Physics 880A20 Winter Quarter 2003
Dr. Herbst

HOMEWORK ASSIGNMENT # 1

DUE: Wednesday, 22 January

1. Determine the rotational selection rules for transitions allowed by the electric quadrupolar moment of a rigid diatomic molecule. For an electric field parallel to Z, the component of the quadrupolar tensor which you should investigate goes as YZ. Hint: break the matrix elements down into dipolar matrix elements.

2. A rigid diatomic molecule is placed in a strong and uniform electric field E_z (Stark Effect). Determine the energy levels of the system as a function of □, J, and M using second-order perturbation theory. Draw the dependence of the energy on electric field strength for the J=0 and 1 levels.

3. A 300 K sample of normal-H_2 (3:1 ortho to para) is cooled to 10 K. Calculate the fraction of H_2 in the J=1 state assuming (i) normal Boltzmann equilibrium pertains (ignore spin completely), (ii) there is no catalyst for ortho-para conversion, and (iii) there is a catalyst for ortho-para conversion such that the two are in equilibrium.
B_e = 60.809 cm^{-1} k/hc = 0.6950 cm^{-1}/K

4. Starting from the radial equation for *S* shown in class, use perturbation theory to determine the approximate energy levels of a harmonic oscillator – rigid rotor system, The idea is to expand the centrifugal term in the effective potential (the one that goes as $1/r^2$) in powers of x/r_e through x^2, where $r = r_e + x$. First rewrite this term as $hB_eJ(J+1)/r^2r_e^{-2}$. Treat the non-rigid rotor terms as perturbations. You need not solve the harmonic oscillator equation; assume that you know the energy levels of the quasi one-dimensional harmonic oscillator. Perform first- and second-order perturbation theory using matrix elements of the harmonic oscillator from a table. Your total energy-expression should contain terms for both centrifugal distortion (D_e) and vibration-rotation interaction (□$_e$). What is wrong with the term for vibration-rotation interaction?

5. Determine the maximum absorption coefficient for the $J = 1$ □ 0 transition of CO, considered as a rigid molecule with internuclear separation 1.1282 Å. You may assume □□ to be 1 MHz, the pressure to be 0.01 Torr (1 Torr = 1/760 atm) and the temperature to be 300 K. What is the percentage absorption along a 100 cm path at the center frequency? The dipole moment of CO is 0.1 D (1 D = 10^{-18} esu-cm). Use cgs units.
k/h = 20.836 GHz/K.