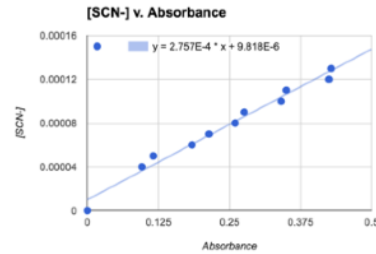
NS H2 Spectrometry − Investigating Atoms, Molecules, and Solutions

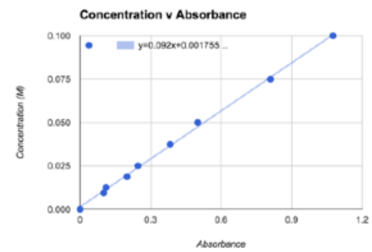
Name____________________ Per___

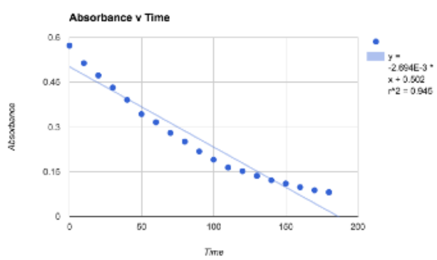
Atoms, molecules, and ions are so very tiny that we can not see them, and as a result of this, one way to probe matter is with radiation. The readouts or graphs from this probing are call spectra (or spectrum, singular). Through the year we have directly and indirectly, both in lab and in the text come across various spectra which will be summarized below.

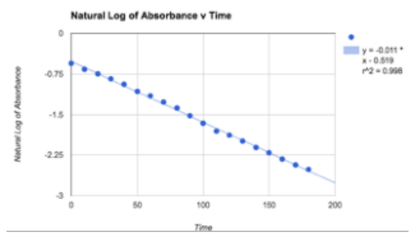
Visible (and UltraViolet) Spectrometry

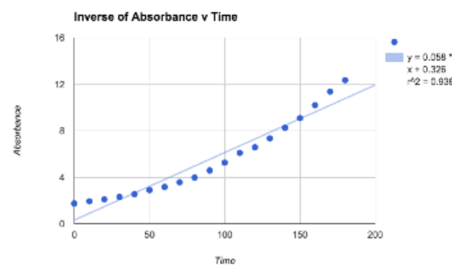
Visible and ultraviolet light packs enough energy to cause electron transitions within atoms. You should be most familiar with this tool that we used to study the concentration of solutions. We used this tool in Lab B1 Concentration of Copper in Brass, ~~Lab F1 The K_c of $FeSCN^+$ ion~~, and Lab E2 Study of the Kinetics of Crystal Violet. The connection between all of these labs is that we used the visible spectrophotometer to measure the absorbance of a colored solution. The important fact is that visible light (and ultraviolet light) of particular wavelengths can be used to cause electrons in a substance to become excited, and when dropping back down to the ground state will give off visible light of a particular color. The intensity of the light absorbed by a solute in a solution will give information about the concentration of that solute in the solution. In lab B1 we prepared a known concentration graph of Cu^{2+} ions which is linear due to Beers law, and then tested unknown solutions for which we could determine their concentration. In lab F1 we prepared only one known concentration of the $FeSCN^+$ ion and used a ratio to determine the concentration of an unknown. For lab E2, we simply gathered data for the decline of absorbance over time which we could then re-graph to linearize in order to determine the kinetic order of the reaction.



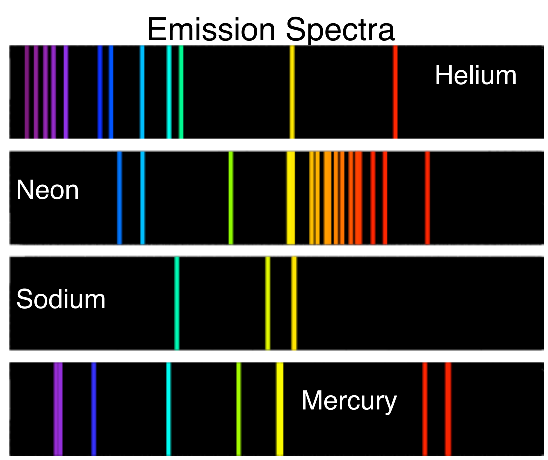




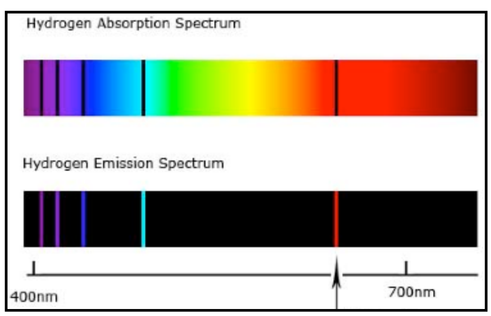




Although we did not study emission spectra any further in AP Chemistry, we should also note that visible spectrum that emit from excited elements give off unique, characteristic spectra that can be used to identify elements.

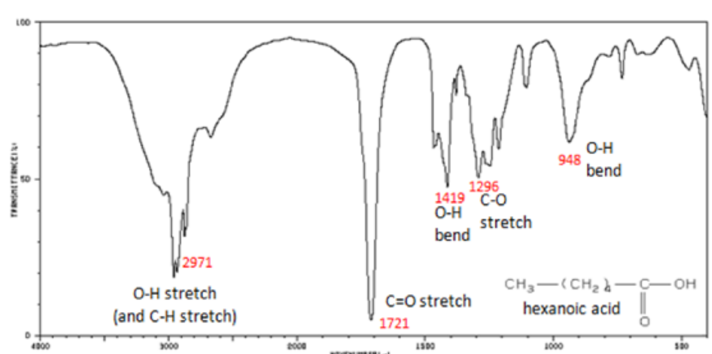


You may find it interesting to take note of the relationship between the absorption and emission spectra of hydrogen.



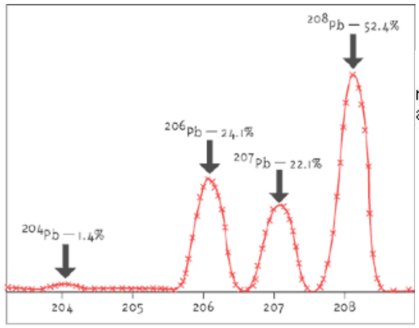
Infrared Spectrometry (affect vibrational motion of molecules)

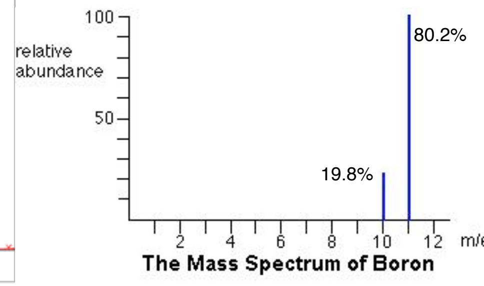
The energy of infrared radiation is lower energy and is not large enough to excite electrons, but may induce **vibrational** excitation of covalently bonded atoms and groups of atoms. The covalent bonds in molecules are not rigid sticks or rods, such as found in our molecular model kits, but are more like stiff springs that can be stretched and bent. The use of infrared spectroscopy is extremely useful in organic chemistry in the identification of certain bonds and functional groups. An IR spectrum of hexanoic acid is shown to the right. While it is very, very unlikely that you would have to read such a spectrum for the AP Chemistry Exam, it is important that you know that **IR radiation induces the vibrational** movements of molecules, **which is the bending and stretching of chemical bonds.**



NS H2 Spectrometry − Investigating Atoms, Molecules, and Solutions Name____________________Per___

Mass Spectrometry



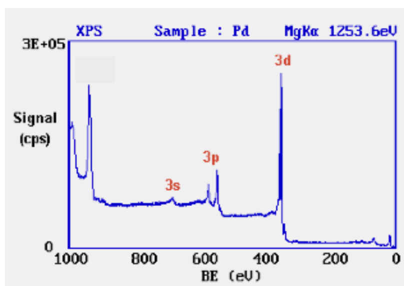


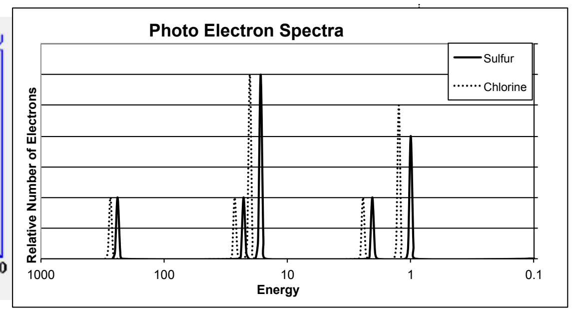
Mass spectrometry is an analytical technique that ionizes a substance then sorts the resulting ions based on their mass to charge ratio. This means that a sample of a substance can be sorted according to the various masses that may be within a sample. The mass spectrometry is particularly useful to determine the various isotopes and the respective amount of each isotope within an sample of an element. The mass spectrum on the right shows that there are four naturally occurring isotopes of lead of various percentages resulting in the average molar mass of 207.2 g/mol. You are more likely to see a simplified mass spectrum on the AP exam (with narrower peaks) such as the spectrum shown for boron which naturally occurs as two isotopes resulting in an average molar mass of 10.81 g/mol.

X-Rays PhotoElectron Spectroscopy (PES)

The use of X-Rays to eject all electrons (not just valence electrons) to determine the binding energy of electrons within an atom. The graph shown to the right shows the binding energy (BE) for the third energy electrons of palladium.

You are far more likely to see a "cleaned up" and simplified PES such as the one shown to the far right for sulfur and chlorine. You may be asked to identify such elements or explain why the 3s peaks for the chlorine demonstrate a higher BE (further left) than the 3s peaks for sulfur.





Microwaves (affect rotational and thus translational motion of molecules)

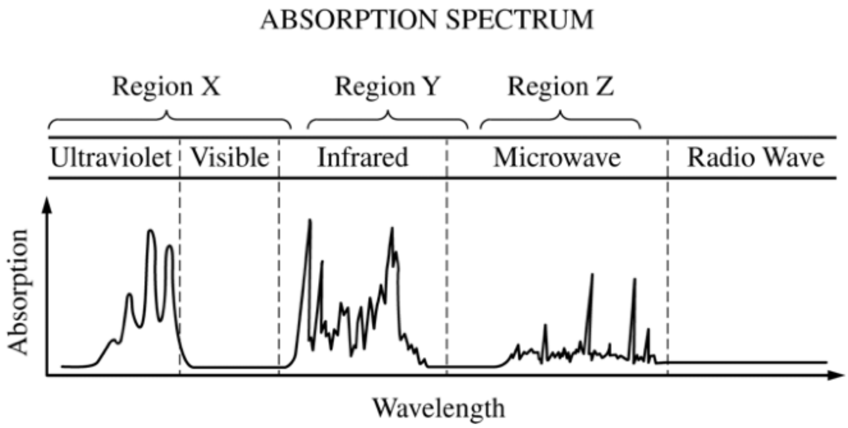
Polar molecules absorb energy from microwaves in a microwave oven. Microwave ovens produce, well, microwaves which is energy within a particular frequency range. Many molecules, including those of water are dipoles, meaning that they have a partial positive charge at one end and a partial negative charge at the other, and and will **rotate** as they try to align themselves with the alternating electric field of the microwaves. In liquids in particular, the rotation of individual molecules will hit other molecules that push them into **translational** motion, thus dispersing the energy. The more polar the molecule (greater dipole moment), then the greater the effect the microwaves will have on the molecule. This is what makes water particularly susceptible to the heating action of microwaves.

Summary Chart

Type	ν / λ	Relative Energy	Effect on atom or molecule	Information Acquired	Name of Spectroscopy
X-Ray	higher ν shorter λ	very high	removes core e⁻ can exam nuclei arrangement	binding energy, how tightly electrons are held	PES and Xray crystal-ography
UV		high	excites valence electrons	emission spectrum, identity of elements	UV
Visible		medium	excites valence electrons	Beers Law, concentration of colored species	visible
Infrared		low	changes bond vibrations (vibrational motion)	types of bonds / atoms / functional groups in molecules	IR
Micro-wave	lower ν longer λ	quite low	changes movement (rotational & translational motion)	location of H atoms in molecules	microwave

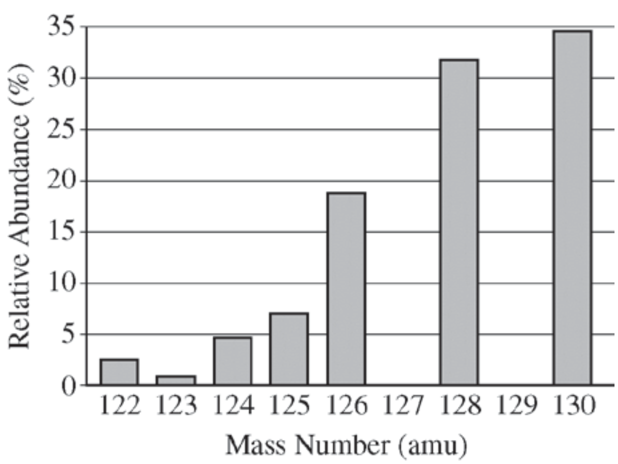
NS H2 Spectrometry − Investigating Atoms, Molecules, and Solutions Name____________________Per___

The following questions found on recent exams are what prompted me to write the previous summary sheet.



1. The diagram above represents the absorption spectrum for a pure molecular substance. Which of the following correctly indicates the type of transition observed for the substance in each of the regions of the absorption spectrum?

	Region X	Region Y	Region Z
(A)	Molecular vibration	Molecular rotation	Electronic transition
(B)	Electronic transition	Molecular rotation	Molecular vibration
(C)	Molecular rotation	Molecular vibration	Electronic transition
(D)	Electronic transition	Molecular vibration	Molecular rotation



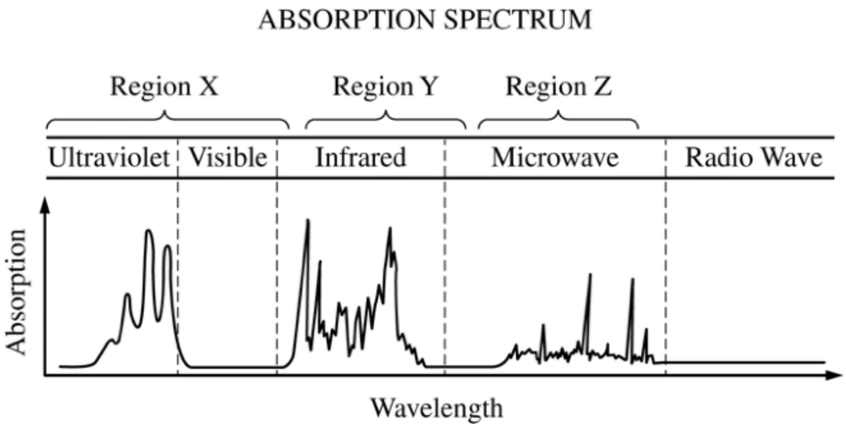
2. The elements I and Te have similar average atomic masses. A sample that was believed to be a mixture of I and Te was run through a mass spectrometer, resulting in the data above. All of the following statements are true. Which one would be the best basis for concluding that the sample was pure Te?
   A) Te forms ions with a −2 charge, whereas I forms ions with a −1 charge.
   B) Te is more abundant than I in the universe.
   C) I consists of only one naturally occurring isotope with 74 neutrons, whereas Te has more than one isotope.
   D) I has a higher first ionization energy than Te does.

3. N_2 molecules absorb ultraviolet light but not visible light. I_2 molecules absorb both visible and ultraviolet light. Which of the following statements explains the observations?
   A) More energy is required to make N_2 molecules vibrate than is required to make I_2 molecules vibrate.
   B) More energy is required to remove an electron from an I_2 molecule than is required to remove an electron from an N_2 molecule.
   C) Visible light does not produce transitions between electronic energy levels in the N_2 molecule but does produce transitions in the I_2 molecule.
   D) The molecular mass of I_2 is greater than the molecular mass of N_2.

4. Which of the following is the electron configuration of an excited atom that is likely to emit a quantum of energy?
   A) $1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^1$
   B) $1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^5$
   C) $1s^2\ 2s^2\ 2p^6\ 3s^2$
   D) $1s^2\ 2s^2\ 2p^6\ 3s^1$
   E) $1s^2\ 2s^2\ 2p^6\ 3s^1\ 3p^1$

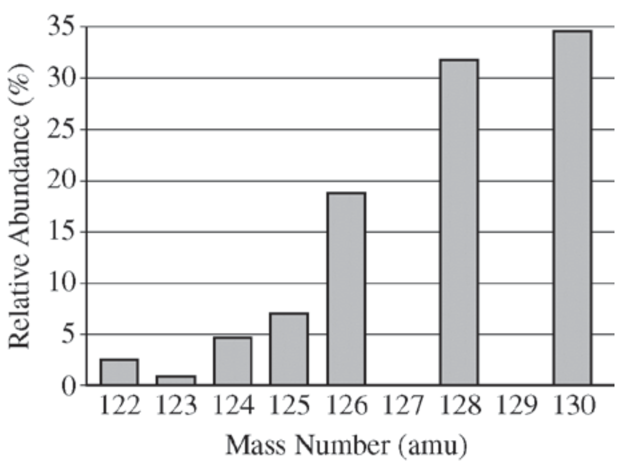
NS H2 Spectrometry − Investigating Atoms, Molecules, and Solutions Name____________________Per___

The following questions found on recent exams are what prompted me to write the previous summary sheet.



5. The diagram above represents the absorption spectrum for a pure molecular substance. Which of the following correctly indicates the type of transition observed for the substance in each of the regions of the absorption spectrum?

	Region X	Region Y	Region Z
(A)	Molecular vibration	Molecular rotation	Electronic transition
(B)	Electronic transition	Molecular rotation	Molecular vibration
(C)	Molecular rotation	Molecular vibration	Electronic transition
(D)	Electronic transition	Molecular vibration	Molecular rotation



6. The elements I and Te have similar average atomic masses. A sample that was believed to be a mixture of I and Te was run through a mass spectrometer, resulting in the data above. All of the following statements are true. Which one would be the best basis for concluding that the sample was pure Te?

   A) Te forms ions with a −2 charge, whereas I forms ions with a −1 charge.

   B) Te is more abundant than I in the universe.

   C) I consists of only one naturally occurring isotope with 74 neutrons, whereas Te has more than one isotope.

   D) I has a higher first ionization energy than Te does.

7. N_2 molecules absorb ultraviolet light but not visible light. I_2 molecules absorb both visible and ultraviolet light. Which of the following statements explains the observations?

   A) More energy is required to make N_2 molecules vibrate than is required to make I_2 molecules vibrate.

   B) More energy is required to remove an electron from an I_2 molecule than is required to remove an electron from an N_2 molecule.

   C) Visible light does not produce transitions between electronic energy levels in the N_2 molecule but does produce transitions in the I_2 molecule.

   D) The molecular mass of I_2 is greater than the molecular mass of N_2.

8. Which of the following is the electron configuration of an excited atom that is likely to emit a quantum of energy?

   A) $1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^1$

   B) $1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^5$

   C) $1s^2\ 2s^2\ 2p^6\ 3s^2$

   D) $1s^2\ 2s^2\ 2p^6\ 3s^1$

   E) $1s^2\ 2s^2\ 2p^6\ 3s^1\ 3p^1$