CHEM106: Assignment 7

Rigid Rotor

1. For the rigid rotor system, the solution of the Schrödinger equation leads to the quantized energy .

A. Define the zero-point energy of the system.

The zero-point energy (ZPE) for a quantum mechanical system is defined as the lowest possible energy allowed. In the case of the rigid rotor, the energy depends on the quantum number J, and J = 0, 1, 2, 3, . . . .

Thus, 

B. Determine the energy gap between energy level J + 1 and J.

The energy gap between energy level J + 1 and J is

 

The energy gap between the neighboring levels for the rigid rotor increases as the quantum number J increases. It is worth noting that this energy gap is related to the frequency of light in the molecular rotational spectrum (see Unit 7, Section 7.2).

C. What is the degeneracy of the energy level EJ?

The degeneracy of an energy level equals to the number of quantum states for the given energy. For each quantum number J, there exist 2J + 1m quantum numbers. So the degeneracy for the energy level EJ is 2J + 1.

2. For the particle on a ring system, the solution of the Schrödinger equation generates the normalized wavefunction . Show that is an eigenfunction of the z-component of the angular momentum operator (), and determine the corresponding eigenvalue.

For a given operator, its eigenfunction must satisfy the relation , where a is a constant.



Thus, is an eigenfunction of, with an eigenvalue of .

3. The solution of the Schrödinger equation for the particle on a sphere system results in the wavefunction  that is commonly referred to as the spherical harmonics. For l = 1, m = +1, the spherical harmonics is given by .

1. Show that is normalized.

Since the Schrödinger equation for the particle on a sphere system is solved in the spherical polar coordinate system, the integration must be carried out using the same system.

We need to evaluate the integral . If M = 1, then the wavefunction is normalized.



Thus,  is normalized.

1. Set up an equation for calculating the average value of the Y component of the angular momentum for the system [No need to calculate the integral].

Given the operator for the Y component of the angular momentum

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its average value can be calculated as



4. Explain/Illustrate how the rigid rotor model can be applied to the determination of bond length of diatomic molecules.

Looking back at the solution to question 1B above, the energy gap between neighboring level of the rigid rotor is

 ,

where the momentum of inertia.

 We also know that the energy gap is related to frequency of the photon by

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 Thus, we can follow the path



to determine the bond length.