## AST 393F Assignment 3

## Due Friday 9/18

1. Let's consider four ionization states of oxygen commonly observed by astronomers: OI, OII, OIII, and OIV. We haven't covered enough to answer the following questions from first principles, but you can make some reasonable guesses and then look up the answers in books in Peridier (like Atomic Energy Levels and Grotrian Diagrams).

a) For each ionization state, write down the ground electron configuration and make guesses at the next two higher energy configurations.

b) For the ground configuration of each ion, what terms  $(^{2S+1}L_J)$  occur, and which is the ground term?

c) Between which configurations or terms do allowed (electric dipole) transitions occur? Pick a few transitions for each ion you think will occur by magnetic dipole and electric quadrupole radiation. Find a table of wavelengths and A coefficients that will tell you whether you got this right.

d) For astronomers working in the visible, what transitions do you think would be most useful in measuring the abundance of each of these ions? How about UV astronomers? Or IR astronomers? (One trick here: OII recombination lines tell you the abundance of  $O^{++}$ , or OIII. Why is that?)

2. We won't have time to get to the corrections to the rigid rotor and harmonic oscillator model of the diatomic molecule, but the corrections are mostly classical, so you can do them pretty easily. Note: you can treat a diatomic molecule as a particle of mass equal to the reduced mass,  $\mu$ , moving in the interatomic potential, V(R).

a) Assume the potential between the atoms of a diatomic molecule is quadratic:  $V(R) = 1/2 \text{ k } (R-R_e)^2$ . (R is the interatomic distance, and  $R_e$  is the spacing at the minimum of the potential.) If the molecule is rotating, the effective potential is  $V_{eff} = V(R) + h^2 J(J+1)/(2\mu R^2)$ . The centrifugal potential causes a shift in the potential minimum to larger R. Calculate  $R_{min}$ , where  $V_{eff}(R)$  is a minimum. (You will have to make an approximation to solve for  $R_{min}$ .) Calculate  $V_{eff}(R_{min})$ . This is the rotational energy including centrifugal stretching. It is normally written as:

 $E = hc B_e J(J+1) - hc D_e J^2 (J+1)^2$ , where  $B_e$  and  $D_e$  are in units of cm<sup>-1</sup>. Get your answer into this form, and calculate  $B_e$  and  $D_e$  (in terms of k,  $R_e$ , h, and  $\mu$ ). Look up the values of  $B_e$  and  $D_e$  for CO in a Herzberg book and use your formulas to calculate k and  $R_e$ . b) k can also be derived from the vibrational frequency. Do that. Does the value derived in that way agree with that from centrifugal stretching?

c) Next let's add an anharmonic potential term, k'  $(R-R_e)^3$  to V(R). I claim that this term doesn't change the harmonic oscillator energy levels to first order (that is, in first order perturbation theory) except through its effect on the centrifugal stretching. We didn't talk much about time-independent perturbation theory this year, but if you know enough about it, give an argument that my claim is correct (or that it is incorrect). What sort of an anharmonicity would affect the vibrational energies?

d) Next, we want to ask how a cubic anharmonicity interacts with centrifugal stretching. Calculate  $k_{eff}(R_{min}) = d^2/dR^2 V_{eff}(R)$ , including both centrifugal stretching and the cubic anharmonicity in  $V_{eff}$ . This is the effective spring constant at the minimum of the effective potential. The vibrational frequency at the shifted potential minimum is  $v_{vib} = 1/2\pi (k_{eff}/\mu)^{1/2}$ . Calculate  $v_{vib}$ . This is the vibrational frequency including vibration-rotation interaction.  $E_{vib} = h v_{vib} (v+1/2)$  is written as:  $E_{vib} = h c \omega_e (v+1/2)$  - hc

 $\alpha_e$  (v+1/2)J(J+1). Calculate formulas for  $\omega_e$  and  $\alpha_e$ . (Note that both have units of cm<sup>-1</sup>, not radians/s.) We'll talk in class about the effects of  $D_e$  and  $\alpha_e$  on the spectrum of CO.