Ge/Ay 132

Problem set # 3

You are allowed to use the class notes and books to solve these problems. Collaboration is permitted, please write up your own solutions however. The questions are worth 30, 40, 15 and 15 points. Due Friday, November 16^{th}.

1. From the following wave numbers of the P and R branches of the 1–0 infrared vibrational band of $^1H^{127}I$ in the X $^1\Sigma^+$ state, obtain values for the rotational constants B_0, B_1 and B_e (in cm^{-1}), the band center $\tilde{\nu}_0$ (in cm^{-1}), the vibration–rotation interaction constant α (in cm^{-1}), and the internuclear distance R_e (in Å). How does the value for R_e compare with the value R_e=1.607775 Å for $^2H^{127}I$? How should it compare? Why? Given that the band center of the 2–0 band is at 4379.0 cm^{-1}, determine ω_e and $\omega_e x_e$ in cm^{-1}.

$v = 0 \rightarrow 1$ Rovibrational Transitions for $^1H^{127}I$

Transition	Frequency (cm^{-1})	Transition	Frequency (cm^{-1})
R(0)	2242.087	P(1)	2216.723
R(1)	2254.257	P(2)	2203.541
R(2)	2266.071	P(3)	2190.025
R(3)	2277.510	P(4)	2176.168

2. The figure below presents the rotational spectrum of CH_3CN observed toward the Orion molecular cloud. Using the JPL catalog, which may be found at

http : //spec.jpl.nasa.gov,

answer the following:

a. Label the tick marks on the plot with the corrected rotational transition quantum numbers.

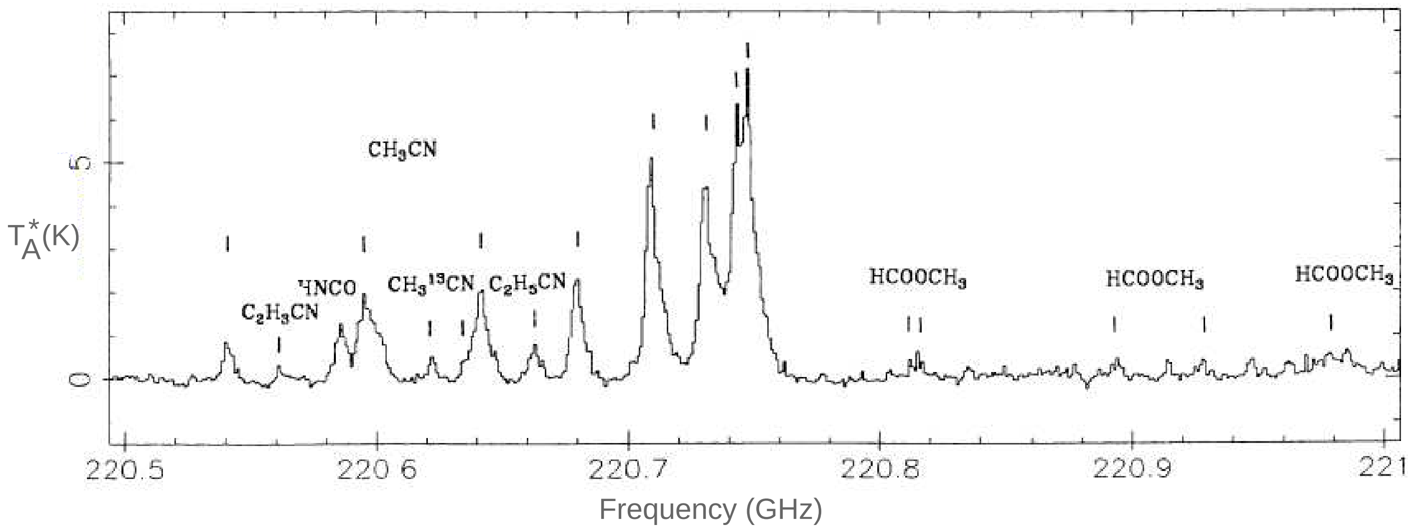
b. Assume local thermodynamic equilibrium is maintained. What temperature best fits the distribution of K-subcomponent projections in this spectrum?

c. Use the temperature found in b and the rotational partition function to estimate the total column density of CH_3CN in the Orion cloud.

In parts b and c, the following will be helpful: For optically thin rotational transitions on the so-called antenna temperature scale, the integrated intensity is given by

$$\int T_A^* dv \quad = \quad \frac{hc^3}{8\pi k \nu^2} A_{ul} g_u \frac{N_T}{Q(T_{ex})} e^{-E_u/kT_{ex}} \quad ,$$

where the integrated intensity $\int T_A^* dv$ is given in (K km/s), ν is the line frequency, A_{ul} is the Einstein A coefficient, g_u is the degeneracy of the upper state, N_T is the total column density (molecules cm^{-2}), Q is the rotational partition function, and E_u is the energy of the upper state. By taking the ln of both sides you'll get an equation of a straight line whose slope is related to the excitation temperature and whose intercept is related to



Problem #2– Observed CH_3CN spectrum toward the Orion-KL molecular cloud.

the total column density. You can find the rotational partition function data under the Catalog directory with links button, while the interface to the catalog itself is at

`http://spec.jpl.nasa.gov/ftp/pub/catalog/catform.html`

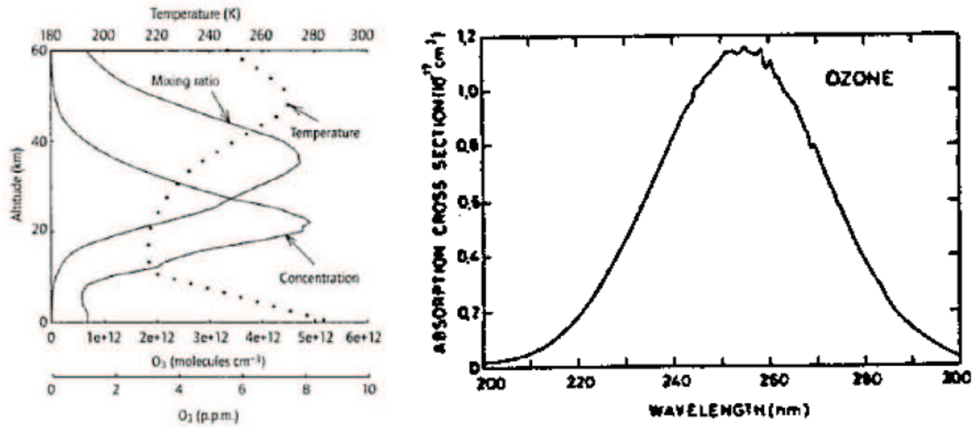
The catalog presents the frequencies and energies of the transitions along with the $\log_{10}$ of an intensity at 300 K which is related to the Einstein A coefficient (A_{ul}) for the transition by:

$$A_{ul} = \frac{1.748\times10^{-9}\ \nu(\mathrm{MHz}) I_{cat}(\mathrm{T}_0)\ Q(\mathrm{T}_0)}{g_u e^{-E_u/k\mathrm{T}_0}} \qquad \mathrm{s}^{-1}$$

where $\mathrm{T}_0 = 300$ K. This equation lets you derive the value of A_{ul} that is defined in a consistent way with the partition function Q for the equation above. Further information on the format of the catalog can be found in the README file on the main catalog page. You can assume the lines are Gaussian in shape, and can therefore simply use the peak height and FWHM to get the integrated area.

3. Suppose (unrealistically) that a grain of 1000 Å diameter is a perfect blackbody with its effective cross section equal to its geometrical cross section at all wavelengths. It is in the vicinity (400 astronomical units away) of a young star of luminosity 10^{37} egs/sec. (a) Calculate the effective temperature of the grain. How does this temperature vary with distance if nothing blocks the stellar radiation from reaching the grains? (b) Pick your favorite material's heat capacity (remember water is 1 cal gm^{-1}, rock is closer to 3). Assume all the energy of a 10 eV photon is instantaneously deposited into the above sized grain through processes such as internal conversion. What is the temperature jump that would ensue? What about 100 and 10 Å grains? What is the distance dependence of the temperature jump?

4.An "average" ozone abundance profile in the Earth's atmosphere is shown below, along with ozone UV absorption cross sections (the units are in 10^{-17} cm^2). What is the optical



Problem #4– Vertical abundance profile of ozone in the Earth's stratosphere (left), and the absorption cross sections in the so-called ozone Hartley band (right).

depth provided by the ozone layer at 250 nm? Treat the ozone layer as a Guassian to get the column density; that is, just use the peak concentration times the FWHM of the vertical extent. At 250 nm the extinction coefficient of liquid water is 0.0168 cm^1. How thick a layer of liquid water is needed to equal the UV extinction of ozone, at this wavelength (which is close to the maximum of the radiation damage yield of DNA)? Does the calculated optical depth help you explain the temperature profile in the stratosphere, also presented in the figure at left?