AS – 6342 Spectroscopic Reactive Flow Diagnostics
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Assignment–1, Total: 45, Weightage: 15%, Due: Apr 01, 2018 NOON.

NOTE: For physical data about specific molecules refer to the website for Q data.

1. Consider a gas with 30% CO and the rest N2. The gas is at 1 atm, 300 K.
(a) Find the microwave absorption spectrum for this gas. Assume that the fraction of molecules that goto lower level from a given level by emitting light is approximately 1e-15. [3]
(b) Find the IR absorption spectrum of the gas in the range 0.9 to 5.0 microns. Assume that for all the lines rotation correction or vibration correction are negligible. Draw only lines that have strengths above 1e-25. Assume that the fraction of molecules that goto lower level from a given level by emitting light is approximately 1e-14. Assume for each level of overtone, there is another factor of 0.01 multiplying the emission fraction. [5]
(c) Repeat the all the above for T=500K, and 1000K, plot all the spectra on top of each other for comparison. Also show them independently. [4]

2. Assume only Doppler broadening, redraw the IR spectrum of CO from Question1, for the fundamental band alone, only for 300K and 1000K. Draw the spectrum as will be seen by an infinite resolution spectrometer for the full range of the band. Comment on the plots. [5]

3. Overlay the curves for collision broadening on the plot for Question 2, for both the cases, for two pressures. Answer this question with two plots, one for 300K with two pressures, and another for 1000K with two pressures. In both of these, have the appropriate plots from question 2 also. Comment on the results. [7]

4. Draw the full shape including collision and Doppler broadening for the first three lines in the R branch of the fundamental band. At 300K and 1000K for two pressures (1 atm and 5 atm). [8]

5. Using the molecular data given below for CO,
(a) list the line positions of CO R-branch of vibration spectrum. [5]
(b) find the band head wavelength [2]
(c) find the J" for the band head transition. [1]
B_o=2.01cm^{-1}, α_e=0.033, ω_e'=2169.32 cm^{-1}, $\omega_e x_e$'=13.278, ω_e"=1515.61 cm^{-1}, $\omega_e x_e$"=17.2505.

6. Given that the integrated absorption strength of a specific CO line chosen for detection of small concentrations of CO, is 1e-23 cm-2/atm. If the path length available is 2m, and your detectors can detect a change in intensity of 0.01%, what is the best concentration detectable by this line at pressures 0.1 atm, 0.5 atm, 1 atm, 2 atm, and 10 atm, if integrated absorbance is used to deduce the concentration. [10]