Question Bank

Molecular Spectroscopy

1. Microwave causes molecules to rotate energetically. A molecule absorbs microwave photon of wavelength 40 cm. Calculate the energy difference between the two energy levels in joule.

2. State Born-Oppenheimer approximation. For a diatomic molecule undergoing anharmonic oscillations, draw energy level diagram showing rotational levels, vibrational levels and electronic levels.

3. What are hot bands?

4. Write symmetric and asymmetric and bending vibrations of CO_2 and H_2O molecules.

5. State which of the following molecules are microwave active: HCl, H_2O, HI, OCS, N_2, H_2, HF.

6. i) Derive an expression for moment of inertia of a rigid diatomic molecule. ii) Write an expression for allowed rotational energy levels of rigid diatomic molecule. Give rotational energy level diagram, show allowed rotational transitions and resulting spectra for the rotation of rigid diatomic molecule.

7. Calculate the reduced mass and moment of inertia of HCl if the bond length is 1.27 Å. Atomic masses of hydrogen = 1.008, Chlorine = 35.45, 1 amu = 1.66×10^{-27} kg, h = 6.6×10^{-34} Js, c = 3×10^{8} ms^{-1}, N = 6.023×10^{23} mol^{-1}.

8. For HBr molecule:

i) The rotational spectrum shows the first line at 17.19 cm^{-1}. Calculate the bond length of HBr

molecule (Use rigid rotor model) (ii) The vibrational spectrum shows fundamental and first overtone at 2559.08 cm^{-1} and 5027.54 cm^{-1} respectively. Calculate the anharmonicity constant for the molecule. (Use anharmonic oscillator model). (1 amu=1.66 x 10^{-27} kg, h = 6.627x10^{-34} Js, c = 3 x 10^{10} cms^{-1} , N = 6.023 x 10^{23} mol^{-1}, Gram molar mass of H = 1.0 and Br = 79.9)

9. Assuming a rigid rotor model for a rotating diatomic molecule, draw the rotational energy level diagram and calculate the distance (in cm^{-1}) between two consecutive lines in the rotational spectrum of a diatomic molecule with I = 1.34 x 10^{-47} kgm^2. (h = 6.625 x 10^{-34} Js and c = 3 x 10^{10} cms^{-1})

10. Write an expression for allowed vibrational energy levels of simple harmonic oscillator model of diatomic molecule. Explain the terms. Give energy level diagram, show allowed transitions and resulting spectra for simple harmonic oscillator model of diatomic molecule.

11. Write an expression for allowed vibrational energy levels of anharmonic oscillator model of diatomic molecule. Explain the terms. Give vibrational energy level diagram, show allowed vibrational transitions and resulting spectra for anharmonic oscillator model of diatomic molecule.

12. Using harmonic oscillator model, calculate the zero-point vibrational energy of HCl given that the force constant of HCl is 516 Nm^{-1}.

13. The force constant of CO is 1840 Nm^{-1}. Calculate the oscillation frequency and wave number in cm^{-1}. (1 amu = 1.66 x 10^{-27} kg, c = 3 x 10^8 ms^{-1}, Gram molar mass of C = 12.000 and O = 15.9994)

14. For a KCl molecule undergoing simple harmonic motion the vibrational spectrum shows a fundamental frequency at 378 cm^{-1}.

i) Calculate the reduced mass of KCl ii) Determine force constant of KCl

iii) Determine zero- point energy for KCl molecule.
(c = 3 x 10^{10} cms^{-1} , N = 6.023 x 10^{23} mol^{-1}, Gram molar mass of K =39 and Cl = 35.5)

15. i) Why real molecules do not obey simple harmonic oscillator model?
ii) The force constant of a HF is 970 N/m. Calculate reduced mass and the spacing between two consecutive levels. (Use simple harmonic oscillator model).
(Given: Atomic masses of H = 1.008 and F = 18.99, Avagadro's number = 6.023 x 10^{23}, Speed of light = 3 x 10^{10} cm/s, 1 amu = 1.66 x 10^{-27} kg, Planck's constant = 6.627 x 10^{-34} Js, π = 3.14)

16. Given that the spacing of the lines in the pure rotational spectrum of $^{27}Al^{1}H$ is constant at 12.604 cm^{-1}, calculate the moment of inertia and bond length of the molecule.
(Given: Atomic masses of Al = 26.9815 amu and H = 1.008 amu, Avagadro's number = 6.023 x 10^{23}, Speed of light = 3 x 10^{10} cm/s, π = 3.14, Planck's constant = 6.627 x 10^{-34} Js, 1 amu = 1.66 x 10^{-27} kg)

17. State Franck-Condon principle. With the help of suitable diagram, show the vibrational-electronic transitions and corresponding spectra for the following cases.
i) Transitions takes place from $v'' = 0$ to $v' = 2$.
ii) Transitions takes place from $v'' = 0$ to beyond the dissociation energy of the molecule.

18. For HBr molecule : i) Calculate the reduced mass and force constant in N/m, when it shows harmonic oscillations, if the vibrational spectrum of the molecules show a single intense line at 2649 cm^{-1}. ii) If the same molecule shows anharmonic oscillations, calculate the wave number of fundamental absorption and first overtone if the anharmonicity constant for the molecule is 0.017 and equilibrium vibrational frequency is 2649 cm-1. (Given: Atomic masses of H = 1.0 amu and Br = 80.0 amu, Avogadro's number = 6.023 x 10^{23}, Speed of light = 3 x 10^{10} cm/s, π = 3.14, Planck's constant = 6.627 x 10^{-34} Js, 1 amu = 1.66 x 10^{-27} kg)

19. For a rigid rotor diatomic molecule :

i) Derive an expression for moment of inertia.

ii) Draw the energy level diagram for a rigid rotor diatomic molecule up to J = 5.

iii) Calculate the energy required (in cm^{-1}) for the molecule to move from J = 3 to J = 4 level if B = 10.93 cm^{-1}.

20. The rotational constant of $^{127}ICl^{35}$ is 0.1142 cm^{-1}. Calculate the ICl bond length, (Given: Atomic masses of I = 126.9amu and Cl = 34.9688 amu, Avogadro's number = 6.023 x 10^{23}, Speed of light = 3 x 10^{10} cm/s, π = 3.14, Planck's constant = 6.627 x 10^{-34} Js, 1 amu = 1.66 x 10^{-27} kg)

21. The force constant of a HI is 294 N/m. Calculate reduced mass and the spacing between two consecutive levels. (Use simple harmonic oscillator model). (Given: Atomic masses of H = 1.008 and I = 126.9, Avogadro's number = 6.023 x 10^{23}, Speed of light = 3 x 10^{10} cm/s, 1 amu = 1.66 x 10^{-27} kg, Planck's constant = 6.627 x 10^{-34} Js, π = 3.14)

Phase Equilibria

1. Define chemical potential.

2. Give an example of an equilibrium system of i) 2- phase, ii) an invariant system

3. Calculate the degrees of freedom. i) Two partially miscible liquids in the absence of vapor.
   ii) A solution of a solid in a liquid in equilibrium with solvent vapor

4. How many phases and components present for the following system?
   $MgCO_3(s) \rightleftharpoons MgO(s) + CO_2$ (closed system)

5. What are the number of phases and components for the following reaction in a closed system? $NH_4Cl(s) \rightleftharpoons NH_3(g) + HCl(g)$

6. Draw a labeled phase diagram of water system and calculate degree of freedom at triple point and on the vaporization curve.

7. Derive phase rule using thermodynamic principles.

8. In the one component water system why does the fusion curve has a negative slope?

9. What are the phases in equilibrium with each other on the meta stable curve in water system phase diagram?

10. What is reduced phase rule? Describe lead-silver system with the help of a neat labeled diagram. Calculate the degrees of freedom at eutectic point.

11. What is desilverisation of lead?

12. What are cooling curves? How are they useful in construction of phase diagrams?

13. For Pb-Ag system, calculate the degrees of freedom at eutectic point and mention the temperature and pressure corresponding to eutectic point

Computational Chemistry

1. What is computational chemistry?
2. What are the different types of computational chemistry methods?
3. Give the difference between classical and quantum methods of computational chemistry

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