PG Even Semester Examination, May 2025

PHYSICS

(4th Semester)

Course No.: PHY-403

(Molecular Spectroscopy)

Full Marks: 70

Pass Marks: 28

Time: 3 hours

The figures in the right margin indicate full marks for the question. Answer any five questions selecting one from each unit.

UNIT-I

1. Determine the wavefunctions and total energy of H_2^+ molecure using the LCAO method. What will be the wavefunctions of the H_2^+ molecure if the two nuclei are at infinite distance. 12+2=14

2. (a) Write short notes on bonding and antibonding orbitals. 3+3=6

   (b) Explain why He_2 molecule is unstable in its ground state but its excited state exists. 4

   (c) Write the limitations of valence bond theory. 4

UNIT-II

3. (a) Will H_2 and N_2 molecules exhibit rotatonal spectra? Why? 1+3=4

(b) The spacing of a series of lines in the microwave spectrum of AlH is constant at 12.604 cm^{-1}. Calculate the moment of inertia of the AlH molecule. What are the energy of rotation and the rate of rotation when J=10? 6

(c) Write the salient features of rorational spectra. 4

4. (a) Explain the isotopic effect on rotational spectra. 4

(b) Discuss the rotational spectra for linear diatomic molecule considering it to be a non-rigid rotator. 10

UNIT-III

5. Discuss the fine structure of IR bands of diatomic. Why are they all degraded towards red. 12+2=14

6. Considering the molecule to be a anharmonic oscillator discuss the formation of fundamental, first overtone and second overtone vibrational bands in a diatomic molecule. 14

UNIT-IV

7. (a) Explain the Franck condon Principle. 8

(b) What are 'progressions' and 'sequences'? Explain with illustration. 3+3=6

8. Discuss the three branches in the rotational structure of electronic bands. 14

UNIT-V

9. (a) Write the two basic theorems of density functional theory. 6

(b) Discuss the merits and demerits of density functional theory over the conventional quantum mechanical approach. 6

(c) What is electron-correlation functionals. 2

10. Describe the calculation of ground state energy and wave function of a system using Hartee-Fock method. 14

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