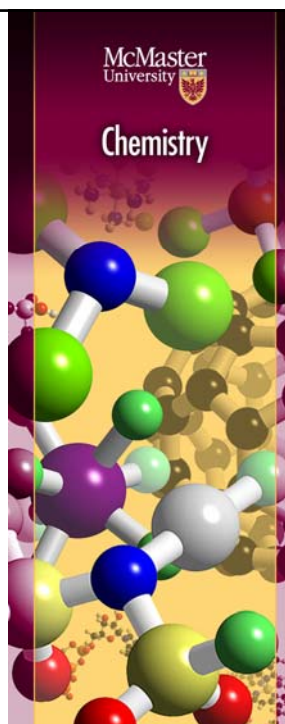
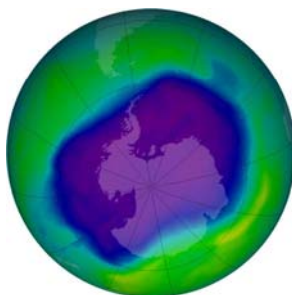


CHEM 1A03: Intro. Chemistry I

Essential Elements: Chemistry, Life & Health

Ch.8: *Electrons in Atoms*



Chemistry that's out of this world!

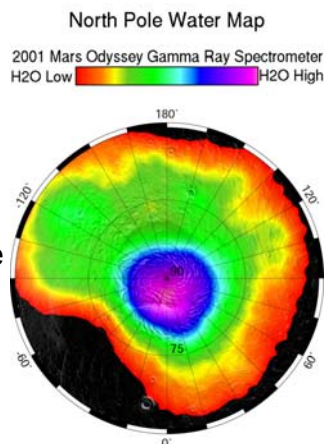
Life on Mars?

Odyssey Mission (Launch 2001): From space, mapped the amount/distribution of elements and minerals that make up the martian surface.

Maps of **H distribution** infer the presence of vast amounts of water ice buried beneath the surface in the polar regions.

Current: Mars Phoenix Lander Mission (Launch: Aug. 4/07, Landing: May 25/08)

Gamma Ray Spectrometer – detects an excited element's characteristic emission of energy.



Spectroscopy

What is spectroscopy?

The study of the interaction of radiation and matter

What types of radiation?

Electromagnetic radiation

What is electromagnetic radiation?

Energy transmission propagated as waves with perpendicular magnetic and electrical components

Petrucci, 9th edition, p. 278

Department of **3**
Chemistry

Review of Wave Properties & Light: Physics

Wave properties: Figure 8-2

Wavelength (λ , nm)

Frequency (ν , s⁻¹ or Hz)

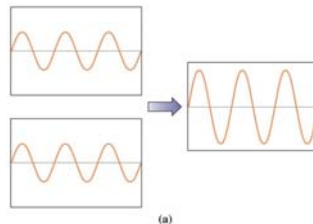
Amplitude

Wave Properties of Light:

Interference - Fig. 8-5

Diffraction - Fig. 8-4b

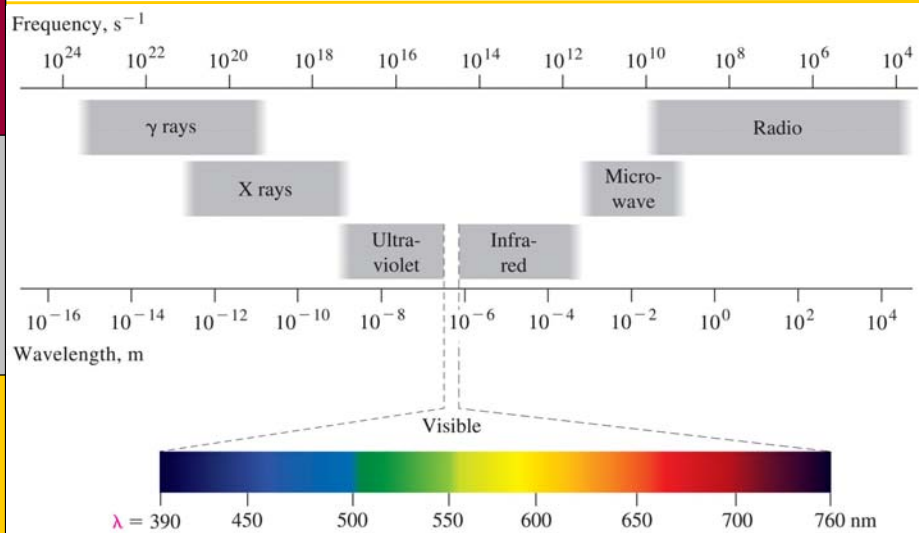
Refraction - Fig. 8-7a



p. 279-283

Department of **4**
Chemistry

Electromagnetic Spectrum (Fig. 8-3)

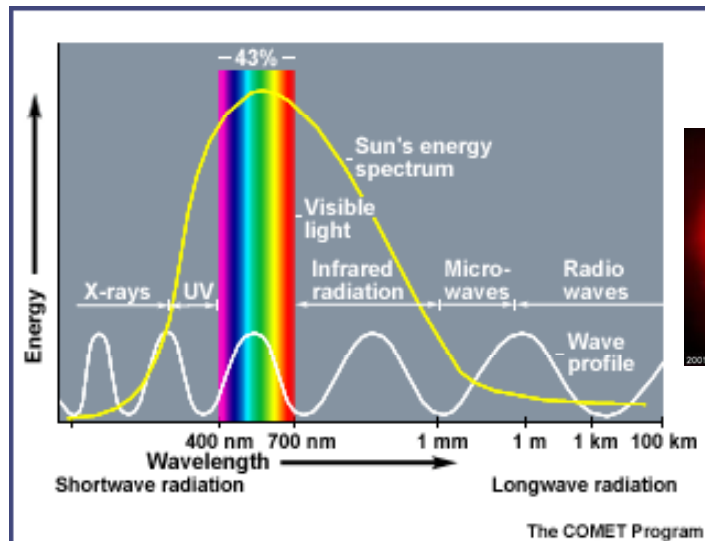


Department of **5**
Chemistry

i-Clicker Question#1

Department of **6**
Chemistry

Sun's Emission Spectrum



Sun ($T = 6,000K$)

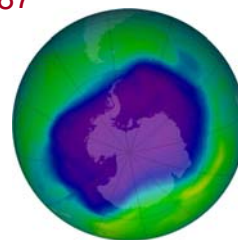
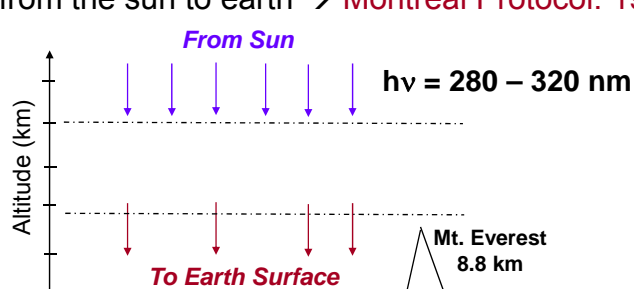


Department of 7
Chemistry

Earth's Protective Shield: Ozone

A. Ozone & UV Exposure

- **UVB radiation** (280-320 nm) from the sun is selectively absorbed by O_3 (ozone) in stratosphere
- **Photolysis of O_3** absorbs $\approx 90\%$ **UV B** radiation with peak at about 20km from Earth's surface
- **Lower O_3 levels** increase the transmittance of **UV B radiation** from the sun to earth \rightarrow **Montreal Protocol: 1987**



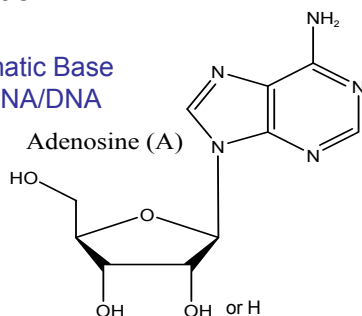
Department of 8
Chemistry

Ozone Depletion & UV Exposure

B. Biological Impacts

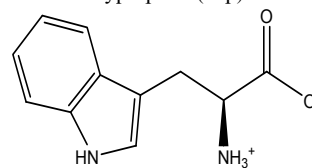
- UV B radiation can **ionize** biological molecules
- **Chronic exposure** to UVB transmission increases chance of skin cancer, cataracts & genetic mutations
- Body's response: produce **melanin** (dark pigment) to filter UV B radiation.

Aromatic Base
in RNA/DNA



Aromatic Amino Acid
in Protein

Tryptophan (Trp)

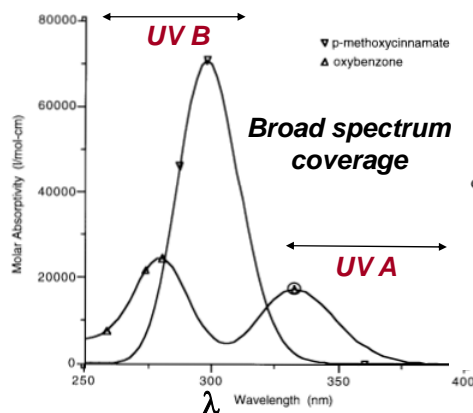


Department of **9**
Chemistry

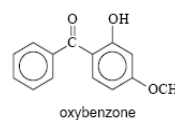
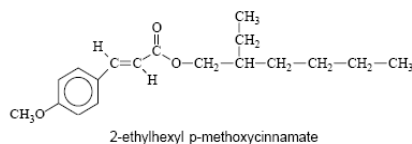
UV Exposure & Sunscreen

C. Chemistry of Sunscreen

- Propose alternative ways to **decrease exposure** to UV radiation?
- Use of sunscreen/cosmetics containing **UV absorbing chemicals**



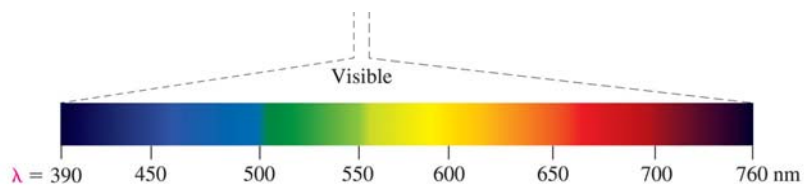
2 Major Chemical Sunscreens:



Department of **10**
Chemistry

Continuous vs. Discontinuous Spectra

- Continuous: e.g. visible spectrum



- Discontinuous: e.g. visible Na emission lines



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589.0, 589.6 nm

Department of **11**
Chemistry

Atomic spectra

- *Discontinuous* (Line) spectra of atoms; few λ
 - Observed by experiment (Fig. 8-8)
 - Unique for each element (characteristic λ produced)
 - Samples are excited by electric discharge or gas flame



H₂

He

Li salt

Na salt

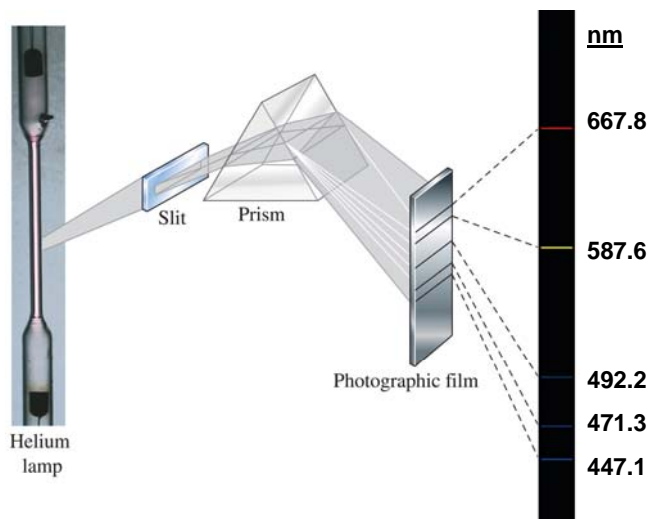
K salt

<http://youtube.com/watch?v=d8hpUtRnsYc&mode=related&search>

Department of **12**
Chemistry

Atomic spectrum experiment (Fig. 8-9)

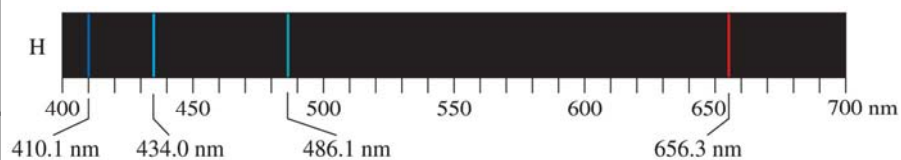
- Emission spectrum of excited He:
- Light from the discharge is filtered through a slit, passed through a prism (refraction, p. 282)
- Only certain λ of visible light observed



p. 284

Department of 13
Chemistry

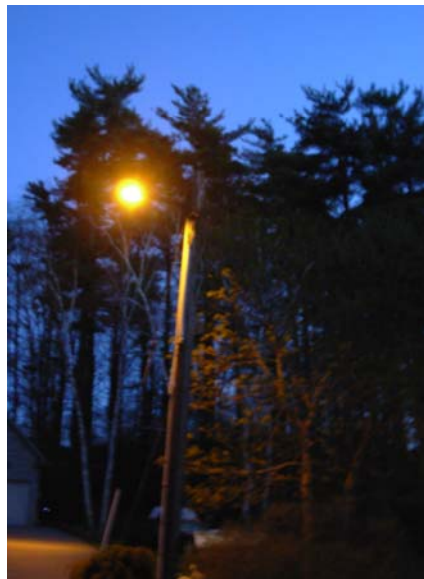
Atomic spectrum of H (Fig. 8-10)



- **H**: Most abundant element in universe!
- Johann Balmer (1885) calculated the λ of the 4 visible spectral lines for hydrogen
- In terms of frequency:

Department of 14
Chemistry

Na Emission in Streetlamps



Streetlamp
Na D-lines
(589.0, 589.6 nm)

Department of 15
Chemistry

Problems with classical physics

- Classical physics could not address certain phenomena
 - discontinuous spectra
 - blackbody radiation (where radiation is emitted by hot objects *but* intensity of radiation does not increase indefinitely)
- **Problem:** Classical physics imposes no limit on the amount of energy a system may possess
- **Solution:**

p. 285

Department of 16
Chemistry

Quantum: Theory & Experiment

- Max Planck proposed (1900): energy, like matter, is discontinuous (quantized)



$E = \text{energy}, \nu = \text{frequency}$

$h = \text{Planck's constant}, 6.626 \times 10^{-34} \text{ J s}$

- This idea was used by Einstein (Nobel Prize) to explain Hertz's experiment...

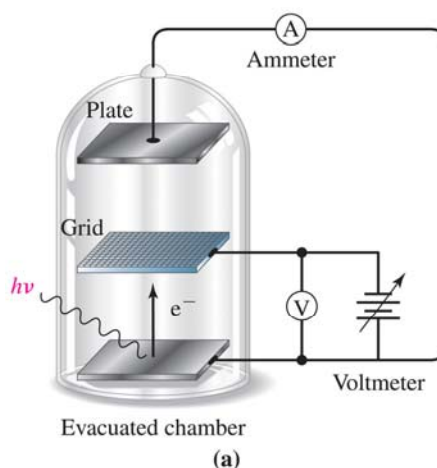


p. 285

Department of 17
Chemistry

Photoelectric effect (Fig. 8-12 a)

- Single λ light strikes a metal surface to which a voltage is applied.
- If $E_{\text{photon}} > \text{Threshold Energy of metal}$, e^- are ejected with KE
- Measured current (ammeter) determines # of e^- emitted
- If a negative potential on grid is applied, e^- stop at the grid. The voltage gives a measure of the KE of the e^- .



p. 286-289

Department of 18
Chemistry

Key observations – Photoelectric effect

- Work function (threshold energy, $h\nu_0$) of the metal must be overcome for e^- to be emitted
- When incident light frequency exceeds a **threshold value** (ν_0), e^- are emitted
- # of electrons (current) emitted depends on light intensity (# of photons)
- K.E. of emitted electrons depends on E (or ν) of light

Department of **19**
Chemistry

i-Clicker Question#2

Department of **20**
Chemistry

i-Clicker Question#3

Department of 21
Chemistry

Einstein's proposal

- Light is quantized like a particle (photons)
- $E_{\text{photon}} = h\nu$ and
 $E_{\text{photon}} = \Delta E_{\text{atom}}$
 \therefore

p. 288

- Related application of photoelectric effect: solar cells
<http://science.howstuffworks.com/solar-cell.htm>

Putting together all relationships thus far ($\nu = c/\lambda$):

Department of 22
Chemistry

Bohr model of the H atom

- Electrons circle the nucleus in fixed set of orbits ($n = 1, n = 2 \dots$ where n is a quantum number)
- Electron passes from one orbit to another, absorbing or emitting a quantum of energy (a photon)
- The Bohr radius for an orbit: $r_n = n^2 a_0$
 $n = 1, 2, \dots$
 $a_0 = 53\text{pm} (5.3 \times 10^{-12} \text{m})$

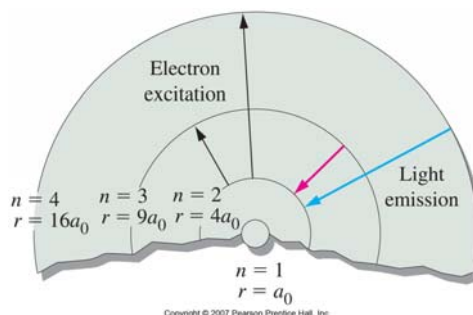


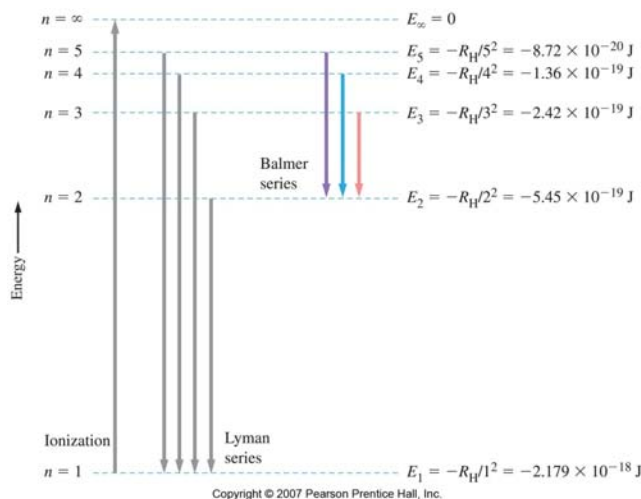
Fig. 8-13

p. 290

Department of **23**
Chemistry

H atom energy levels (Fig. 8-14)

- Energy of e^- in orbital, n , is given by
- R_H is the Rydberg constant for H, $2.179 \times 10^{-18} \text{J}$
- Convention: zero energy is when the e^- is removed from the atom



p. 291

Department of **24**
Chemistry

H atom energy changes

- n = quantum number
 - $n = 1$ e^- in ground state
 - $n > 1$ e^- in excited state, $n = \infty$ e^- is ionized
- For e^- going from n_{initial} to n_{final} , unique quantity of energy is absorbed or emitted (ΔE = energy difference between levels)

p. 292

and $E_{\text{photon}} = h\nu$, whether absorption or emission

- Good model for understanding emission spectra (discrete lines), as only certain ΔE are possible.

Department of **25**
Chemistry

i-Clicker Question#4

Department of **26**
Chemistry

Ionization of Hydrogen

- When an H atom is ionized, its electron absorbs enough energy to escape the atom:
- The e^- moves from its initial n state (n_i) to a final n state (n_f), where $n_f = \infty$
- But from $\Delta E = E_f - E_i$, we can see that

The energy it takes to free the electron is

p. 294

Department of **27**
Chemistry

H and Extra-solar Planet HD 209458 b: The 1st Extra-Solar Planet known to have an atmosphere

- Feb. 2007: Detection of hot H by the Hubble Space Telescope
- “The hot hydrogen consists of hydrogen atoms in the first excited state ($n=2$ energy level). Most of the hydrogen atoms in HD 209458b's extended upper atmosphere are in the ground state ($n=1$ energy level).”
- “The Balmer jump, at 364.6 nm, is at the spectral edge where hot hydrogen atoms start absorbing light into the ionization continuum.”
- <http://vega.lpl.arizona.edu/~gilda/extrass.html>



Department of **28**
Chemistry

i-Clicker Question#5

H atom calculations based on HD 209458 b

Department of 29
Chemistry

Evolution of Quantum Mechanics

- Bohr's model explains the H atom spectrum well, but does not explain multi-electron atoms
- The idea of orbits belongs to classical physics
- Quantum mechanics moves beyond this
- Missing piece is wave-particle duality of electrons

p. 295

Department of 30
Chemistry

Wave-Particle Duality: Theory



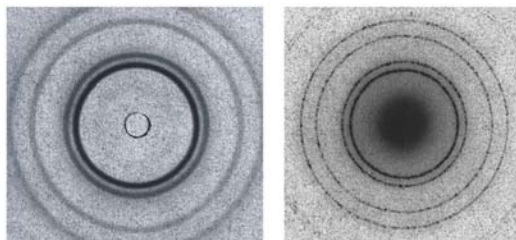
- Louis de Broglie: particles (e^-) display wave properties
 - From $E = mc^2$ (Einstein), $E = h\nu$ (Planck), and $\nu\lambda = c$
- Particles should display wave properties, e.g. diffraction
 - If distance between objects that the waves scatter is \sim same as the radiation λ , diffraction occurs

p. 296

Department of **31**
Chemistry

Thomson's Experiment (Nobel prize)

- Evidence: (Fig. 8-16)
 - Radiation and object spacing are similar
 - X-rays, $\lambda = 100$ pm
 - Metal foil, regular array of metal atoms, 200 pm spacing



(a)

(b)

- (a) X-ray diffraction by metal foil
- (b) Electron diffraction by metal foil.

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Department of **32**
Chemistry

i-Clicker Question#6

Department of 33
Chemistry

From classical to wave mechanics

- Classical physics gives precise predictions on the macroscale, BUT
- For sub-atomic particles:
- Bohr's model of constrained circular electron orbits is invalid
 - There is uncertainty: position and momentum cannot simultaneously be measured with great precision
(Heisenberg – Nobel Prize, & Bohr)



p. 298-299

Department of 34
Chemistry

Quantum Numbers

- Section 8.6 [not part of the course] introduces:
 - Schrödinger equation: combines ideas of particle & wave behaviour to describe energy of e^- in atom
- We'll use the results of 8.6 - Orbitals
 - Orbitals are wavefunctions, ψ , solutions to the Schrödinger equation
 - Orbitals are described by 3 quantum numbers
 - Orbitals describe regions of high probability of finding an electron (high charge density)

Department of **35**
Chemistry

Quantum Numbers – Review Questions

1. Which quantum represents subshell?
2. Which is the magnetic quantum number?
3. Which quantum number can have the value $-1/2$?

Department of **36**
Chemistry

Orbitals - Review Questions

4. Which shell is at higher energy: $n=3$ or 4 ?
5. What orbitals, and how many of each, are available if $n = 3$?
6. How many electrons can be accommodated in the $n=2$ shell?

Department of **37**
Chemistry

Electron Configurations - Review Questions

7. Which is an excited state configuration for Ne? (element #10)
 - (a) $1s^2 2s^2 2p^6$
 - (b) $1s^2 2s^2 2p^5 3p^1$
 - (c) $1s^2 2s^2 2p^6 3p^1$
7. Write an orbital box electron configuration for O (element # 8).
8. Write the electron configuration for Ca (element #20), using $1s^2 \dots$ notation.

Department of **38**
Chemistry

Review: Quantum Numbers, Orbitals, Electron Configurations

- The following slides (42-53) review material on:
 - Quantum Numbers, Atomic Orbitals, Electron Configurations
 - Please review this material as needed. You are responsible for it.

n

- Principal quantum number, n
 - n describes orbital energy and distance from nucleus
 - Larger n value = orbital is further from nucleus, e^- in orbital is at higher energy
 - $n = 1, 2, 3, 4, \dots$
 - n describes a principal *shell*

l, m_l

- Orbital angular momentum quantum number, l
 - l describes orbital shape (angular distribution)
 - $l = 0, 1, 2, 3 \dots n-1$
 - $l = 0$ (s orbital), $l = 1$ (p), $l = 2$ (d), $l = 3$ (f)
 - Number of l values = number of *subshells* in a given n shell
- Magnetic quantum number, m_l
 - m_l describes orbital orientation
 - $m_l = -l, \dots, 0, \dots, +l$
 - There are $(2l + 1)$ values

p. 304-305

Department of **41**
Chemistry

Hydrogen atom example (Fig. 8-23)

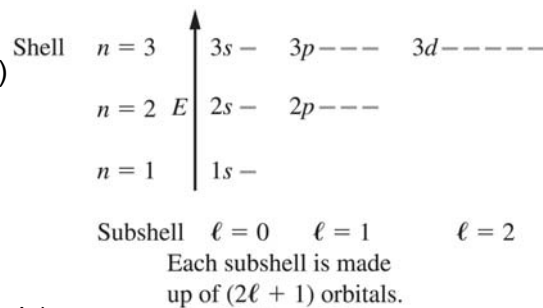
- Orbital energy increases with n

For $n = 3$ shell:
 $l = 0, 1, 2$ (3 subshells)

For $l = 2$,
 $m_l = -2, -1, 0, 1, 2$
(5 3d orbitals)

For $l = 1$,
 $m_l = -1, 0, 1$ (3 3p orbitals)

For $l = 0$,
 $m_l = 0$ (1 3s orbital)



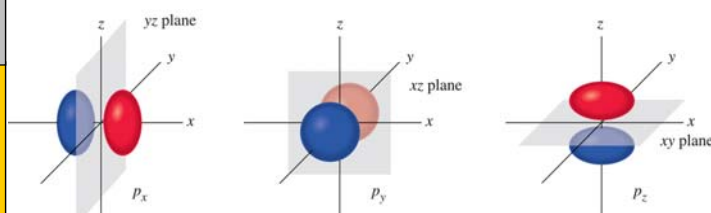
For H: subshells in a given shell have the same energy. This is not true for multi-electron atoms.

p. 305

Department of **42**
Chemistry

Orbital pictures*

- S orbitals are spherical
- 1s, 2s, 3s at 95% probability:



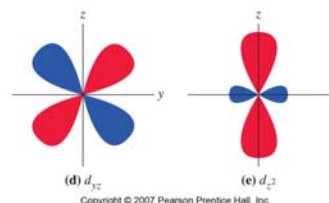
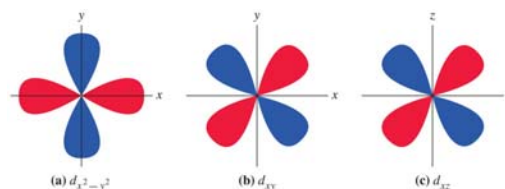
- P orbitals (p_x , p_y , p_z)
- 1 node (0 probability of finding electron)

*Section 8-8 is formally not covered, but we will use these Figures, p. 309, 311.

Department of 43
Chemistry

Orbital pictures*

- d orbitals (cross section):
- 2 nodes
- Possible in $n = 3$ and above



*Pictures are from section 8-8 (p. 311). Know the number & shapes of each type, not the mathematical derivations.

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Department of 44
Chemistry

Electron Spin Quantum Number, m_s

- Electrons have spin, thus generating a magnetic field:
 - Values of $m_s = +1/2$ or $-1/2$
 - A pair of electrons with opposite spins has no magnetic field
- Atoms (or ions) with
 - all spins *paired* are diamagnetic
 - 1 or more *unpaired* electrons are paramagnetic
- We can identify any electron with these 4 quantum numbers

p. 313-314

Department of 45
Chemistry

i-Clicker Question#7

Department of 46
Chemistry

H vs. Multi-electron atoms

- For H all subshells have the same energy – they are *degenerate*
- For multi-electron atoms the subshell energies differ (because of electron screening and effective nuclear charge*)

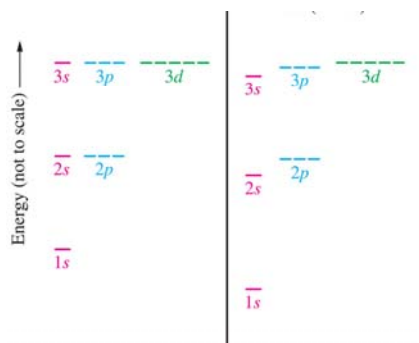


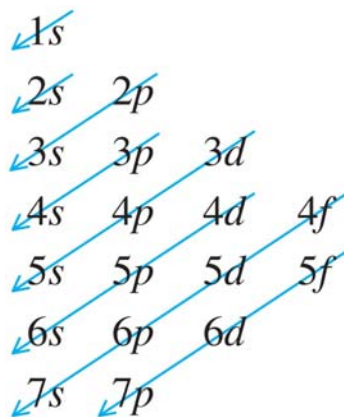
Fig. 8-36, p. 316

* These topics are discussed in 8-10, which is not formally covered, but we use the results to write electron configurations.

Electron Configurations

- Rules for distributing e^- into shells & subshells:

(1) Occupy orbitals so that atom's energy is minimized. We order orbitals according to energy:



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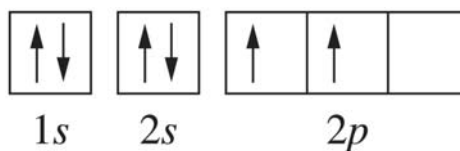
Fig. 8-37

Pauli, Hund

(2) Pauli exclusion principle: every e^- has unique set of 4 quantum numbers, thus 2 e^- in same orbital have opposite spins.

(3) Hund's rule: occupy orbitals of the same energy singly, then pair e^- .

e.g. Carbon: $1s^2 2s^2 2p^2$



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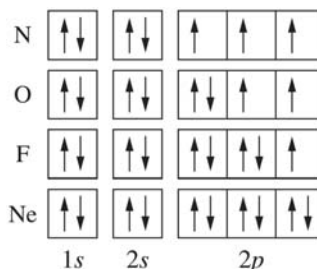
p. 317

Department of **49**
Chemistry

The Aufbau (building up) Process

- Ground state electron configurations of all atoms are based on the rules above.

e.g. N to Ne:



- Noble gas shorthand:
N is $1s^2 2s^2 2p^3$ or $[\text{He}] 2s^2 2p^3$
Ne is $1s^2 2s^2 2p^6$ or $[\text{Ne}]$

- Excited state electron configurations do not follow the orbital filling rules,
e.g. $1s^2 2s^2 2p^5 3s^1$ would be an excited state of Ne

p. 318-320

*Note: not responsible for electron configurations of transition elements & their ions.

Department of **50**
Chemistry

Building the Periodic Table

Main-group elements

s block		Transition elements										p block					
1												18					
(1s)												(1s)					
H												He					
3												5					
(2s)		d block										(2p)					
Li												B					
Be												C					
11												13					
(3s)		3d										(3p)					
Na												Al					
Mg												Si					
19												15					
(4s)		4d										(4p)					
K												P					
Ca												S					
37												17					
(5s)		5d										(5p)					
Rb												Cl					
Sr												Ar					
55												31					
(6s)		6d										(6p)					
Cs												Ga					
Ba												Ge					
87												33					
(7s)		7d										(7p)					
Fr												As					
Ra												Se					
88												35					
(6d)		Inner-transition elements						f block									
Fr								5f									
Ra								6f									
Ac								7f									
Rf								8f									
Db								9f									
Sg								10f									
Bh								11f									
Hs								12f									
Mt								13f									
89								14f									
106								15f									
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