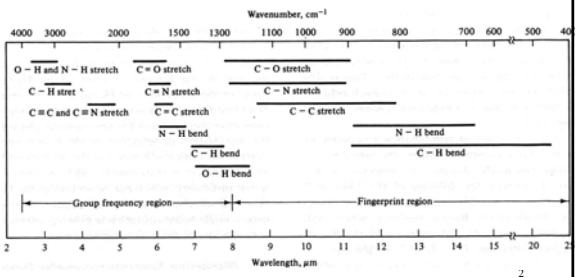
March 11, 2005

- **Exam #2**
  - **Next Wednesday (7 pm, B104)**
  - **Review Session: Sunday, 7pm, B203**
  - **Info Page *now online*!**
  - **Prob Set #3 Solutions *now online*!**
  - ***With Real Blueberry Bursts (artificially flavored)!***
- **Office Hours** – ***modifications this week***
  - **Friday: 1:15 – 1:45 pm (A223 Cook)**

Qualitative Analysis

- Group Frequencies:



More Qual Analysis

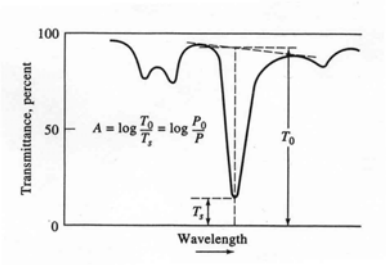
- Must have spectrum of a ***pure compound***
- Use group frequencies as a guide
- Use *correlation chart* for more compound specific functional group analysis
- Use computerized spectral search engines
- Use IR assignments *in conjunction with other info* (e.g., chemical, physical, spectroscopic)

Quantitative Analysis

- **The Good Side:**
  - -Almost all compounds absorb in IR
  - -solids, liquids and gases are all accessible
- **The Problems:**
  - Poor sensistivity and short cell pathlengths mandate relatively high solution concentrations (1-2% or more) results in *Beer's Law deviations*
  - Narrow absorption bands and complex spectra (with overlapping bands) can cause polychromatic errors

Accurate Absorbance Measurements

- Solution cells are difficult to match exactly, so 100%T is not necessarily an absorbance of zero:



IR Spectrometry Applications

- **Qualitative Analysis**
  - Most significant use of IR spec: *structural analysis*
  - Computerized spectral I.D.
  - Use in conjunction with other methods for confirmation
- **Quantitative Analysis**
  - Limited use but, with care, can obtain reasonable results
  - Can get trace (ppm) detection limits with gases (with excellent *selectivity*)

Spectroscopy:
Atomic Absorption and Emission Spectrometry

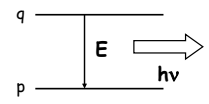
Chem 221

Instrumental Analysis

Spring 2005

Fundamentals

- ***Atoms*** can also absorb and emit EMR:

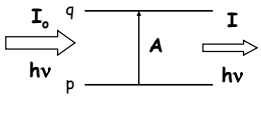


Atomic Emission Spectroscopy (AES)

-emission rate depends on:

N_q and A_{qp}

-Intensity $\propto$ concentration



Atomic Absorption Spectroscopy (AAS)

-absorption rate depends on:

N_p and B_{pq}

-Absorbance $\propto$ concentration

AAS versus AES?

- **AAS:** Absorbance $\propto N_p$
- **AES:** Emission Int. $\propto N_q$

But: *concentration* $\propto N_T$

For a *thermal* population distribution, we use the Boltzmann Equation to relate N_p and N_q to N_T:

$$\frac{N_q}{N_T} = \frac{g_q\, e^{-(E_q/kT)}}{\Sigma(g_i\, e^{-(E_i/kT)})}$$

Where: T = absolute temp., k = Boltzmann's constant, and g_i = statistical weight of state i