PG Even Semester (CBCS) Exam., May—2017

PHYSICS

(4th Semester)

Course No. : PHYCC–403

(Molecular Spectroscopy)

Full Marks : 70
Pass Marks : 28

Time : 3 hours

The figures in the margin indicate full marks for the questions

Answer **five** questions, taking **one** from each Unit

UNIT—I

1. Find the total energy of H_2 for the symmetric and antisymmetric wave functions using LCAO method. 14

2. *(a)* Define ionic and covalent bond. 3

(b) Write the ground state configuration of He_2 and He_2 and discuss their stability. 6

(c) Define bond order. Find bond order of *(i)* C—H bond in CH_4, *(ii)* C—C bond in C_2H_4 and *(iii)* C—C bond in C_6H_6. 5

UNIT—II

3. *(a)* Identify which of these molecules will show pure rotational spectra :

O_2, H—F, CH_3Cl, N_2, H_2O

Show the reason also. 5

(b) Write the principal features of rotational spectra of a diatomic molecule. 3

(c) Discuss the temperature dependence and isotopic effect on rotational spectra. 6

4. *(a)* What is luminescence? Discuss the mechanism of fluorescent emission. Why is fluorescence in general a more powerful technique than absorption? 11

(b) The far-infra-red spectrum of HBr consists of a series of lines spaced 17 cm^{-1} apart. Find the internuclear distance of HBr. 3

UNIT—III

5. *(a)* Give an account of the salient features of vibrational spectra of a diatomic molecule. 4

(b) Discuss how the vibrational spectrum of a diatomic molecule enables us to determine vibrational and anharmonicity constants. 10

6. *(a)* What is Raman effect? Which of the following molecules are Raman active?

H_2, NO, HCl, N_2 4

(b) In a vibrational-rotational spectra, prove that the intensity difference between the maxima of R and P branches is

$$\overset{\max}{R} \quad \overset{\max}{P} \quad 2\ 3583\ \sqrt{BT}$$

where B and T are rotational constant and temperature respectively. 10

UNIT—IV

7. Discuss the rotational structure of three branches (P, Q and R) in electronic transition. On the basis of Fortrat parabola, explain the band-head formation. 14

8. *(a)* State Franck-Condon principle. Describe the quantum-mechanical formulation of Franck-Condon principle. 11

(b) Discuss the isotopic effect on electronic spectra. 3

UNIT—V

9. Describe in detail, how Hartree-Fock method is used to calculate the ground state energy and wave function of a system. 14

10. *(a)* Write the two basic theorems of density functional theory. 5

(b) Explain the merits and demerits of density functional theory over traditional wave function-based method. 6

(c) Write two pure functional and two hybrid functional. 3

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