Molecular physics

Tutorial 1: Elementary theory of rotational, vibrational and electronic spectra of diatomic molecules, Frank-Condon principle and applications, Raman effect and molecular structure; Laser Raman spectroscopy

Q1:

) Why are Raman active vibrations and infrared vibrations in CO_2 molecule complementary to each other ? 30

) In a Raman spectrum of a linear triatomic molecule, the first three lines are 4·86, 8·14 and 11·36 cm^{-1}. Calculate the rotational constant, B and the moment of inertia of the molecule. 10

(Given $h = 6{\cdot}626\times10^{-27}$J.s, $C = 3{\cdot}0\times10^{10}$ cm/sec.) 10

2013

Q2:

Given that the spacing between vibrational levels of CO molecules is 8.45×10^{-2} eV of energy. Find the force constant of the molecule. 10

2014

Q3:

Discuss the vibrational spectra of a diatomic molecule treating it as an anharmonic oscillator. 20

2014

Q4:

Two successive lines in the rotational emission spectrum of HCl molecule appear at wave numbers 83.5 cm^{-1} and 104.1 cm^{-1}. Calculate the position of the next line appearing at the higher wave number. 10

2015

Q5:

Hydrogen molecule is diatomic. Obtain the rotational energy levels of this molecule. Write down the selection rules. Obtain the smallest energy required to excite the lowest rotational mode. 30

2015

Q6:

The observed vibrational frequency of CO molecule is 6.42×10^{13} Hz. What is the effective force constant of the molecule ? 10

2015

Q7:

What is Raman effect ? Describe briefly the chief characteristics of pure rotational spectra. The small rotational Raman displacement for HCl molecule is 41·6 cm^{-1}. Find the internuclear distance between the atoms forming the molecule. *10+10+10=30*

2016

Q8:

Show that the lines in the absorption spectra corresponding to the rotational transitions from two adjacent energy levels of a medium sized molecule at room temperature have comparable intensities. 10

2017

Q9:

Given the force constant of HCl molecule = 516 Nm^{-1}, determine the wave number of the fundamental mode of vibration of the molecule. How many transition lines one can expect in the vibration spectra of HCl molecule at room temperature ? 10

2017

Q10:

Explain Stokes and anti-Stokes Raman scattering with the help of energy level diagram. For a diatomic molecule, obtain expressions for transition energies of its Raman spectra with rotational fine structure and hence the wave numbers of the Stokes lines. 20

2017

Q11:

Explain why lines in some Raman spectra are found to be plane polarized to different extents even though the exciting radiation is completely unpolarized ? 10

2017

Q12:

Why is population inversion in general not possible in a two-level laser system? Explain it. 10

2019

Q13:

Why are Raman active vibrations and IR vibrations in CO_2 molecule complementary to each other? 10

2019

Q14:

What is Franck-Condon principle? Discuss the intensity distribution in the vibrational electronic spectra of a diatomic molecule on the basis of this principle. 15

2019

Q15:

The potential energy of a diatomic molecule in terms of the interatomic spacing R is given by

$$U(R) = \frac{-A}{R^2} + \frac{B}{R^{10}}$$

where $A = 1{\cdot}44 \times 10^{-39}\ \text{J m}^2$ and $B = 2{\cdot}19 \times 10^{-115}\ \text{J m}^{10}$. Calculate the equilibrium spacing, R_e and the dissociation energy. 20

2020

Q16:

The first line in the pure rotational spectrum of HCl appears at $21{\cdot}18\ \text{cm}^{-1}$. Calculate bond length of the molecule. Given atomic masses of H and Cl are 1·008 and 35·45 amu, respectively. 10

2021

Q17:

In observing the Raman spectrum of a sample using 3637Å as the exciting line, one gets stoke line at 3980Å. Deduce the Raman shift in m^{-1} units. Compute the wavelength in Å for corresponding stokes and antistokes lines if the exciting line is 6465Å. 20

2021

Q18:

Define Franck-Condon principle. How does it help in explaining the intensity distribution of vibrational-electronic spectra of diatomic molecules. 15

2022

Q19:

(i) In a diatomic molecule when one constituent atom is replaced by one of its heavier isotopes, what change takes place in the rotational spectrum ?
(ii) Calculate the change in rotational constant B when hydrogen is replaced by deuterium in the hydrogen molecule.
(iii) Draw the spectra of rigid and non-rigid rotors by using the schematic representation of the rotational energy levels and comment on it. 20

2022

Q20:

(i) Briefly explain the effect of anharmonicity on the vibrational spectra of diatomic molecules.
(ii) Calculate the average period of rotation of HCl molecule if it is in the $J = 3$ state. The internuclear distance and the moment of inertia of HCl are 0·1274 nm and $0{\cdot}0264 \times 10^{-45}$ kg.m^2 respectively. 15

2022

Q21:

What is Raman effect ? Explain Quantum theory of Raman effect and Rotational Structure of a Raman spectrum. 5+10+5=20

2023

Q22.

How do Stokes lines appear in Raman spectrum as per classical and quantum theory of Raman effect ? *20*

2024

Q23.

Show that for a diatomic molecule with two nuclei of mass 'M' separated by a distance 'a', the rotational energy of nuclear motion is lower than electronic energy by a factor of $\frac{m_e}{M}$. *15*

2024

Q24.

In case of pure rotational states, if the temperature will be doubled, then calculate the rotational quantum number corresponding to maximum population density.

[Assume that temperature is high] 10

2025

Q25.

From the pure rotational absorption spectra of a diatomic molecule (HF), the wave number difference between the consecutive rotational lines is found to be $\Delta\bar{\nu} = 4050\ m^{-1}$. Calculate the following :

(1) Rotational constant

(2) Moment of inertia

(3) Distance between two atoms (bond length)

[Given, $M_H = 1\ u$, $M_F = 19\ u$] 10

2025

Q26.

The force constant of HCl molecule is $4{\cdot}8 \times 10^5$ dyne/cm. Calculate the wave numbers of Stokes and anti-Stokes lines, when excited with a radiation of wavelength 4358 Å.

[Given, $\mu_{HCl} = 1{\cdot}61 \times 10^{-24}$ g] 10

2025