Welcome CHEM 232

Instructor: Prof. Duncan Wardrop

Time/Day: T & R, 12:30-1:45 p.m.

January 12, 2010

Course Website

http://www.chem.uic.edu/chem232

- ☑ Syllabus
- ☑ Course Policies
- ☑ TA office hours and info
- ☑ Lecture slides (updated each week)
- ☑ Other handouts
- ☑ Announcements (Course News)
- ☑ Course Calendar

Assessment

- ☑ Quizzes: 25 x 10 points = 250 points (25%)
- ☑ Exams: 3 x 150 points = 450 points (50%)
- ☑ Final Exam: 250 points (25%)

To Do This Week

☑ **1. Attend your discussion section.**

☑ a. Check your course registration against TA roster.

☑ b. Master functional groups. Prepare for quiz.

☑ **2. Purchase *Carey* and Molecular Models**

☑ **3. Read Chapter 1 from *Carey*.**

☑ **4. Read Handouts on Website**

Keys to Success

- ☑ 1. Attend all lectures and discussion sections.
- ☑ 2. Don't fall behind. Organic chemistry is easy, but each topic builds on the previous.
- ☑ 3. Don't memorize. Organic chemistry is conceptual.
- ☑ 4. Work through homework carefully. Take notes.
- ☑ 5. Always ask yourself "Why" for everything you read or hear. You may not always find the answer, but just asking will help you to find connections and remember more.

Origins and Examples of Organic Chemistry

Introduction

Vitalism

Living

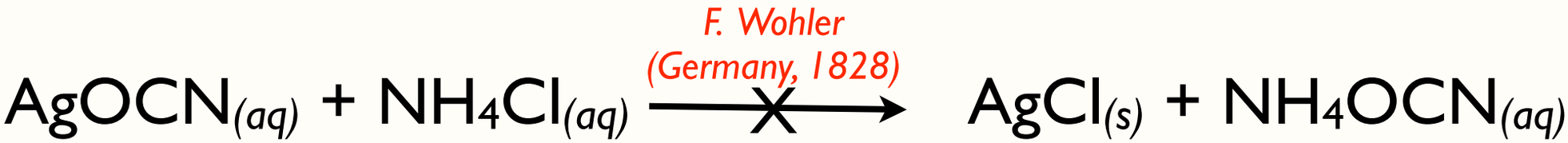
- posses vital force
- compounds derived from are "organic" (coined by J. Berzelius, 1807)
- could not be synthesized in the laboratory

vs.

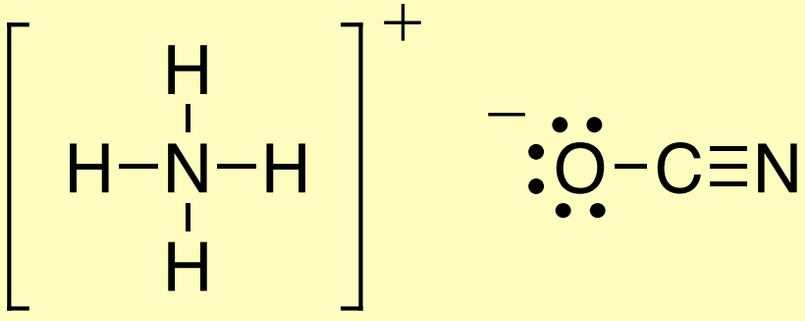
Nonliving.

- termed "inorganic"
- derived from *nonliving* matter
- can be synthesized in the lab

Wohler Synthesis Debunks Vitalism

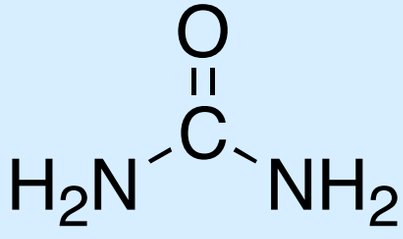


Expected Product



ammonium cyanate
(inorganic)

Actual Product



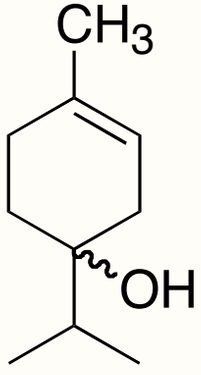
urea
(organic)

Self Test Question

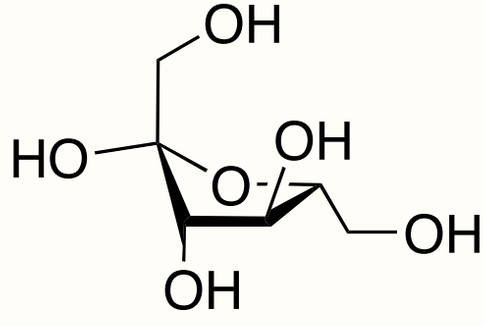
What is the minimum requirement, *today*, for a *chemical substance* to be classified as *organic*?

A. derived from living matter
B. contains carbon
C. cannot be synthesized
D. bought at *Whole Foods*
E. combustion yields SO_2

Vitalism Lives On. . .

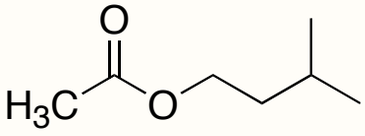


terpinen-4-ol
sold as tea tree oil
or Melaleuca oil

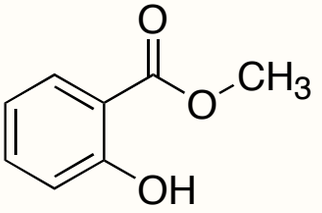


fructose
"fruit sugar"
also in HFCS

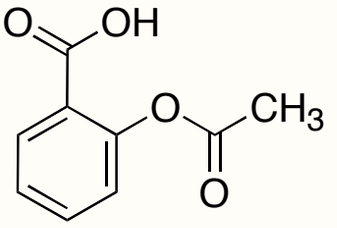
Organic Chemistry Everywhere



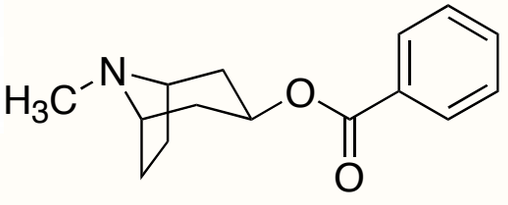
3-methylbutyl acetate
(bananas)



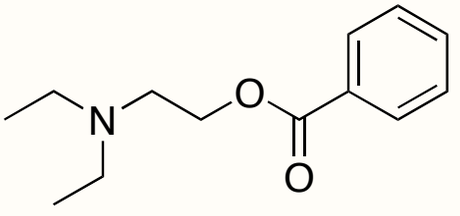
methyl salicylate
(oil of wintergreen)



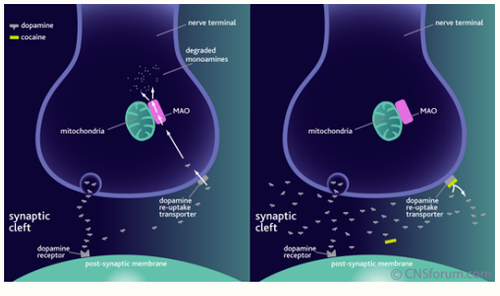
aspirin
(analgesic)



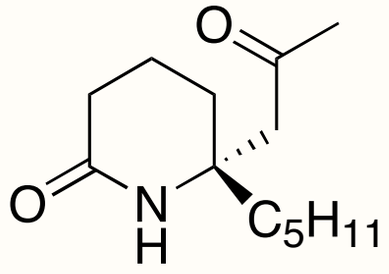
cocaine
(analgesic)



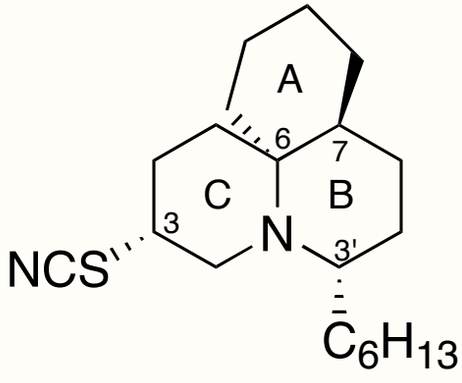
procaine, "Novocaine"
(analgesic)



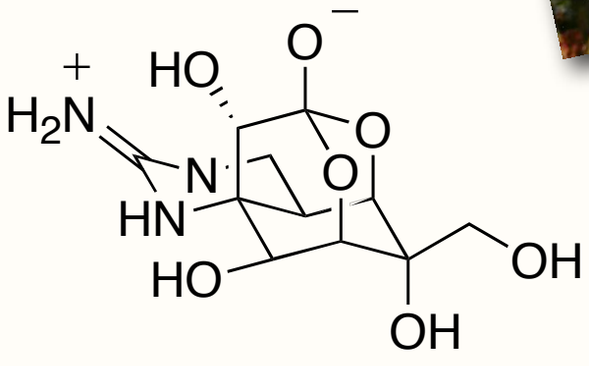
Natural Products



(-)-adalinine

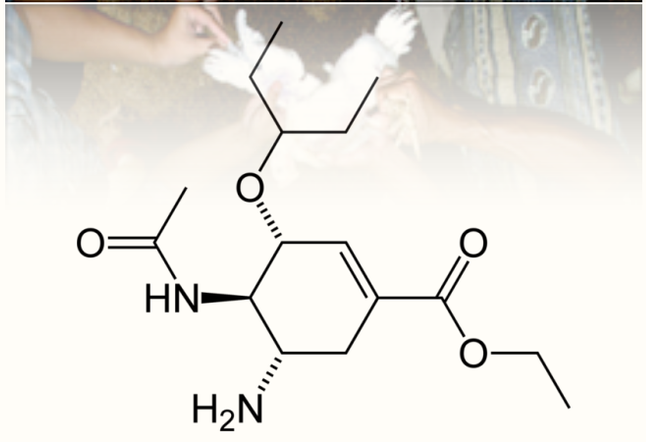


fasicularin

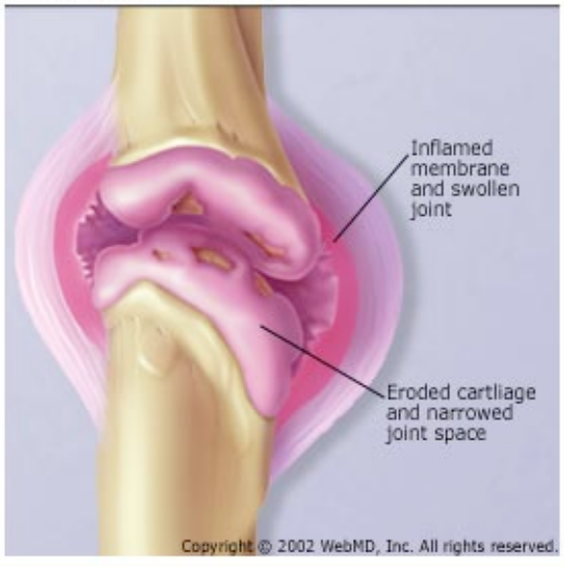


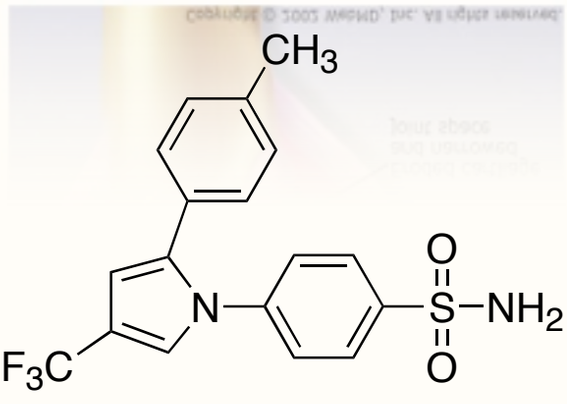
(-)-tetrodotoxin

Pharmaceuticals

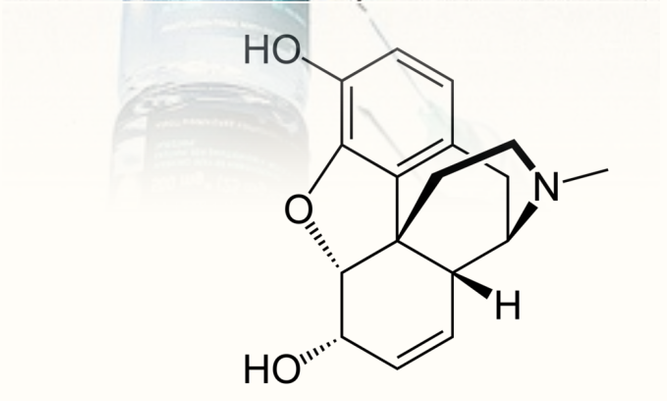


Tamiflu
(influenza)



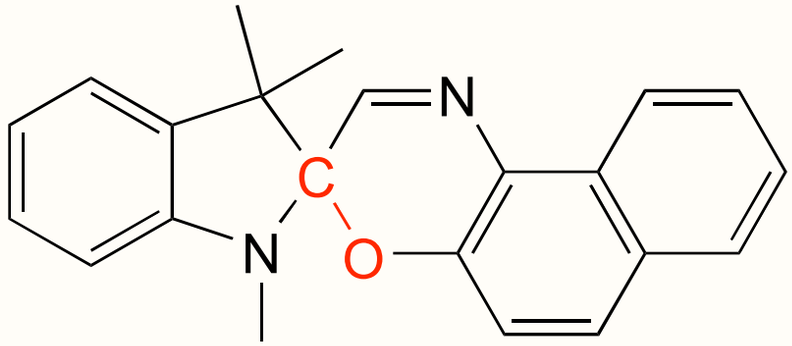


Celebrex
(arthritis)



Morphine
(analgesic)

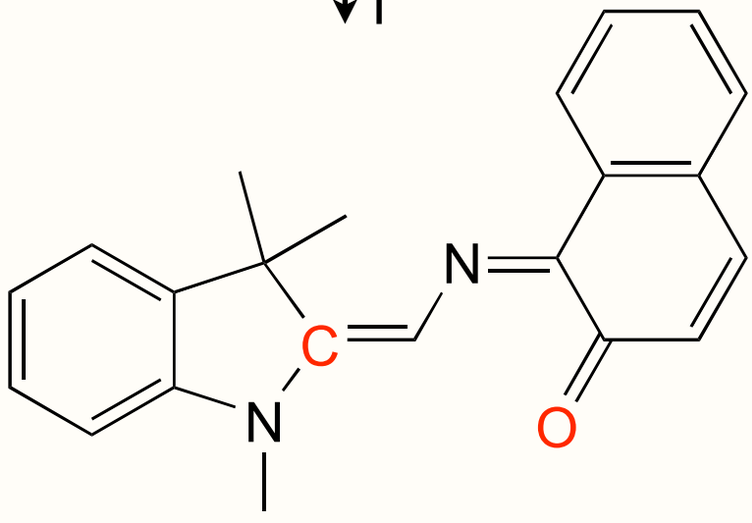
Optics - Transition Lenses?



does not absorb visible light

UV light

heat

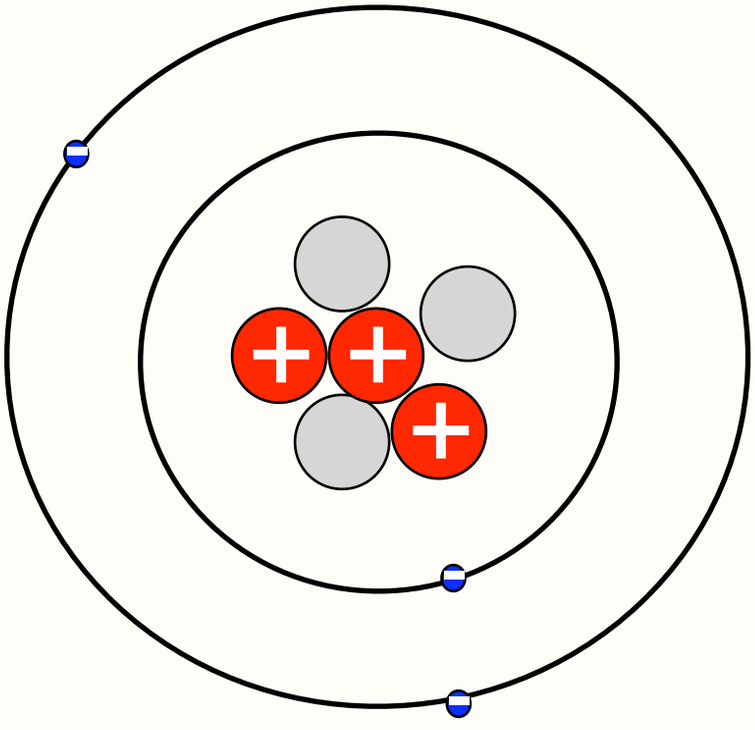


does absorb visible light

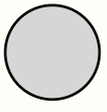
Atomic Structure
A General Chemistry Review

Section: 1.1

Atomic Composition



Bohr Model

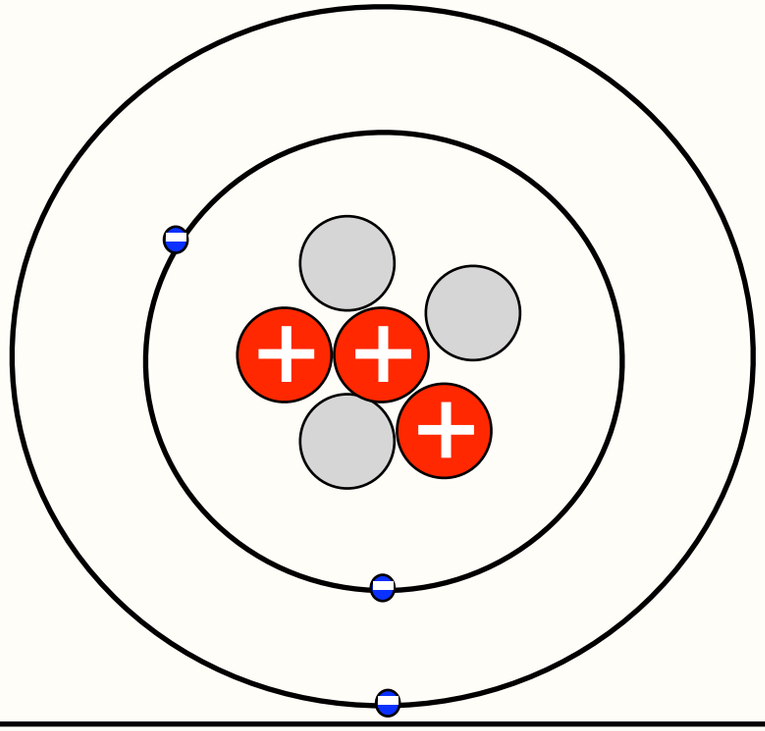
	particle	charge	mass molar mass	symbol
	proton	positive	1.6726×10^{-24} g 1.0073 g/mol	p
	neutron	neutral	1.6750×10^{-24} g 1.0087 g/mol	n
	electron	negative	9.1096×10^{-38} g 5.486 x 10-4 g/mol	e^-

Atomic Number & Mass Number

$$ {}^{A}_{Z}X $$

A = protons + neutrons

Z = protons



$$ {}^{6}_{3}Li $$

For neutral molecules, the number of electrons equals the number of protons.

Self Test Question

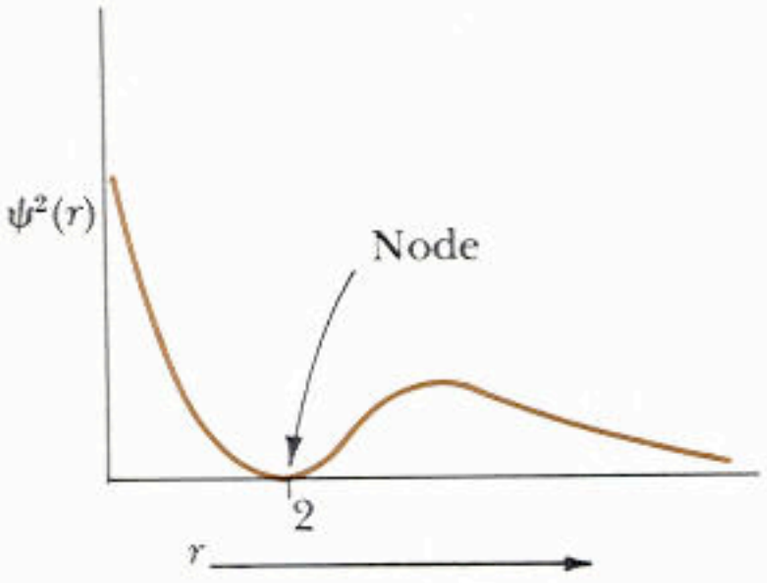
How many neutrons are in the following atom:

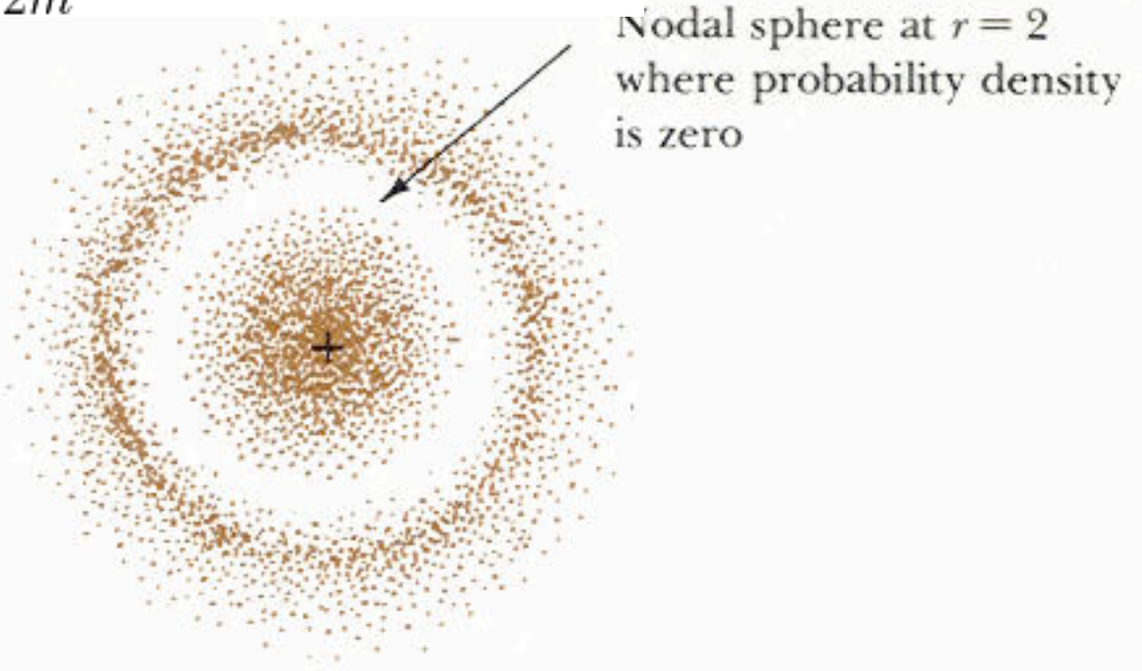
$^{14}_{6}C$

A. 14
B. 6
C. 8
D. 20
E. cannot be determined

Tenets of Schrödinger Equation

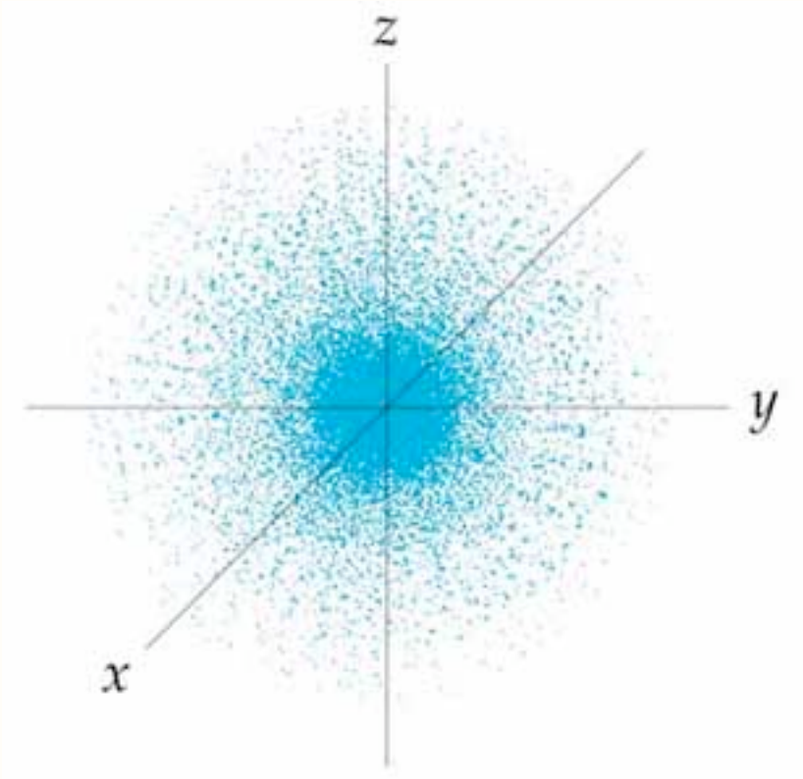
$$i\frac{\partial}{\partial t}\Psi(x,t) = -\frac{1}{2m}\nabla^2\Psi(x,t) + V(x)\Psi(x,t).$$



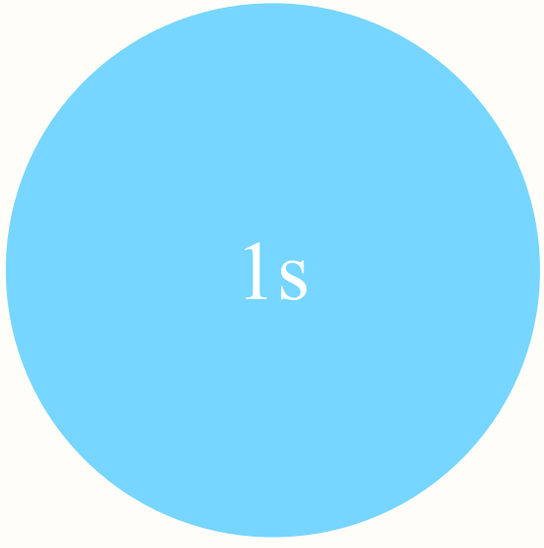


- electrons have wave properties
- wave equation gives energy of electron at a location
- solutions to wave equation are wave functions (Ψ); a.k.a orbitals
- probability distribution = Ψ^2 (Heisenburg uncertainty principle)

Probability Distribution vs. Boundary Surface



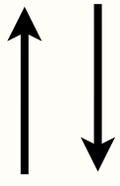
Probability distribution (Ψ^2)
("electron cloud")



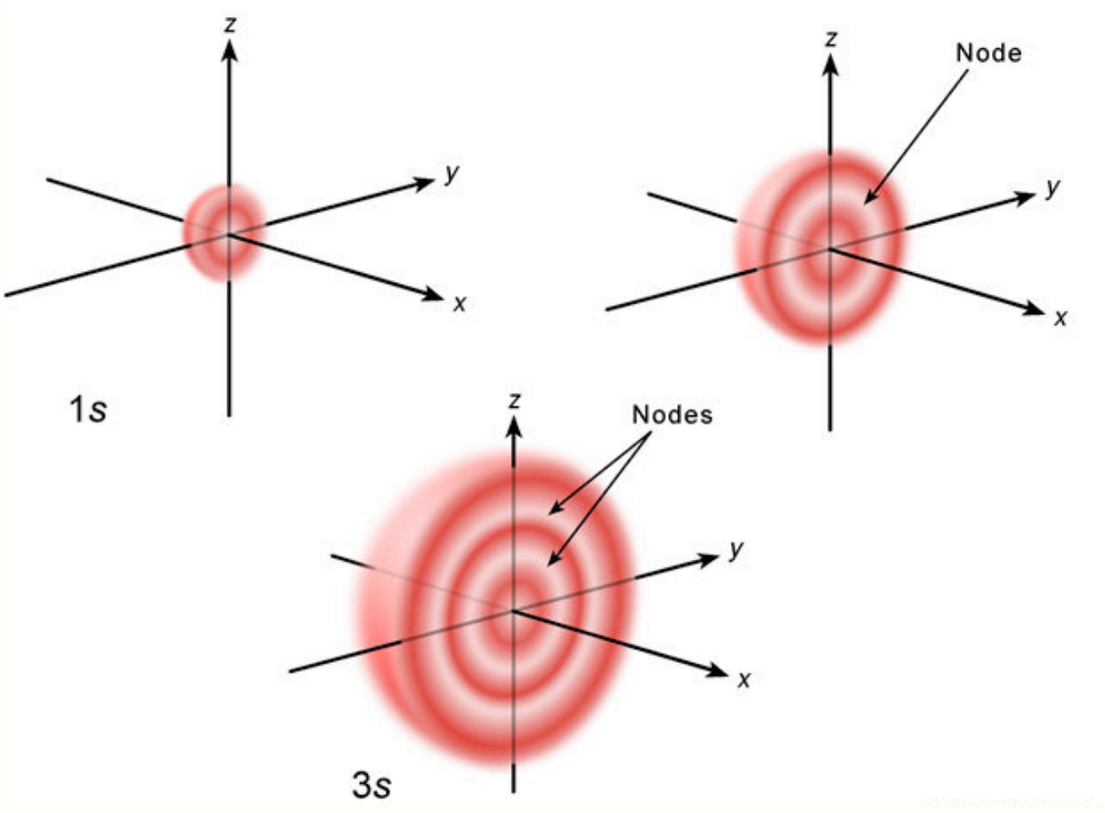
Boundary Surface (1s orbital)
(where the probability = 90-95%)

Wave Function Values: Quantum Numbers

- Shrodinger equation → wave function (orbital, Ψ)
- many solutions for Ψ, energies of electrons in atom

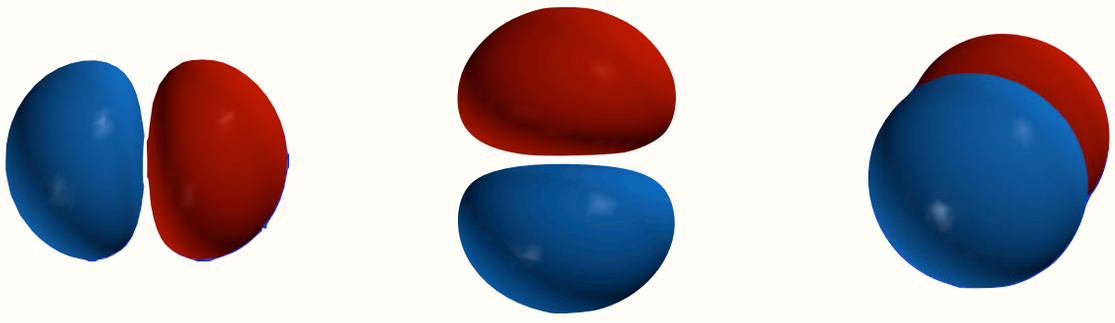
quantum number	principle	orbital	magnetic	spin
symbol	n	l	m_ℓ	m_s
values	1, 2, 3. . .	0, 1, . . . n-1	($m_\ell = -\ell, -\ell+1$ ... 0 ... $\ell-1$, l)	+1/2 or -1/2
examples/ abbreviations		l= 0, s l = 1, p l = 2, d l = 3, f	s: 1 orbital p: three orbitals d: five orbitals f: seven orbitals	

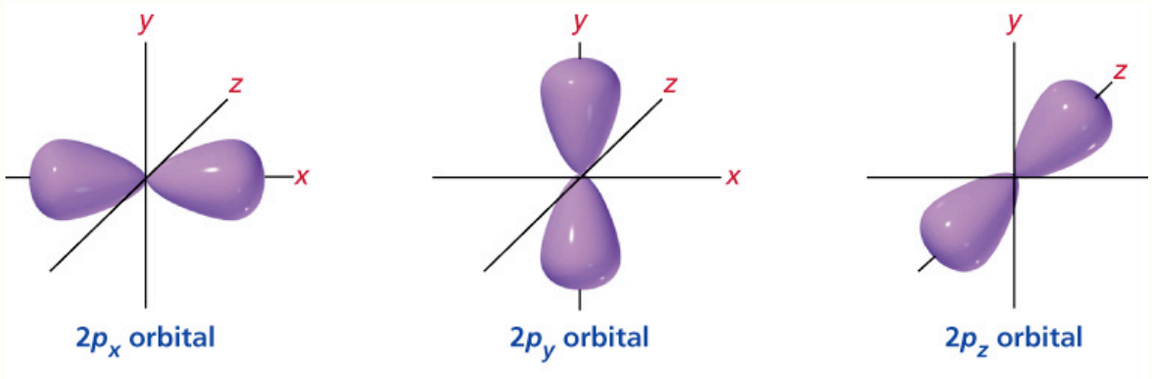
s-Orbitals



- spherically symmetric
- possible for $n \geq 1$
- 1 s-orbitals for each value of n
- 1s = no nodes, 2s = 1 nodes, 3s = 2 nodes, etc.
- probability of finding s-electron at nodal surface = 0
- s-orbital energy increases with increasing nodes (as n increases)

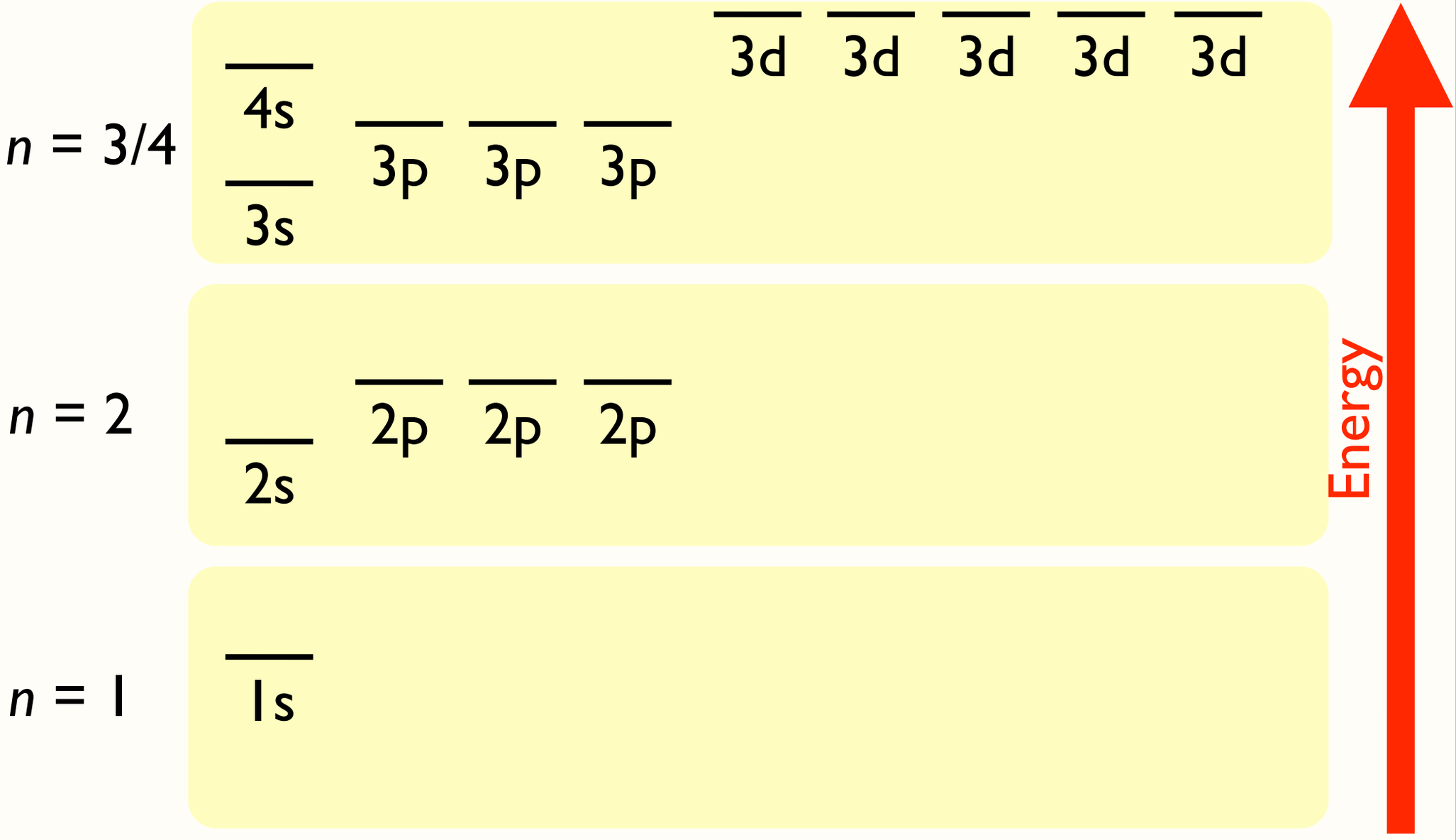
p-Orbitals





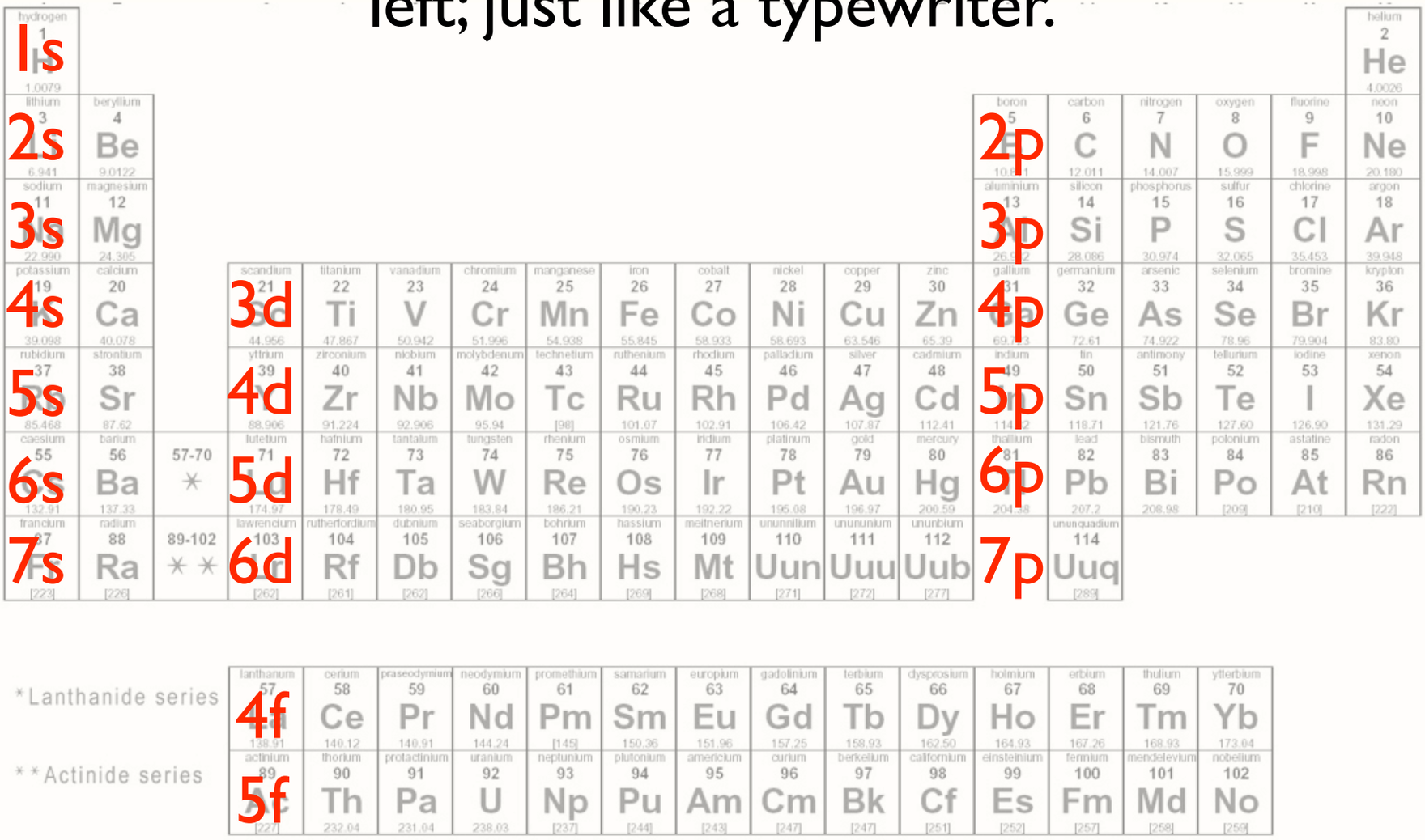
- shaped like dumbells
- not possible for n = 1 (n≥2)
- 3 p-orbitals for each value of n; they are degenerate (equal in energy)
- wave function changes sign at the nucleus (node)
- probability of finding p-electron at nodal plane = 0
- higher in NRG than s-orbitals of the same shell

Relative Energies of Orbitals

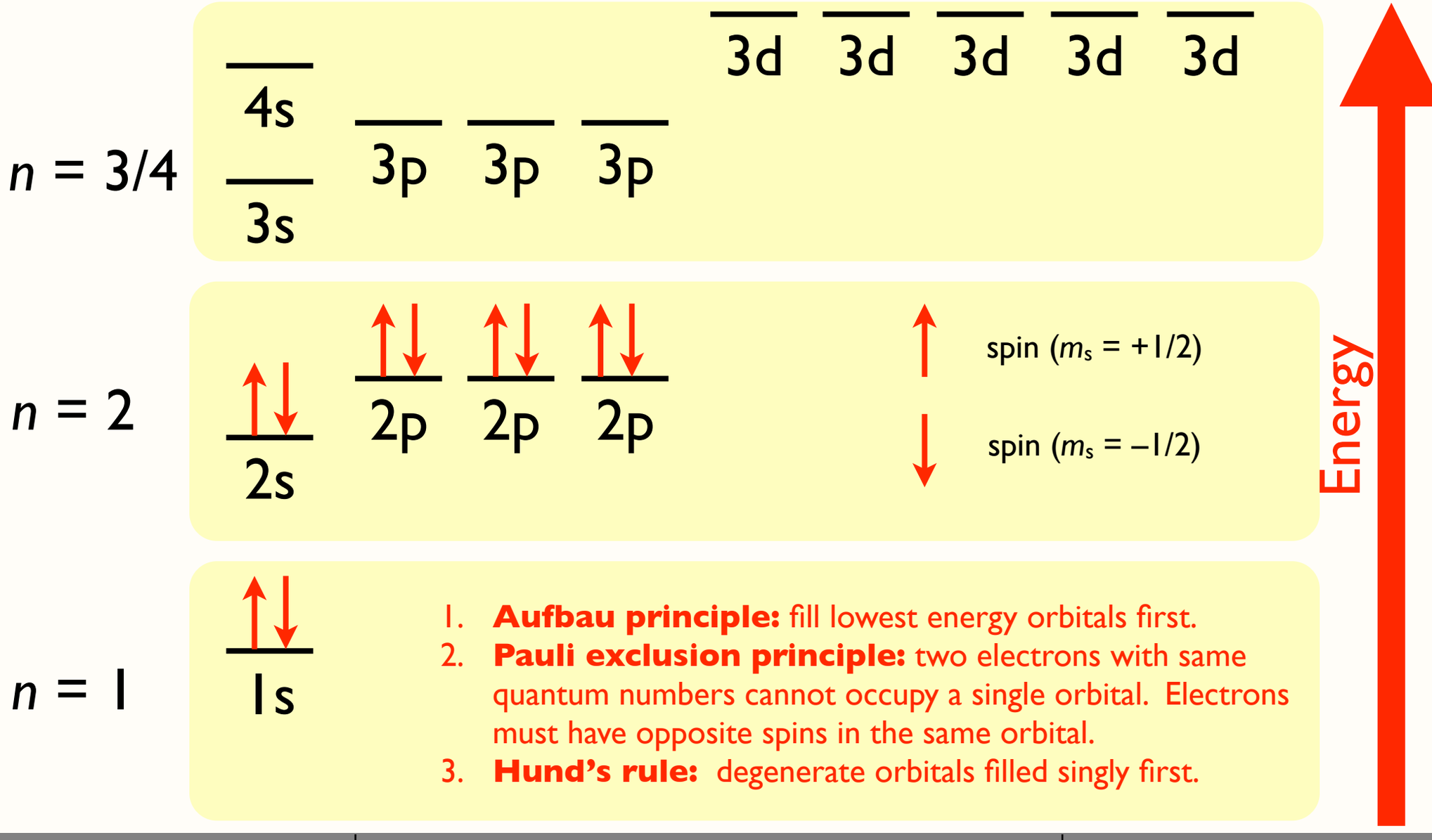


Order of Orbitals from Periodic Table

Read left to right starting at the top left; just like a typewriter.



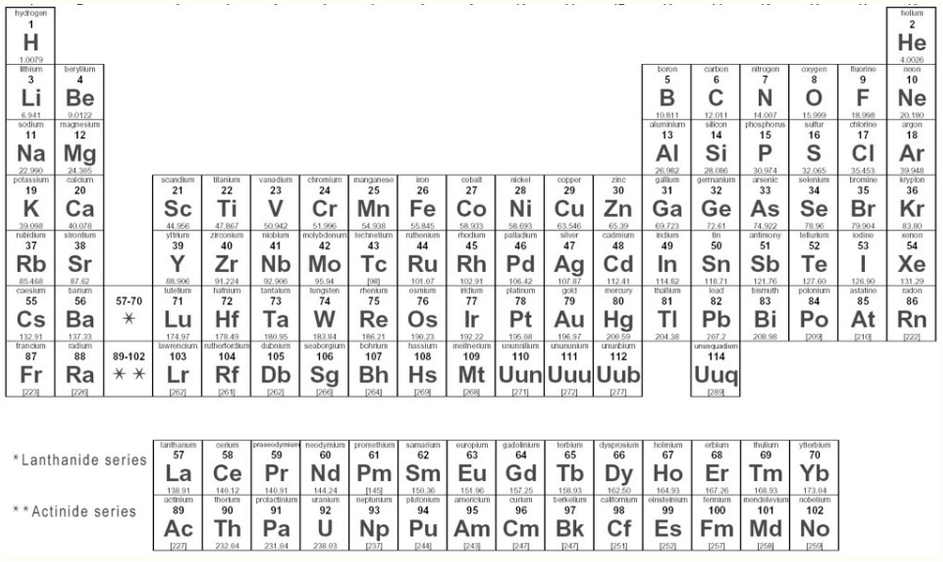
Electron Configuration: Filling Orbitals



1. **Aufbau principle:** fill lowest energy orbitals first.
2. **Pauli exclusion principle:** two electrons with same quantum numbers cannot occupy a single orbital. Electrons must have opposite spins in the same orbital.
3. **Hund's rule:** degenerate orbitals filled singly first.

Self Test Question

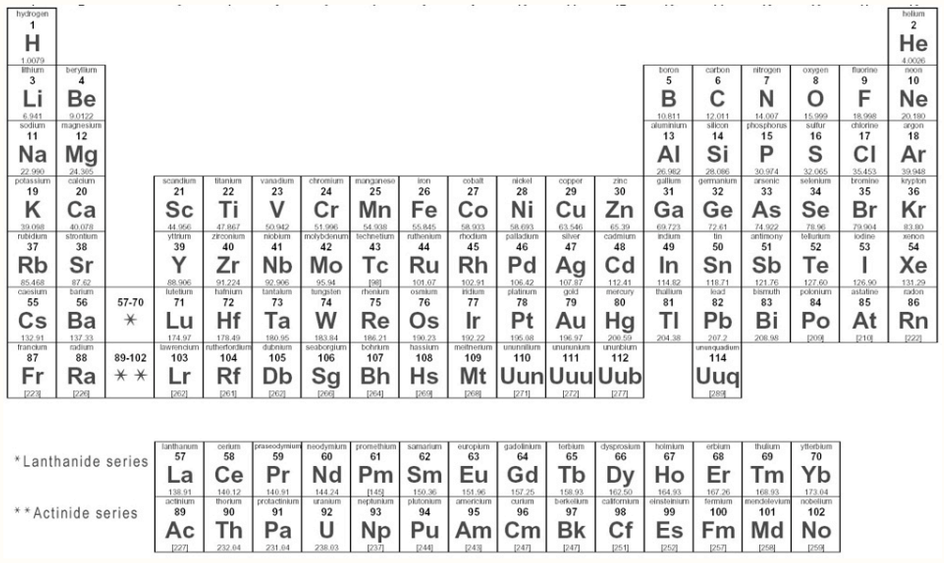
Which of the following orbitals is *highest* in energy?



A. 3f
B. 3p
C. 2s
D. 3s
E. 2d

Self Test Question

Which is the correct electron configuration for carbon?



A. $1s^2, 2s^8$
B. $1s^2, 2s^4$
C. $1s^2, 2s^2, 2s^2$
D. $1s^2, 2s^2, 2p^2$
E. none of the above

Bonding and Molecular Structure

Sections: 2.2, 2.3, 2.4, 1.3, 1.5, 1.6, 1.9

You are responsible for sections 1.2, 1.4, 1.7, 1.10

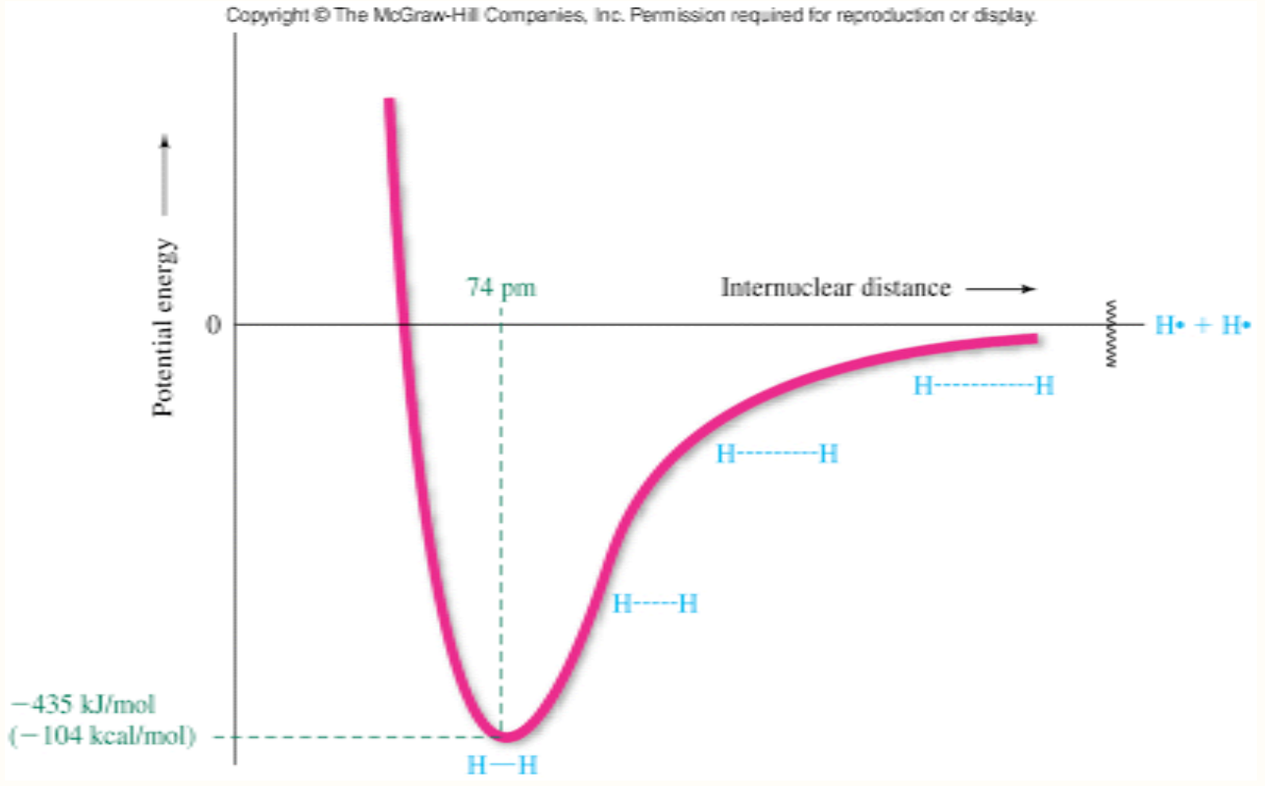
What is a Covalent Chemical Bond?

valent = bonding

covalent = electrons shared between two nuclei

Forces involved:

- electron-electron repulsion
- nucleus-nucleus repulsion
- electron-nucleus attraction

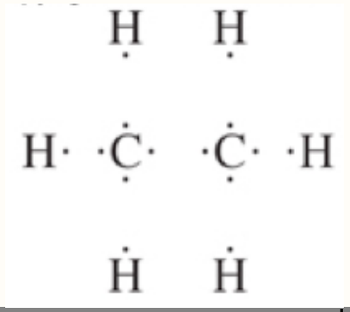
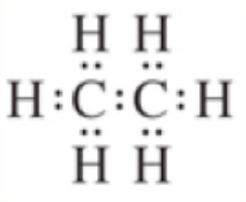
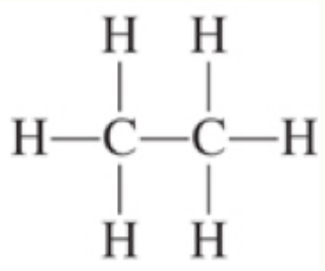


electron-electron repulsion < electron-neutron attraction

Three Models of Bonding

Lewis Model:

- atoms gain, lose or share electrons in order to achieve a closed-shell electron configurations (all orbitals fully occupied)
- closed-shell for row 2 = 8 electrons (octet rule)
- only valence electrons (in outermost shell) are involved in bonding

Atomic Structures	Molecular Lewis Structures	Molecular Lewis Structures
		H–H
		F–F
		

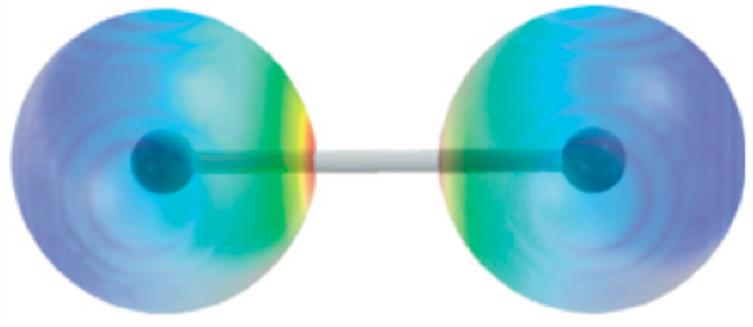
Three Models of Bonding

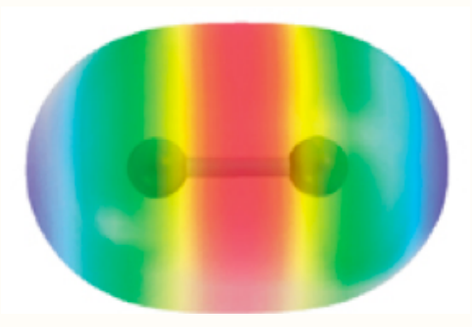
Valence Bond Model:

- in-phase overlap of two half-filled orbitals
- in-phase = constructive interference
- increases probability electrons *between* two nuclei

Boundary Surfaces

Electrostatic Potential maps:
red = negative
blue = postive

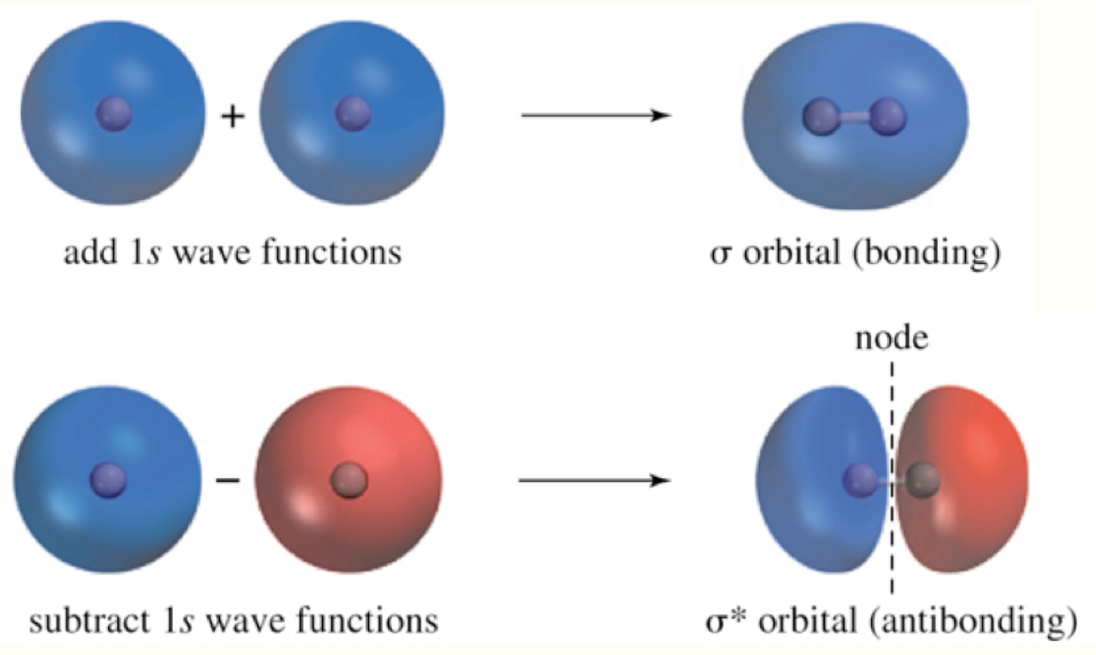




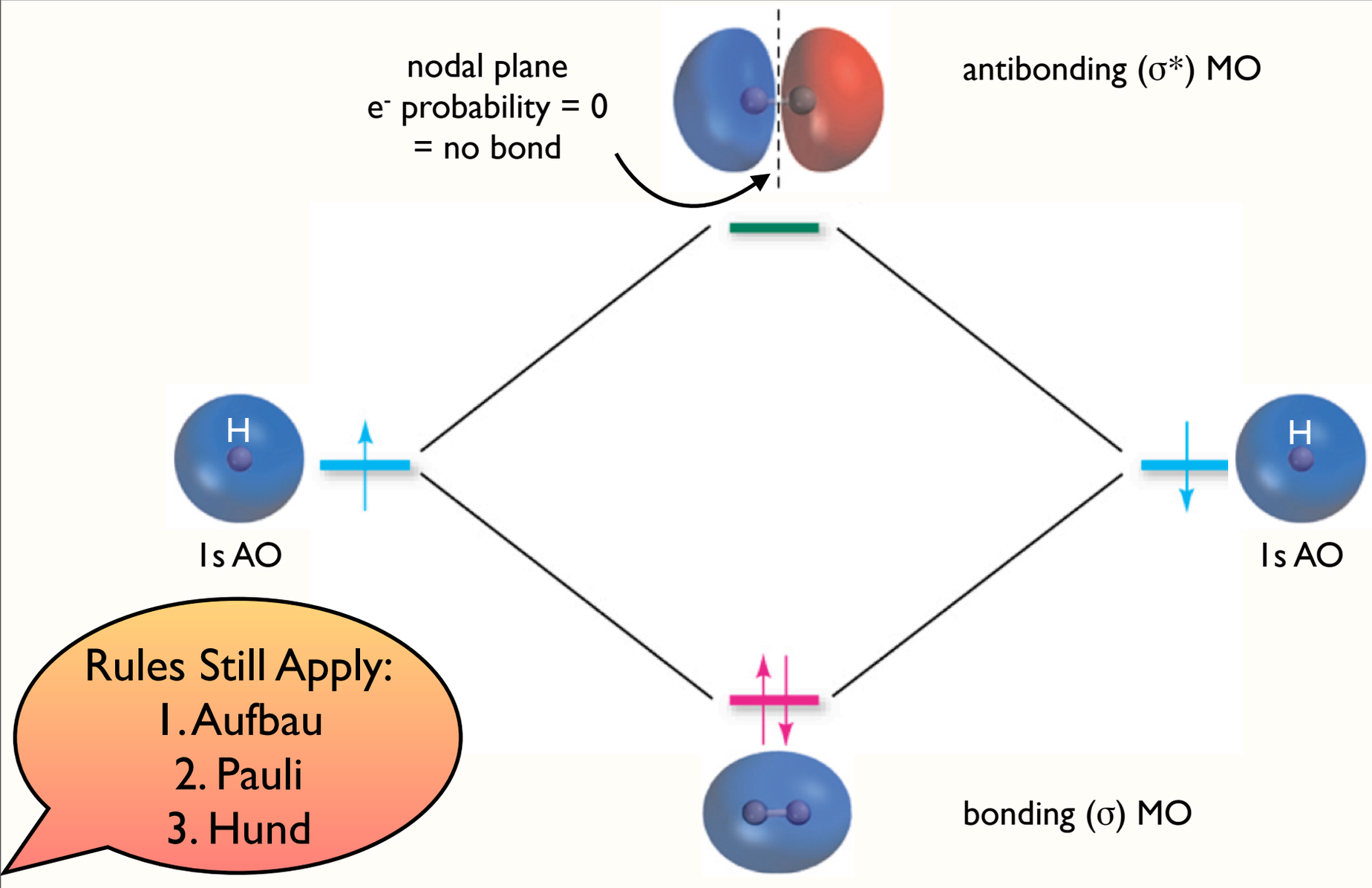
Three Models of Bonding

Molecular Orbital (MO) Model:

- combine atomic orbitals (AO) of all atoms, then extract molecular orbitals
- number of atomic orbitals in equals the number of molecular orbitals out
- combination possibilites:
  - additive = produces bonding molecular orbitals
  - subtractive = produces antibonding molecular orbitals

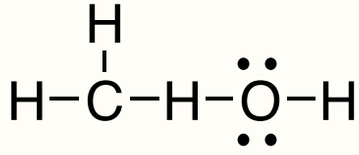


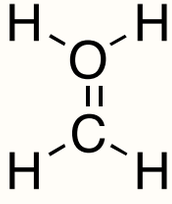
Molecular Orbital Diagram

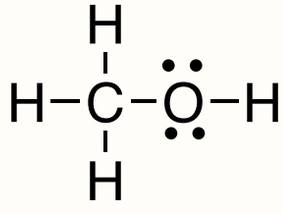


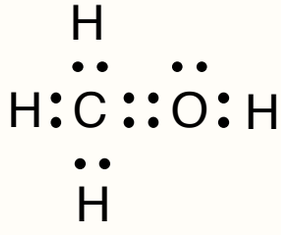
Self Test Question

Which is the correct Lewis dot structure for CH_4O?

A. 

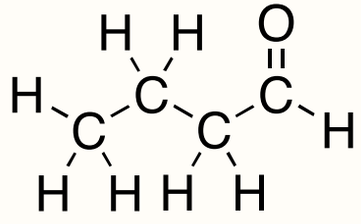
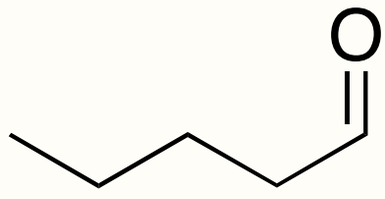
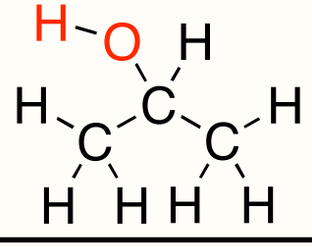
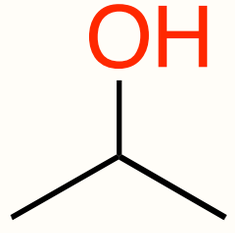
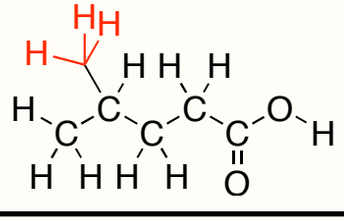
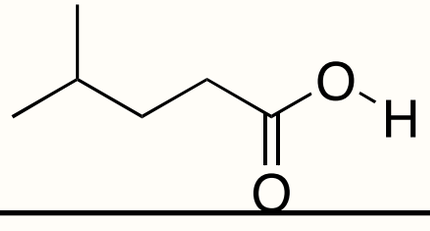
B. 

C. 

D. 

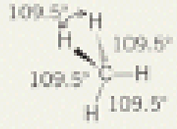
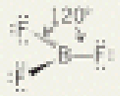
E. none of the above

Structural, Bond-line and Condensed Formulas

Structural	Bond-line	Condensed
•format varies; typically *most* covalent bonds are drawn out •bonds are lines •only lone-pair (nonbonding) electrons are drawn as dots	•only atoms written are those that are *not* C or H bound to C •intersection of two lines is C •terminus of a line is -CH_3 group •# H atoms is assumed for C •chains drawn as "zig-zag"	•all or most covalent bond lines are omitted •groups are separated by parentheses (infers group is attached to carbon with available valency on left or right)
		$CH_3CH_2CH_2CHO$
		$CH_3CH(OH)CH_3$
		$(CH_3)_2CHCH_2CH_2CO_2H$

VSEPR: Quick Review

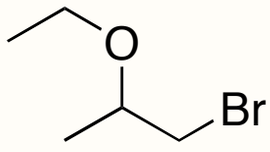
TABLE 1.7 VSEPR and Molecular Geometry

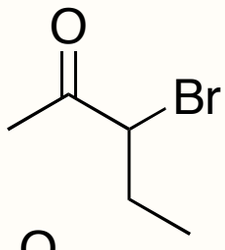
Compound	Structural formula	Repulsive electron pairs	Arrangement of electron pairs	Molecular shape	Molecular model
Methane (CH_4)		Carbon has four bonded pairs	Tetrahedral	**Tetrahedral**	
Water (H_2O)		Oxygen has two bonded pairs + two unshared pairs	Tetrahedral	**Bent**	
Ammonia (NH_3)		Nitrogen has three bonded pairs + one unshared pair	Tetrahedral	**Trigonal pyramidal**	
Boron trifluoride (BF_3)		Boron has three bonded pairs	Trigonal planar	**Trigonal planar**	
Formaldehyde (H_2CO)		Carbon has two bonded pairs + one double bond, which is counted as one bonded pair	Trigonal planar	**Trigonal planar**	
Carbon dioxide (CO_2)		Carbon has two double bonds, which are counted as two bonded pairs	Linear	**Linear**	

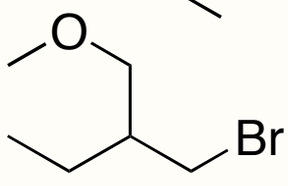
Self Test Question

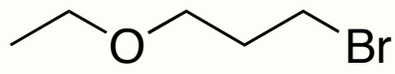
Which bond-line drawing correctly represents the following condensed formula?

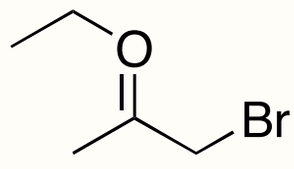
$CH_3CH(OCH_2CH_3)CH_2Br$

A. 

B. 

C. 

D. 

E. 

Functional Groups

Sections: textbook inside cover, Table 4.1 (pg. 140)

Memorize These Functional Groups NOW

functional group: a defined group of atoms with a specific connectivity

- responsible for properties
- predictable reactivity
- well-defined nomenclature

Memorizing: "What is the minimum number of atoms needs to define a functional group and in what order are they bonded?" Flashcards!

Table 4.1, page 140 →

TABLE 4.1 Functional Groups in Some Important Classes of Organic Compounds

Class	Generalized abbreviation*	Representative example	Name of example†
Alcohol	ROH	CH_3CH_2OH	Ethanol
Alkyl halide	RCl	CH_3CH_2Cl	Chloroethane
Amine‡	RNH_2	$CH_3CH_2NH_2$	Ethanamine
Epoxide			Oxirane
Ether	ROR	$CH_3CH_2OCH_2CH_3$	Diethyl ether
Nitrile	RC≡N	$CH_3CH_2C{\equiv}N$	Propanenitrile
Nitroalkane	RNO_2	$CH_3CH_2NO_2$	Nitroethane
Sulfide	RSR	CH_3SCH_3	Dimethyl sulfide
Thiol	RSH	CH_3CH_2SH	Ethanethiol
Aldehyde			Ethanal
Ketone			2-Butanone
Carboxylic acid			Ethanoic acid
Carboxylic acid derivatives			
Acyl halide			Ethanoyl chloride
Acid anhydride			Ethanoic anhydride
Ester			Ethyl ethanoate
Amide			Ethanamide

*When more than one R group is present, the groups may be the same or different.
†Most compounds have more than one acceptable name.
‡The example given is a *primary* amine (RNH_2). *Secondary* amines have the general structure R_2NH; *tertiary* amines are R_3N.

Next Lecture...

Sections: 1.5, 1.8, 1.10-1.17