INDIAN INSTITUTE OF SCIENCE EDUCATION AND RESEARCH PUNE
Quiz–2, Spring 2018

Course Name: Atomic and Molecular Physics — Course Code: PHY420
Date: 28.03.2018 — Duration: 1h
Instructor: Bhas Bapat — Total Marks 20

Solve any *four* of following. Questions carry equal marks.

1. Determine the term symbol for the following ground state configurations (superscript signifies the number of electrons in that orbital, just like the atomic case)
   $B_2 : (1\sigma_g)^2\,(1\sigma_u)^2\,(2\sigma_g)^2\,(2\sigma_u)^2\,(1\pi_u)^2$
   $C_2 : (1\sigma_g)^2\,(1\sigma_u)^2\,(2\sigma_g)^2\,(2\sigma_u)^2\,(1\pi_u)^4$

2. Show that in the P and the R branches of the ro-vibrational spectrum of a diatomic molecule, the lines are equally spaced if ro-vibrational coupling is neglected. Show that the spacings depend quadratically on J if the ro-vibrational coupling is taken into account. You may show this for either the P or the R branch.

3. Show that the J quantum number of the highest populated rotational level of a rigid diatomic molecule is
   $$J_{max} = \left[\frac{kT}{2Bhc}\right]^{1/2} - \frac{1}{2}$$
   If the value of B for HCl is 10.6 cm^{-1}, which state would be the most populated (i) at room temperature, (ii) and at 100 °C? What would be the difficulty in determining the temperature of a sample by merely deducing J_{max} from the spectrum?

4. What is the dependence of the value of the centrifugal distortion term in the ro-vibrational spectrum of a diatomic molecule on the vibrational level?

5. Describe the rotational spectrum of the H_2 molecule. Obtain the approximate position (in wavenumbers) of its lowest line, and the spacing between the first and the second line. Is it right to ignore the ro-vibrational coupling for this molecule?

6. Lines in the vibrational spectrum of HCl lie at 2886, 5668, 8347, 10923 cm^{-1}. Are these values in agreement with the prediction based on the Morse potential? The Morse potential is given by
   $$U(R) = D_e[1 - \exp(-\alpha(R - R_e))]^2.$$
   which gives the energy eigenvalues
   $$G(v) = \omega_e(v + \frac{1}{2}) - x_e\omega_e(v + \frac{1}{2})^2$$