

## Ge/Ay 132

### Problem set # 3

You are allowed to use the class notes and books to solve these problems. Limited collaboration is permitted. The questions are worth 30, 30, and 40 points. Due Friday, February 20th.

1. Consider the molecule thioformaldehyde,  $\text{H}_2\text{CS}$ .

- Using the asymmetric rotor energy level formulas given in Table 8.4, calculate the first few ( $J=0, 1$  and  $2$ ) rotational energy levels of the molecule. The inertial moments are  $A= 291291.641$  MHz,  $B=17699.628$  MHz, and  $C= 16651.83$  MHz. Draw an energy level diagram.
- The molecule can be classified as a near-prolate top. Using the approximate selection rules for this case, indicate in the diagram which transitions are electric dipole allowed.
- Do the transitions lie in the centimeter, millimeter, submillimeter or far-infrared part of the spectrum?

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

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

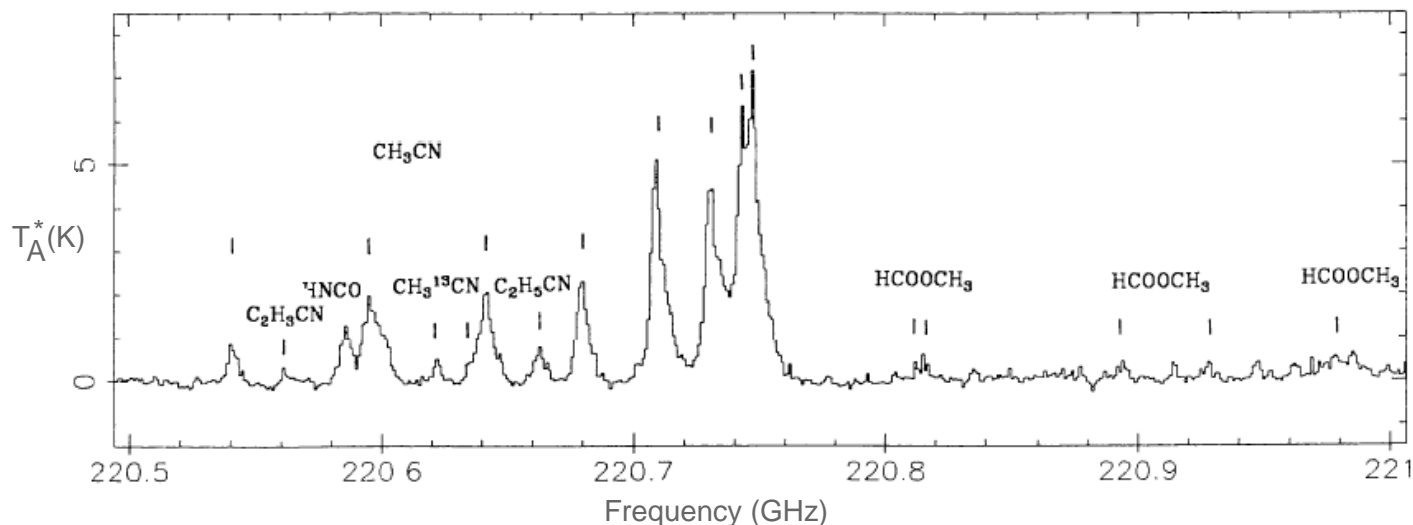
Transition	Frequency ( $\text{cm}^{-1}$ )	Transition	Frequency ( $\text{cm}^{-1}$ )
R(0)	2242.087	P(1)	2216.723
R(1)	2254.257	P(2)	2203.541
R(2)	2266.071	P(3)	2190.025
R(3)	2277.510	P(4)	2176.168

3. The figure below presents the rotational spectrum of  $\text{CH}_3\text{CN}$  observed toward the Orion molecular cloud. Using the JPL catalog, which may be found at

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

answer the following:

- Label the tick marks on the plot with the corrected rotational transition quantum numbers.
- Assume local thermodynamic equilibrium is maintained. What temperature best fits the distribution of K-subcomponent projections in this spectrum?
- Use the temperature found in b and the rotational partition function to estimate the total column density of  $\text{CH}_3\text{CN}$  in the Orion cloud.



**Problem #3**– Observed CH<sub>3</sub>CN spectrum toward the Orion-KL molecular 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

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

where the integrated intensity  $\int T_A^* dv$  is given in (K km/s),  $\nu$  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<sup>-2</sup>),  $Q$  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 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:

$$A_{ul} = \frac{1.748 \times 10^{-9} \nu(\text{MHz}) I_{cat}(T_0) Q(T_0)}{g_u e^{-E_u/kT_0}} \text{ s}^{-1}$$

where  $T_0 = 300$  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.