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4) Briefly explain what reversed-phase partition chromatography is:

5) List several ways to increase the resolution and efficiency of a chromatographic column:

6) What is gradient elution (as used in this HPLC experiment):

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- 5) Write the Beer–Lambert Law that relates absorbance, pathlength, and concentration. Imagine that you plot absorbance as a function of concentration. A form of the equation that is useful for fitting this experimental plot is: “ $y = mx + b$ ”. Relate the variables and linear fit parameter (y , m , x , and b) to the constants used in Beer’s Law.
- 6) Dilution of solutions is very common in “wet” labs. In this lab, a nitrite (NO_2^-) solution of approximately $5 \mu\text{g/mL}$ will be used to make 4 standard solutions of varying concentrations. If $500.0 \mu\text{L}$ of the $5 \mu\text{g/mL}$ solution is diluted to 25.00 mL in a volumetric flask, what is the resulting concentration of the diluted standard solution in $\mu\text{g/mL}$. (Remember the dilution equation: $C_1V_1 = C_2V_2$ where C = concentration; V = volume).

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(3) What are the main molecular precursors to photochemical smog formation?

(4) If you had the authority to regulate atmospheric emissions of one chosen air pollutant, which air pollutant would you pick in order to have the largest impact on the air quality?

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Computational Chemistry Prelab

Last modified: June 17, 2014

Recommended reading:

AirUCI Manual: Computational Chemistry Lab (Spartan)

Environmental Chemistry Text: Pages: 175–179, 184–187 and 193–196
on Molecular Vibrations

Prelab Questions:

- 1) What is the overall goal of this lab?
- 2) What computer program will be used for the computations?
- 3) What region of the electromagnetic spectrum can induce molecular vibrations:
- 4) Convert the wavenumber (similar to a “frequency”) 1000 cm^{-1} to a wavelength in μm .
- 5) What is a dipole?
- 6) What is the model chemistry (i.e., theoretical model and basis set) that will be used for the calculations in this lab:
- 7) What do the terms HOMO and LUMO stand for?