Final Exam

• Thursday, Dec. 11, 2003
  – 8:00 PM to 10:50 PM
  – Chem Annex Room 16
• Final 25% of Overall grade
  – Multiple Choice, no partial credit, no extra credit
• Chapters covered
  – Part A Chapters 1-6
  – Part B Chapters 7-10
  – Part C Chapters 11-14
  – Part D Chapters 16-17
• Crib Sheets allowed
  – 4 pages A-D above
  – single sided, handwritten
• Grade Improvement Plan
  – If Part A > Exam 1, Part A score replaces E1
  – If Part B > Exam 2, Part B score replaces E2
  – If Part C > Exam 3, Part C score replaces E3
  – Will use Final Exam total, as sum Parts A+B+C+D
Chapter 16
Quantum Mechanics and the Hydrogen Atom

• 16-1 Waves and Light
• 16-2 (skip) Paradoxes in Classical Physics
• 16-3 Planck, Einstein and Bohr
• 16-4 Waves, Particles and the Schrödinger Equation
  – only Schrödinger equation
• 16-5 The Hydrogen Atom
16-1 Waves and Light
“A Light Version”

- Electromagnetic Radiation
  - Energy travels through space by electromagnetic radiation
  - Examples, sunlight, microwave ovens, cell phones, X-rays, radiant heat from a fireplace, AM/FM radio, colors from fireworks
  - All travel as waves
  - All travel as the speed of light
Figure 16–4 Light consists of waves of oscillating electric (E) and magnetic (H) fields that are perpendicular to one another and to the direction of propagation of the light.
The electro magnetic spectrum.

The frequency doubles 80 times from right to left in the top diagram

The wavelength doubles 80 times from left to right in the top diagram

Visible light is confined within a single doubling near the middle
Important Equations

\[ c = 3 \times 10^8 \text{ m per second} \]
\[ \lambda = \text{wavelength} \]
\[ \nu = \text{frequency} \]

\[ h = \text{Planck’s constant} \]
\[ h = 6.62 \times 10^{-34} \text{ Js} \]
\[ \text{or} \]
\[ h = 6.62 \times 10^{-34} \text{ kg m}^2 \text{ s}^{-1} \]
Radio Waves

\[ c = \lambda \nu \]

- **AM 890 kHz**
  - 890,000 waves per second
  - Wavelength is 337 meters (about 1/5 mile)

- **FM 99.1 MHz**
  - 99,100,000 waves per second
  - Wavelength is 3 meters (about 10 feet)
Problems: General given two values, calculate the third,  c is constant 3 \( \times 10^8 \) m/s

Problem

The laser in an audio compact disc (CD) player uses light with a wavelength of 780 nm. What is the frequency of the light emitted from the laser?
Problem

The brilliant red color seen in fireworks displays is due to $4.62 \times 10^{14} \text{ s}^{-1}$ strontium emission. Calculate the wavelength of the light emitted.
16-2 (skip) Paradoxes in Classical Physics
16-3 Planck, Einstein, and Bohr

• 1901 Max Planck found that light (or energy) was quantized
  – Quite a surprise as light was thought to be continuous
• Energy can be gained or lost only in integer multiples of $hv$.

\[ n \text{ are whole numbers (1,2,3,...)} \]

• $H$ is Planck’s constant
• Determined experimentally
  \[ h = 6.628 \times 10^{-34} \text{ J s} \]
• Each unit of size $hv$ is called a packet or quantum
Problem

Blue fireworks (typically CuCl) emit light of 450 nm. What is the energy of the light emitted at 450 nm

\[ c = \lambda \nu \quad E = h \nu \]

Rearrange and combine

\[
E = h \left( \frac{c}{\lambda} \right) = 6.67 \times 10^{-34} \text{ J} \cdot \text{s} \left( \frac{3 \times 10^8 \text{ m/s}}{450 \times 10^{-9} \text{ m}} \right) = 4.41 \times 10^{-19} \text{ J}
\]
• 1905 Einstein suggested that electromagnetic radiation can be viewed as a "stream of particles" called photons

• About the same time, Einstein derived his famous equation
  \[ E = mc^2 \]

• The main significance is that energy has mass
\[ E = mc^2 \]

- Rearrange

\[ m = \frac{E}{c^2} \]

where \( E = h\nu = h\left(\frac{c}{\lambda}\right) \)

**mass of a photon**

\[
m = \frac{E}{c^2} = \frac{h}{\lambda c}
\]
Atomic Spectra of Hydrogen

1.) \( \text{H}_2 \xrightarrow{\text{High Energy Spark}} \text{H} \bullet^* \text{ (Excited State)} \)

2.) \( \text{H} \bullet^* \text{ (Excited State)} \xrightarrow{\text{Radiative Decay}} \text{hv emission} \)

\[ E_n = \frac{hc}{\lambda_n} \quad \text{quantized energy} \]

\( n \) is excited state orbitals

\( N = 1, 2, 3, \ldots \)

\[ E_3 = \frac{hc}{\lambda_3} \quad \text{blue emission} \]

\[ E_2 = \frac{hc}{\lambda_2} \quad \text{green emission} \]

\[ E_1 = \frac{hc}{\lambda_3} \quad \text{red emission} \]
Quantized Emissions

\[ E_1 = \frac{hc}{\lambda_1} \text{ red emission} \]

\[ E_2 = \frac{hc}{\lambda_2} \text{ green emission} \]

\[ E_3 = \frac{hc}{\lambda_3} \text{ blue emission} \]

Figure 16-11 Atoms of hydrogen, mercury, and neon emit light at discrete wavelengths. The pattern seen is characteristic of the element under study. (1 Å = 10^{-10} m; see page 659.)
The Bohr Model

called a Planetary Model

Orbital Transition Diagram

\[ E_n = \frac{hc}{\lambda_n} \]

\[ E_n = \frac{hc}{\lambda_n} \text{ green emission} \]

\[ E_n = \frac{hc}{\lambda_n} \text{ red emission} \]
Bohr calculated the angular momentum, radius and energy of the electrons traveling in discrete orbits.

**Angular Momentum** = \( m_e v r \)

\[
= n \frac{h}{2\pi} \quad n = 1, 2, 3, ... 
\]

\( r_n = \frac{n^2}{Z} a_0 \) = radius of each orbital  

\( a_0 \) called the bohr radius, a constant

\( n = \) orbitals, excited states  

\( n = 1, 2, 3, ... \quad n = 1 \) called ground state

\( Z \) is the positive charge on the nucleus  

(1 of H, 2 for He, etc.)

\[
E_n = -\frac{Z^2}{n^2} (2.18 \times 10^{-18} \text{ J})
\]

Calculated levels match those on the photographic plate shown earlier.
Schrödinger Equation
\[ \hat{H}\psi = E\psi \]
Results in many solutions, each solution consists of a wave function, \( \psi (n, l, m_l) \) called **quantum numbers**

\( \psi = \) a wave function which defines an electron's position in 3D space \((x, y, z)\), called an **orbital**

\( \psi^2 = \) the probability that an electron is in a certain region of space

This defines the shape of the orbital \((s, p, d, f)\)
Solutions to the Schrödinger Equation

\[ \psi (n, l, m_l) \]

- **n = principal quantum number**
  
  \[ n = 1, 2, 3, \ldots \]
  
  *n* is related to the size and energy of the orbital

- **l = azimuthal quantum number**
  
  \[ l = 0, 1, \ldots (n-1) \]
  
  *l* is related to the shape of the orbital

  - \( l = 0 \) is called an *s* orbital
  - \( l = 1 \) is called a *p* orbital
  - \( l = 2 \) is called a *d* orbital
  - \( l = 3 \) is called an *f* orbital
  - \( l = 4 \) is called a *g* orbital
Solutions to the Schrödinger Equation

- \( m_l = \text{magnetic quantum number} \)
  \[ m_l = -l, \ldots, 0, \ldots, +l \]
  \( m_l \) relates to the orientation of the orbital

- Although not a solution to the Schrödinger Equation, a 4th quantum number is
  \( m_s = \text{electron spin quantum number} \)
  \[ m_s = +1/2, -1/2 \] denoted by \( \uparrow \downarrow \)
### First four levels of Orbitals in hydrogen

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<th>l</th>
<th>orbital designation</th>
<th>$m_l$</th>
<th># of orbitals</th>
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<tr>
<td></td>
<td>3</td>
<td>4f</td>
<td>-3, -2, -1, 0, +1, +2, +3</td>
<td>7</td>
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</table>

- **n** is related to the size and energy of the orbital
- **l** is related to the shape of the orbital
- **$m_l$** relates to the orientation of the orbital
Figure 16–20 Three representations of hydrogen s-orbitals. (a) An electron-density representation of a hydrogen atom in its 1s, 2s, and 3s states. The spheres are cut off at a radius that encloses 90% of the total electron density. (b) The wave functions graphed against distance from the nucleus $r$. (c) The radial probability distribution, equal to $r^2|\psi|^2$. The distance $a_0$ is the Bohr radius (0.529 Å).
- **n** is related to the size and energy of the orbital
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F- Orbitals
G-Orbitals

http://www.shef.ac.uk/chemistry/orbitron/
Chapter 16
Quantum Mechanics and the Hydrogen Atom

• Example / exercise
  16-1, 16-5

• Problems
  14, 16, 22, 28, 34, 41
Chapter 17
Many-Electron Atoms and Chemical Bonding

• 17-1 Many-Electron Atoms and the Periodic Table
• 17-2 Experimental Measures of Orbital Energies
• 17-3 Sizes of Atoms and Ions
• 17-4 Properties of the Chemical Bond
• 17-5 Ionic and Covalent Bonds
• 17-6 Oxidation States and Chemical Bonding
Chapter 17
Many Electron Atoms and Chemical Bonding

ψ (n, l, m_l) called quantum numbers
– n is related to the size and energy of the orbital
– l is related to the shape of the orbital
– m_l relates to the orientation of the orbital
– m_s is electron spin quantum number

• Aufbau Principle (building up)
• Pauli Exclusion Principle
  – No 2 electrons in an atom can have the same set of quantum numbers
  
n, l m_l, m_s
Chapter 17
Many Electron Atoms and Chemical Bonding

• Aufbau Principle (building up)
• Pauli Exclusion Principle
  – No 2 electrons in an atom can have the same set of quantum numbers 
    \[ n, l, m_l, m_s \]
• Hund’s Rule
  – When several orbitals are of equal energy, a single electron enters each orbital before a second electron.
  – In addition, the spins remain parallel until the second orbital enters the orbital.
H: 1s

He: 1s²

Li: 1s² 2s¹

Be: 1s² 2s²

B: 1s² 2s² 2pₓ¹

C: 1s² 2s² 2pₓ¹ 2pᵧ¹

N: 1s² 2s² 2pₓ¹ 2pᵧ¹ 2p₂¹

O: 1s² 2s² 2pₓ² 2pᵧ¹ 2p₂¹

F: 1s² 2s² 2pₓ² 2pᵧ² 2p₂¹

Ne: 1s² 2s² 2pₓ² 2pᵧ² 2p₂²

11/20/2003
• Hund’s Rule
  – When several orbitals are of equal energy, a single electron enters each orbital before a second electron.
  – In addition, the spins remain parallel until the second orbital enters the orbital.
Paramagnetic:

Attracted into a magnetic field
Have one or more un-paired electrons

Diamagnetic:

Pushed out of a magnetic field
Have paired electrons

**Carbon**

(Z = 6)

*paramagnetic*

**Beryllium**

(Z = 4)

*diamagnetic*
**Figure 17-3** The filling of subshells and the structure of the periodic table. Anomalous ground-state electron configurations are indicated explicitly; all others can be derived from the position of the element in the table.
Exercise (pg 730):

The ground-state electron configuration of an atom is $1s^22s^22p^63s^23p^3$. Name the atom. Is it paramagnetic? If so, state how many unpaired electrons it has.

15-electron Phosphorus atom;

\[
\begin{array}{cccccccc}
1s & 2s & 2p_x & 2p_y & 2p_z & 3s & 3p_x & 3p_y & 3p_z \\
\uparrow \downarrow & \uparrow \downarrow & \uparrow \downarrow & \uparrow \downarrow & \uparrow \downarrow & \uparrow & \uparrow & \uparrow & \uparrow \\
\end{array}
\]

This is paramagnetic with three unpaired electrons.
• **Valence Electrons**
  – Are electrons that can become directly involved in chemical bonding
  – They occupy the outermost (highest energy) shell of an atom
  – Beyond the immediately preceding noble-gas configuration
  – Among the *s*-block and *p*-block elements, the valence electrons include electrons in *s* and *p* sub shells only
• **Valence Electrons**
  
  – Among the **s-block and p-block** elements, the valence electrons include electrons in **s** and **p** sub shells only
  
  – Among **d-block and f-block** (transition elements), valence electrons usually consist of electrons in **s orbitals** plus electrons in unfilled **d** and **f** sub shells

![Figure 17-3](image) The filling of subshells and the structure of the periodic table. Anomalous ground-state electron configurations are indicated explicitly; all others can be derived from the position of the element in the table.
Problem:

Write the valance-electron configuration and state the number of valence electrons in each of the following atoms and ions: (a) Y, (b) Lu, (c) Mg$^{2+}$

(a) Y (Yttrium): atomic number $Z = 39$

\[ \text{[Kr]} \ 5s^2 \ 4d^1 \quad \text{3 valence electrons} \]

(b) Lu (Lutetium): $Z = 71$

\[ \text{[Xe]} \ 6s^2 \ 4f^{14} \ 5d^1 \quad \text{3 valence electrons} \]

Note filled 4f sub shell

(c) Mg$^{2+}$ (Magnesium (II) ion): $Z = 12$

This is the 2+ ion, thus 10 electrons

\[ \text{[Ne]} \text{ configuration or } 1s^2 \ 2s^2 \ 2p^6 \]

0 valence electrons
The filling sub shells and the structure of the periodic table.

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<th>2s-filling</th>
<th>3s-filling</th>
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- Anomalous ground-state electron configurations are indicated explicitly
- All others can be derived from the position of the element in the table

11/20/2003 OFB Chapter 16 & 17
PRS transmitters

- Turn in your transmitters
- Chem Annex Stockroom
- Before the end of Finals week, no extensions.
- Make sure someone signs your form indicating that they received the transmitter
- Otherwise, a $42 charge will be sent to the Bursar.
Chapter 17
Many-Electron Atoms and Chemical Bonding

• Example / exercise
  17-1, 17-2
• HW problems
  1, 3, 5, 7