

## 22.4.1: i. Exercises

### Q1

Consider the molecules  $CCl_4$ ,  $CHCl_3$ , and  $CH_2Cl_2$ .

- What kind of rotor are they (symmetric top, ect; do not bother with oblate, or near-prolate, etc.)
- Will they show pure rotational spectra?
- Assume that ammonia shows a pure rotational spectrum. If the rotational constants are  $9.44$  and  $6.20 \text{ cm}^{-1}$ , use the energy expression:

$$E = (A - B)K^2 + BJ(J + 1),$$

to calculate the energies ( in  $\text{cm}^{-1}$ ) of the first three lines (i.e., those with lowest K, J quantum number for the absorbing level) in the absorption spectrum (ignoring higher order terms in the energy expression).

### Q2

The molecule  $^{11}B^{16}O$  has a vibrational frequency  $\omega_e = 1885 \text{ cm}^{-1}$ , a rotational constant  $B - e = 1,78 \text{ cm}^{-1}$ , and a bond energy from the bottom of the potential well of  $D_e^0 = 8.28 \text{ eV}$ .

Use integral atomic masses in the following:

- In the approximation that the molecule can be represented as a Morse oscillator, calculate the bond length,  $R_e$  in angstroms, the centrifugal distortion constant,  $D_e$  in  $\text{cm}^{-1}$ , the anharmonicity constant,  $\omega_e X_e$  in  $\text{cm}^{-1}$ , the zero-point corrected bond energy,  $D_0^0$  in eV, the vibrational rotation interaction constant,  $\alpha_e$  in  $\text{cm}^{-1}$ , and the vibrational state specific rotation constants,  $B_0$  and  $B_1$  in  $\text{cm}^{-1}$ . Use the vibration-rotation energy expression for a Morse oscillator:

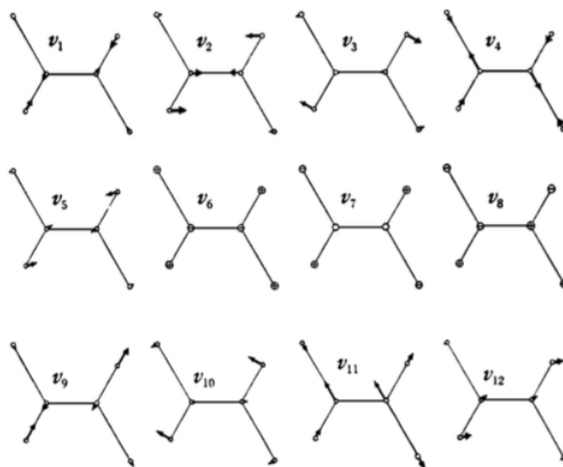
$$E = \hbar\omega_e \left( v + \frac{1}{2} \right) - \hbar\omega_e X_e \left( v + \frac{1}{2} \right)^2 + B_v J(J + 1) - D_e J^2(J + 1)^2, \text{ where} \quad (22.4.1.1)$$

$$B_v = B_e - \alpha_e \left( v + \frac{1}{2} \right), \alpha_e = \frac{-6B_e^2}{\hbar\omega_e} + \frac{6\sqrt{B_e^3 \hbar\omega_e X_e}}{\hbar\omega_e}, \text{ and } D_e = \frac{4B_e^3}{\hbar\omega_e^2} \quad (22.4.1.2)$$

- Will this molecule show a pure rotation spectrum? A vibration-rotation spectrum? Assume that it does, what are the energies ( $\text{in cm}^{-1}$ ) of the first three lines in the P branch ( $\Delta v = +1, \Delta J = -1$ ) of the fundamental absorption?

### Q3

Consider  $\text{trans-}C_2H_2Cl_2$ . The vibrational normal modes of this molecule are shown below. What is the symmetry of the molecule? Label each of the modes with the appropriate irreducible representation.



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