PG Even Semester (CBCS) Exam., May—2018

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. *(a)* Find the energies of H_2 molecule using the LCAO method and discuss its variations with inter-nuclear distance. 12

(b) Why is the triplet states of H_2 molecule unstable? 2

2. *(a)* What are bonding and anti-bonding molecular orbitals? Explain taking examples of *s* and *p* atomic orbitals. 8

(b) Define bond order. Calculate bond orders for CO, O_2 and N_2 molecules. 6

UNIT—II

3. Discuss in brief Born-Oppenheimer approximation. Discuss the origin of different types of molecular spectra within Born-Oppenheimer approximation. 4+10=14

4. *(a)* Distinguish between the mechanisms of fluorescence and phosphorescence emission. 4

(b) The first line (*J* 0) of the pure rotational spectra of CO molecule appears at 3 84cm ^{1}. Calculate the rotational constant and frequency of transition *J* 5 4 considering the molecule to be a rigid rotator. 5

(c) Highlight the changes that occur in rotational energy level and spectra of a diatomic molecule when passing from rigid to non-rigid molecule (rotator). 5

UNIT—III

5. *(a)* Give the classical theory of Raman effect. 8

(b) "In ordinary Raman effect, intensity of anti-Stokes lines are very weak." Explain. 3

(c) What is the general rule for vibrations or rotations to be Raman active? How does it differ from infrared and microwave activity? 3

6. *(a)* Derive analytically the expression for vibrational-rotational spectra of a diatomic molecule. What are *P*, *Q*, *R* branches? 6+3=9

(b) The fundamental and first overtone of CO molecule undergoing anharmonic oscillation is at 2143 cm^{-1} and 2459·7 cm^{-1}, respectively. Calculate anharmonicity constant and equilibrium frequency. 5

UNIT—IV

7. *(a)* Bring out the salient features of vibrational course structure of molecular electronic system. 5

(b) Why do electronic absorption spectra consist of 'progression'? 3

(c) Explain how intensity of vibrational electronic transitions be accounted by Franck-Condon principle. 6

8. *(a)* Discuss the classification scheme of electronic states of a diatomic molecule. 8

(b) Rotational analysis of one band system is given by

$$24762 \quad 25\,m \quad 2\,1\,m^{2}cm^{-1}$$

Deduce the position of band head, the values of *B* and *B* and degradation of the band (symbols have their usual meanings). 6

UNIT—V

9. Outline the Hartree-Fock method for many-body system and show how it can be used to determine the ground state energy and wave function of such systems. 4+5+5=14

10. Write short notes on the following : 7×2=14

(a) Density functional theory

(b) Hohenberg-Kohn theorem

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