

FINAL EXAMINATION (100 POINTS)

DUE: MONDAY, 17 MARCH

1. (20 points) Determine the equilibrium internuclear separation (\AA) for the ground electronic state of CO to 5 significant figures given the following information:

Vibrational State v	$J'-J''$	Frequency (MHz)
0	1-0	115271.2
0	2-1	230538.0
1	1-0	114223.0
1	2-1	228441.5

2. (35 points) Consider the triatomic molecule SO_2 , a bent species with a bond distance of 1.4321\AA and a bond angle of 120 degrees in its ground vibrational state.

- (15 pts) Determine the rotational constants.
- (10 pts) O is a spinless boson. Discuss the spin degeneracy of the states as a function of the pseudo-quantum numbers K_1, K_2 .
- (10 pts) What are the allowed transition frequencies for $J=2$?

3. (15 points) In the PAM method for internal rotation of the methyl group in methanol, the torsional-rotational interaction Hamiltonian is given approximately by the equation

$$H_{\text{int}} = \frac{1}{2} F P_a P_\phi$$

Determine an integrated expression for the first-order correction to the energy.

Remember that the zeroth-order energy can be expressed as $E_T + E_R$, where "T" stands for the torsional energy and "R" for the asymmetric top rotational energy. Use as your zeroth-order function:

$$\psi_{JK_1K_2}^{(v)}$$

4. (20 points) Consider the linear molecule HCN, which possesses a dipole moment μ of 2.98 Debye ($1 \text{ D} = 10^{-18} \text{ esu-cm}$), and a rotational constant B_0 of 44,315.97 MHz.

- (10 pts) What is the critical density for emission of the $J = 1 \rightarrow 0$ transition from an interstellar cloud? Use $k_{\text{up}} (\text{cm}^3 \text{ s}^{-1}) = 3 \times 10^{-11}$.
- (10 pts) What will happen if the density is 0.1 the critical density?

5. (10 points) The pressure broadening coefficient γ for a molecule is 32 MHz/Torr at 300 K. What is the effective rate coefficient for collisions contributing to pressure broadening in units of $\text{cm}^3 \text{ s}^{-1}$?