

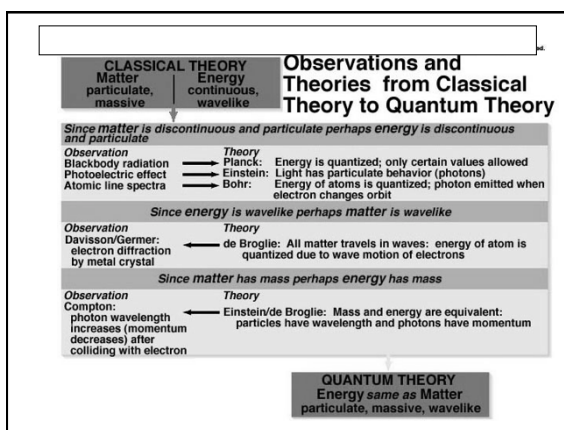
Quantum Chemistry

Chem 108
Electron Configurations
&
The Periodic Table
Dr. Ron Rusay

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Quantum Theory

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



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

Heisenberg Uncertainty Principle

- δ The more accurately we know a particle's position, the less accurately we can know its momentum or vice versa. (NON-intuitive)
- δ **Quantum Entanglement/Superposition**
- δ Schrödinger's Cat: Alive or Dead?
- δ Can something be in two places at the same time?

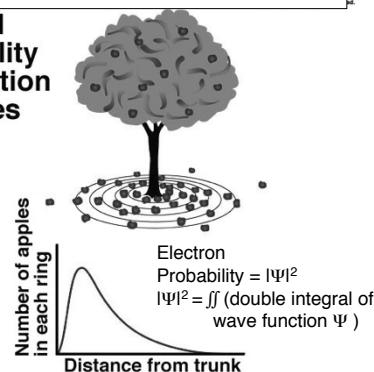


Quantum Numbers (QN) for Electrons (Solutions for the Schrödinger Equation: $H\Psi = E\Psi$) Where: Ψ = Wave function

- δ 1. Principal QN (integer $n = 1, 2, 3, \dots$): relates to size and energy of the orbital.
- δ 2. Angular Momentum QN (integer l or $\lambda = 0$ to $n - 1$): relates to shape of the orbital.
- δ 3. Magnetic QN (integer m_l or $m_\lambda = +l$ to $-l$): relates to orientation of the orbital in space relative to other orbitals.
- δ 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

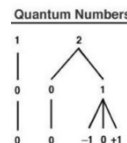


The Hierarchy of Quantum Numbers for Atomic Orbitals			
Name, Symbol (Property)	Allowed Values	Quantum Numbers	
Principal, n (size, energy) $n = 1, 2, 3, \dots$	Positive integer (1, 2, 3, ...)	1	2
Angular momentum, l (shape) $l = 0 \text{ to } n - 1$	0 to $n - 1$	0	1
Magnetic, m_l (orientation) $m_l = +l \text{ to } -l$	$-l, \dots, 0, \dots, +l$	0	1

QUESTION

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

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



QUESTION

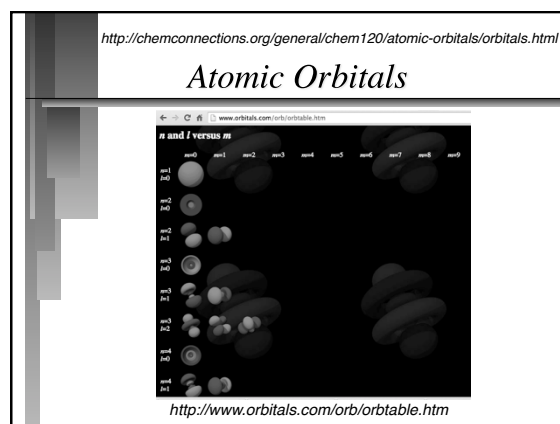
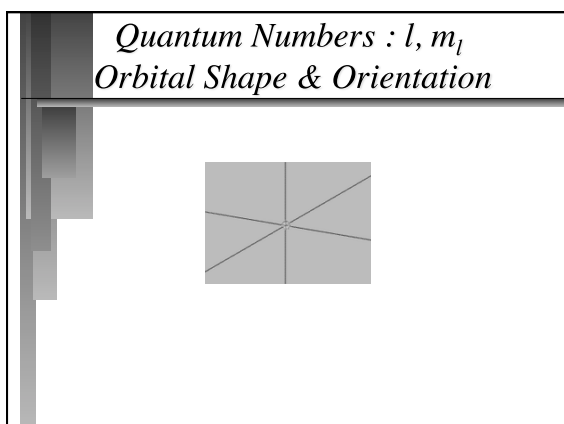
How many f orbitals have the value $n = 3$?

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

QUESTION

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

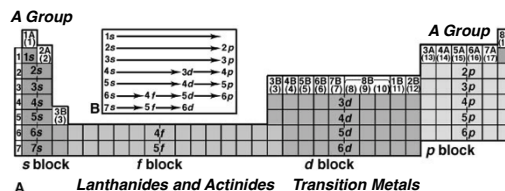
- A) 0
- B) 3
- C) 5
- D) 7
- E) 1



Periodic Table Classifications Electron Configurations & Quantum Numbers

- δ Representative Elements (A Groups):
s ($l=0$) and p ($l=1$) (N, C, Al, Ne, F, O)
- δ Transition Elements: d ($l=2$) orbitals
(Fe, Co, Ni, etc.)
- δ 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

Octet Rule & Electron Configurations

	7A (17)	8A (18)	1A (1)	2A (2)	3A (13)
5A (15)	H ⁻	He	Li ⁺		
6A (16)					
N ³⁻	O ²⁻	F ⁻	Ne	Na ⁺	Mg ²⁺
	S ²⁻	Cl ⁻	Ar	K ⁺	Ca ²⁺
	Br ⁻		Kr	Rb ⁺	Sr ²⁺
	I ⁻		Xe	Cs ⁺	Ba ²⁺

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

Electron Configurations

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

The Bohr Model Explanation of the Three Series of Spectral Lines

The diagram is divided into two parts, A and B.

Part A: A diagram of the Bohr model of a hydrogen atom. It shows a central nucleus with a '+' sign, surrounded by six concentric circular orbits labeled $n=1$ through $n=6$. Three regions are indicated by dashed lines and labels: 'Ultraviolet series' for transitions between $n=1$ and $n=2$ to $n=1$ and $n=6$; 'Visible series' for transitions between $n=2$ and $n=3$ to $n=2$ and $n=6$; and 'Infrared series' for transitions between $n=3$ and $n=4$ to $n=3$ and $n=6$.

Part B: A graph of Energy (in 10^{20} J/atom) versus Wavelength (in nm). The y-axis ranges from 0 to -200, with a specific level at -218. The x-axis ranges from 100 to 200 nm. The graph shows several vertical lines representing spectral lines. The 'Infrared' region is labeled for wavelengths greater than 700 nm. The 'Visible' region is labeled for wavelengths between approximately 400 nm and 700 nm. The 'Ultraviolet' region is labeled for wavelengths less than 400 nm. The lines correspond to the transitions shown in Part A.

Order for Filling Energy Sublevels with Electrons

The diagram illustrates the order in which atomic orbitals are filled with electrons. It features a vertical axis labeled "Energy, E" and a horizontal axis labeled "n". The orbitals are represented by horizontal bars of varying lengths, indicating their relative energy levels. The filling order is as follows:

- 1s
- 2s
- 2p
- 3s
- 3p
- 4s
- 3d
- 4p
- 5s
- 4d
- 5p
- 6s
- 4f
- 5d
- 6p
- 7s
- 5f
- 6d
- 7p

The diagram also shows the number of electrons (n) that can occupy each sublevel: 1s (2), 2s (2), 2p (6), 3s (2), 3p (6), 4s (2), 3d (10), 4p (6), 5s (2), 4d (10), 5p (6), 6s (2), 4f (14), 5d (10), 6p (6), 7s (2), 5f (14), 6d (10), 7p (6).

Multi-electron Electron Configuration

The Period 4 Crossover in Sublevel Energies

The graph shows the energy of the 3d and 4s sublevels as a function of atomic number (Z) from 1 to 60. The 4s sublevel is lower in energy than the 3d sublevel for Z < 20. At Z = 20, the 3d sublevel drops below the 4s sublevel, and this ordering continues for higher Z values.

Energy, E $\uparrow$

Atomic number, Z $\rightarrow$

1 20 40 60

4s

3d

$n=1$ 1s

$n=2$ 2s 2p

$n=3$ 3s 3p 3d

$n=4$ 4s 4p 4d 4f

$n=5$ 5s 5p 5d 5f

$n=6$ 6s 6p 6d 6f

$n=7$ 7s 7p 7d 7f

Los Alamos National Laboratory Chemistry Division

Periodic Table of the Elements

Electron Configuration

1A																	8A			
H																	He			
2A																	10A			
Li	Be															Ne				
3A	4A	5A	6A	7A														Ar		
Na	Mg															Kr				
4A	5A	6A	7A	8A																Xe
K	Ca	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As	Se	Br	Kr			
5A	6A	7A	8A	9A	10A	11A	12A													
Rb	Sr	Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd	In	Sn	Sb	Te	I	Xe			
6A	7A	8A	9A	10A	11A	12A														
Cs	Ba	*	Hf	Ta	W	Re	Os	Ir	Pt	Au	Hg	Tl	Pb	Bi	Po	At	Rn			
7A	8A	9A	10A	11A	12A															
Fr	Ra	**	Rf	Db	Sg	Bh	Hs	Mt	Ds	Rg	Cn	Nh	Fl	Mc	Lv	Ts	Og			

113: Nihonium, 115: Moscovium, 117: Tennessine and 118: Oganesson

Lanthanide Series

23	58	59	60	61	62	63	64	65	66	67	68	69	70	71
La	Ce	Pr	Nd	Pm	Sm	Eu	Gd	Tb	Dy	Ho	Er	Tm	Yb	Lu
89	90	91	92	93	94	95	96	97	98	99	100	101	102	103
Ac	Th	Pa	U	Np	Pu	Am	Cm	Bk	Cf	Es	Fm	Md	No	Lr

Actinide Series

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CHEMISTRY

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 ² 2p ¹	6 C [He] 2s ² 2p ²	7 N [He] 2s ² 2p ³	8 O [He] 2s ² 2p ⁴	9 F [He] 2s ² 2p ⁵	10 Ne [He] 2s ² 2p ⁶
3	11 Na [Ne] 3s ¹	12 Mg [Ne] 3s ²	13 Al [Ne] 3s ² 3p ¹	14 Si [Ne] 3s ² 3p ²	15 P [Ne] 3s ² 3p ³	16 S [Ne] 3s ² 3p ⁴	17 Cl [Ne] 3s ² 3p ⁵	18 Ar [Ne] 3s ² 3p ⁶

Full electron configuration (Spectroscopic notation) ---->

Spectroscopic Notation
Be → (1s)²(2s)²

Legend:
 ■ s-block elements
 ■ p-block elements
 ■ d-block elements
 ■ f-block elements

QUESTION

The electron configuration for the barium atom is:

A) 1s²2s²2p⁶3s²3p⁶3d¹⁰4s²
 B) [Xe] 6s²
 C) 1s²2s²2p⁶3s²3p⁶4s¹
 D) 1s²2s²2p⁶3s²3p⁶4s²
 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)	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.

A)

B)

C)

D)

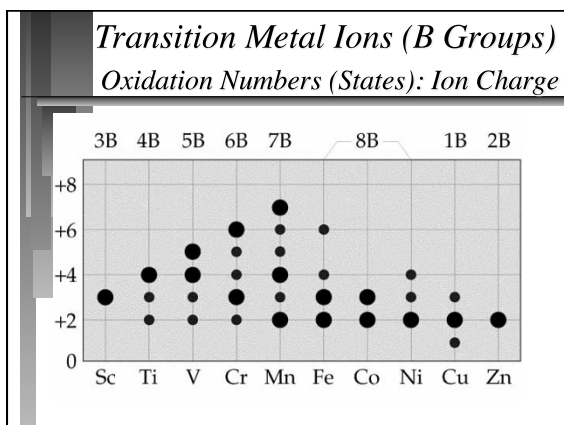
E)

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

A Li [He] 2s¹ + F [He] 2s²2p⁵ → Li⁺ 1s² (or [He]) + F⁻ [He]2s²2p⁶ (or [Ne])

B

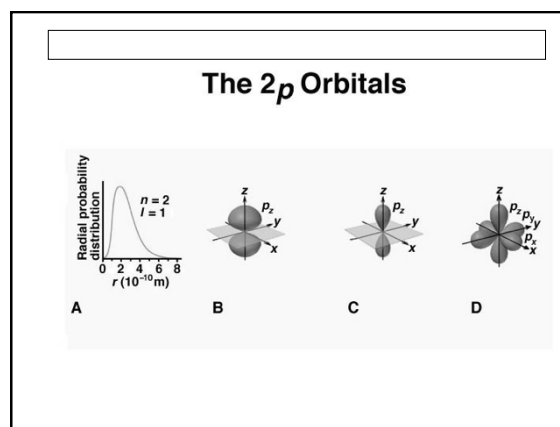
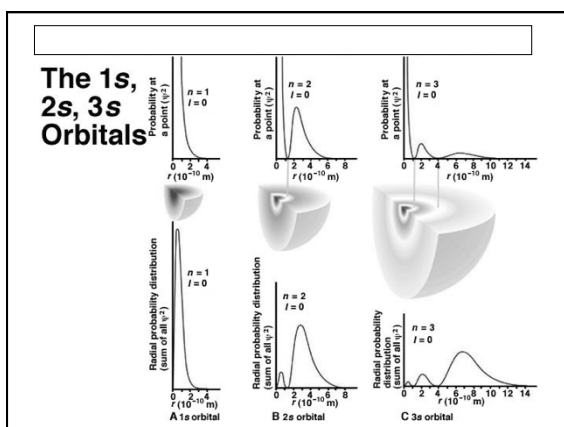
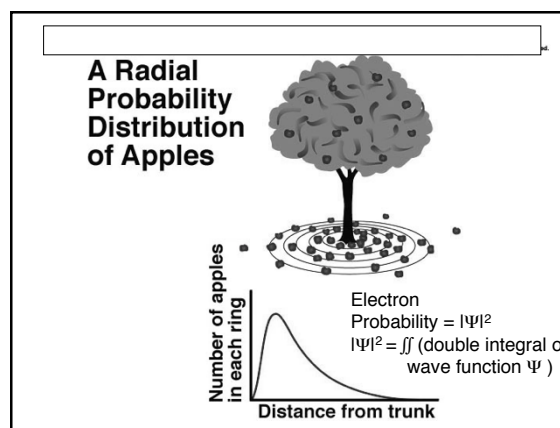


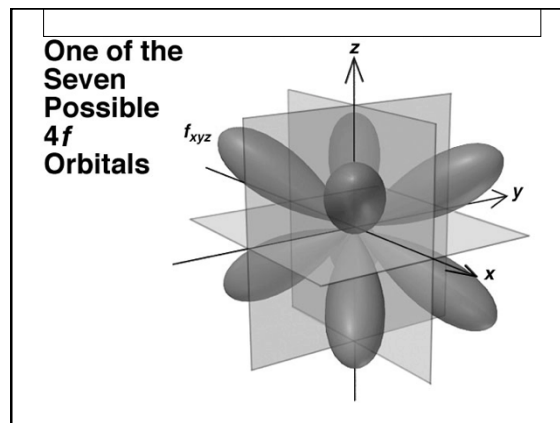
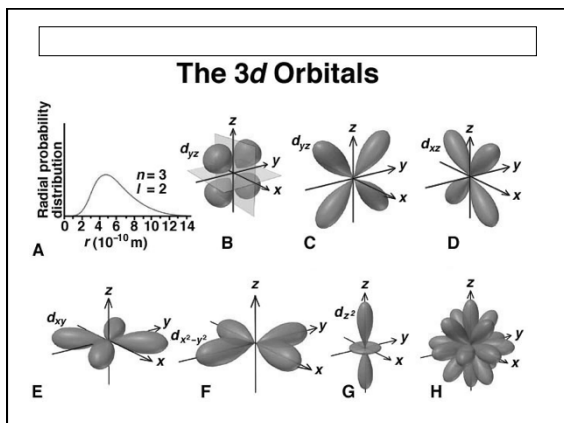
Summary: Information from the Periodic Table

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

This information can be used to:

- δ a. Predict the physical properties and general chemical behavior of the elements.
- δ b. Identify metals and nonmetals.
- δ c. Predict ions & formulas of compounds





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.

Aufbau Principle

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 ->

Boron, 8

1s: $\uparrow\downarrow$
2s: $\uparrow\downarrow$
2p: $\uparrow$ (empty), (empty)