

PHY420 Tutorial 3

Handed out 13.03.2018, Due 16.03.2018

1. In the pure rotational spectrum of (isotopically pure) HCl , it is found that the emission from the $J = 2$ and $J = 3$ levels have equal intensities and that the line spacing is 21.2 cm^{-1} . Find the temperature of the gas sample.
2. The vibrational Hamiltonian using the Morse potential

$$U(R) = D_e[1 - \exp(-a(R - R_e))]^2.$$

gives the energy eigenvalues

$$G(v) = \omega_e(v + \frac{1}{2}) - x_e\omega_e(v + \frac{1}{2})^2$$

Find the value of ω_e in terms of D_e and a by expanding the Morse potential about its minimum. Calculate the first energy of the two lowest vibrational transitions. Compare the 10th vibrational levels in the Morse and Harmonic approximations.

3. CO_2 is a symmetric, linear molecule. Can it have a rotational spectrum? Can it have a pure vibrational spectrum? Will it have strong ro-vibrational couplings? How does that affect the spectrum?
4. Explain why the electronic energy curves $E(R)$ for the ground electronic states of H_2 and D_2 are expected to be nearly identical. Estimate the difference between the dissociation energies of the two molecules and explain the reason for difference. Would the vibrational frequencies of the two molecules in their ground electronic states be the same? If not, how different would they be?
5. Write down the electronic configuration and the term symbol for the ground state of N_2 and O_2 .
6. The fundamental ro-vibrational band in HCl shows the following lines in the P and R branches ($v = 0 \leftrightarrow 1$). Based on these data determine the centrifugal distortion for $J = 5$, and the bond lengths for the states $J = 0$ and $J = 5$.

Line	wavenumber [cm^{-1}]
R(5)	2997.78
R(4)	2980.90
R(3)	2963.24
R(2)	2944.89
R(1)	2925.78
R(0)	2906.25
ν_0 (absent)	2885.90
P(1)	2865.09
P(2)	2843.56
P(3)	2821.49
P(4)	2798.78
P(5)	2775.79
P(6)	2752.03