QUIZ - I

① Consider the vibrational mode that corresponds to the uniform expansion of the benzene ring. Assume this vibration as a simple harmonic motion. Do you think this vibrational excitation satisfies the first Selection rule for vibrational transitions? Justify your answer.

② Consider a Pure rotational transition of a diatomic molecule from $J=2$ to $J=3$ states. How do you calculate the frequency of this transition? Given this frequency, is it possible to estimate the moment of inertia and the bond length of the molecule? How?

③ Consider a system of N non-interacting diatomic molecules at $T = 300K$.

Case-I: Assume that molecules can only vibrate harmonically. Let N_0 and N_1 are the numbers of molecules in the ground and the first excited vibrational states of the system. Calculate N_1/N_0.

Case-II: Assume that molecules can only rotate. Let n_0 and n_1 are the numbers of molecules in the ground and the first excited rotational states of the system. Calculate n_1/n_0.

Compare these ratios.

④ How do you determine the normal modes of a Polyatomic molecule consisting of N atoms? You need to define the Hessian matrix and discuss about the need to diagonalize this matrix and about the vibrational density of states. Consider a special vibrational mode in which the coordinates of atoms change from (x_i, y_i, z_i) to $(x_i + \Delta x, y_i, z_i)$ $(i = 1, 2, \ldots, N)$ and Δx is same for all atoms. What is the frequency of this mode? Justify your answer.

(5) Consider the Potential energy of two one-dimensional harmonic oscillators coupled to each other by a spring of spring constant K_{12}. (Recall the model discussed in the class), which is given by

$$U(x_1, x_2) = \frac{1}{2} K_1 x_1^2 + \frac{1}{2} K_2 x_2^2 + \frac{1}{2} K_{12}(x_1 - x_2)^2$$

Calculate the Hessian for this model system. Determine the frequencies of the normal modes. Plot schematic graphs showing the variation of these frequencies with K_{12}.

(6) In the class, we discussed about electronic energy surfaces of a diatomic molecule as a function of internuclear separation. How do we determine/calculate the ground and first excited electronic energy surfaces? What do they represent physically? Why do you think the energy gap between these two states is greater than that of vibrational and rotational levels?

(7) By rotating a diatomic molecule about an axis passing through the center of gravity, which is perpendicular to the molecular axis, we can break the molecule (dissociate). Do you agree with this statement? Justify your answer.