

Learning Objectives – Molecular and Atomic Spectroscopy

Background Material

After completing this unit the student will be able to:

1. Explain what it means to use spectroscopic methods for qualitative and quantitative analysis.
2. Identify the terms in and describe deviations to Beer's Law.
3. Describe the effect of changing the slit width and the impact it will have on qualitative and quantitative analyses.
4. Qualitatively determine the relative error in absorbance measurements and determine the optimal range for measurement purposes.
5. Describe the desirable features of a radiation source.
6. Explain the advantages of a dual versus single-beam spectrophotometer.
7. Explain the difference between a 3- and 4-level laser and why it is not possible to have a 2-level laser.
8. Compare the output of and advantages of prisms and gratings as dispersing elements.
9. Explain how a photomultiplier tube works.
10. Explain how an array detector works and describe the advantages of using an array detector.

Ultraviolet/Visible Spectroscopy

After completing this unit the student will be able to:

1. Compare and contrast atomic and molecular spectra.
2. Explain why atomic spectra consist of lines whereas molecular spectra at room temperature are broad and continuous.
3. Justify the difference in molecular spectra at room temperature and 10K.
4. Describe the cause of Doppler broadening.
5. Determine the effect of conjugation on a UV/Vis absorption spectrum.
6. Determine the effect of non-bonding electrons on a UV/Vis absorption spectrum.
7. Determine the effect of solvent on the energy of $n-\pi^*$ and $\pi-\pi^*$ transitions.
8. Evaluate the utility of UV/Vis spectroscopy as a qualitative and quantitative method.
9. Describe a procedure by which UV/Vis spectroscopy can be used to determine the pKa of a weak acid.

Molecular Luminescence

After completing this unit the student will be able to:

1. Describe the difference between a singlet and triplet state.
2. Draw an energy level diagram and identify the transitions that correspond to absorption, fluorescence, internal conversion, radiationless decay, intersystem crossing and phosphorescence.
3. Explain why phosphorescence emission is weak in most substances.
4. Draw a diagram that shows the layout of the components of a fluorescence spectrophotometer.
5. Describe the difference between a fluorescence excitation and emission spectrum.
6. Draw representative examples of fluorescence excitation and emission spectra.
7. Describe a procedure for measuring phosphorescence free of any interference from fluorescence.
8. Justify why fluorescence measurements are often more sensitive than absorption measurements.
9. Describe the meaning and consequences of self-absorption.
10. Identify variables including the effect of pH that can influence the intensity of fluorescence.
11. Identify the features that occur in organic molecules that are likely to have high fluorescent quantum yields.
12. Compare two molecules and determine which one will undergo more collisional deactivation.

Infrared Spectroscopy

After completing this unit the student will be able to:

1. Describe the selection rule for infrared-active transitions.
2. Determine the vibrations for a triatomic molecule and identify whether they are infrared-active.
3. Draw the design of a non-dispersive infrared spectrophotometer and describe how it functions.
4. Describe the difference between time and frequency domain spectra.
5. Explain how a Michelson Interferometer can be used to obtain a time domain spectrum.
6. Explain the advantages of Fourier Transform infrared spectroscopy over conventional infrared spectroscopy.

Raman Spectroscopy

After completing this unit the student will be able to:

1. Determine whether the molecular vibrations of a triatomic molecule are Raman active.
2. Explain the difference between Stokes and anti-Stokes lines in a Raman spectrum.
3. Justify the difference in intensity between Stokes and anti-Stokes lines.
4. Draw the Stokes and anti-Stokes lines in a Raman spectrum of a compound when given the energies of the different transitions.

Atomic Spectroscopy

After completing this unit the student will be able to:

1. Compare and contrast the advantages of flame, furnace and inductively coupled plasma atomization sources.
2. Justify why continuum radiation sources are usually not practical to use for atomic absorption spectroscopy.
3. Describe the design of a hollow cathode lamp and justify the reasons for a hollow cathode configuration and low pressure of argon filler gas.
4. Devise an instrumental procedure to account for flame noise in atomic absorption spectroscopy.
5. Devise an instrumental procedure to account for molecular absorption and scatter from particulate matter in atomic absorption spectroscopy.
6. Describe three possible strategies that can be used to overcome the problem of non-volatile metal complexes.
7. Devise a procedure to overcome excessive ionization of an analyte.
8. Devise a procedure to account for matrix effects.