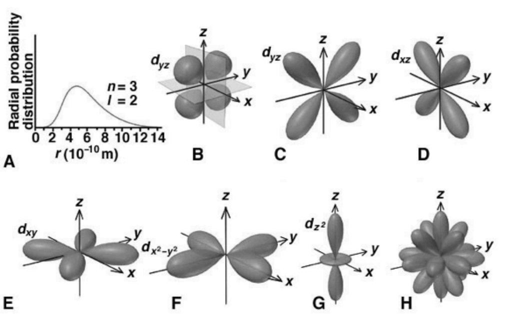
The 1*s*, 2*s*, 3*s* Orbitals



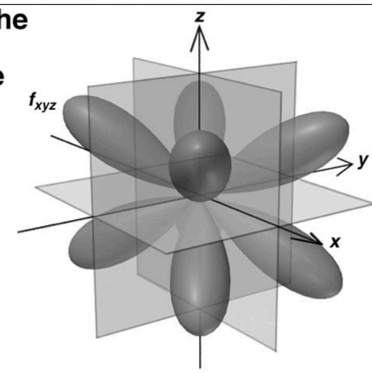
The 2*p* Orbitals



The 3*d* 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 ->