

**Homework #1**

As the first part of this class is “review”, the homework problems from the QM section are loosely based on various chapters of M&S (i.e., 1-13). You should be able to do the problems based on class notes, but if you get stuck, check these chapters for additional information. You can also see me in office hours.

1. The anti-symmetric stretch of CO<sub>2</sub> appears in an IR spectrum at 2349.16 cm<sup>-1</sup>. Translate this value into frequency (in Hz), wavelength (in nm), and energy (in J).
2. The force constant,  $k$ , of <sup>79</sup>Br<sup>79</sup>Br is 240 N·m<sup>-1</sup>.
  - a. Calculate the fundamental vibrational frequency,  $\nu$ , and the zero point energy of <sup>79</sup>Br<sup>79</sup>Br. The following definitions will be useful:

$$\nu = \frac{1}{2\pi} \left( \frac{k}{\mu} \right)^{1/2} \quad \text{and} \quad \mu = \frac{m_1 m_2}{m_1 + m_2}$$

where  $\nu$  is the fundamental vibrational frequency,  $k$  is the force constant, and  $\mu$  is the reduced mass.

- b. The force constant of <sup>14</sup>N<sup>14</sup>N is 2243 N·m<sup>-1</sup>. Why is this value is so much greater for <sup>14</sup>N<sup>14</sup>N than for <sup>79</sup>Br<sup>79</sup>Br?
3. Given that  $\tilde{\nu} = 2330 \text{ cm}^{-1}$  and  $D_0 = 78715 \text{ cm}^{-1}$  for N<sub>2</sub>, calculate  $D_e$ .
4. What is the energy of a ground state electron confined to a 1 nm cube?
5. Determine the number of translational, rotational, and vibrational degrees of freedom in:
  - a. CH<sub>3</sub>Cl
  - b. OCS
  - c. C<sub>6</sub>H<sub>6</sub>
  - d. H<sub>2</sub>CO
6. The energy difference between the J=0 and J=1 rotational levels for carbon monoxide (<sup>12</sup>C<sup>16</sup>O) is  $\nu = 1.153 \times 10^5 \text{ MHz}$ .
  - a. Calculate the energy difference between the J=0 and J=2 rotational levels. Give your answers in Hz, kJ, nm, and cm<sup>-1</sup>.
  - b. Calculate the degeneracy of the first 4 rotational levels.