2019/EVEN/08/21/PHY–403/067

PG Even Semester (CBCS) Exam., May—2019

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)* What is LCAO approximation? Illustrate with examples. List the conditions to be satisfied by the contributing atomic orbitals of generate an effective MO. 4+3=7

(b) Compare the MO wave function of hydrogen molecule with that of the valence bond theory (VBT). 3

(c) Discuss the molecular orbital energy-level diagram of homonuclear diatomic molecules. 4

2. Determine the wave functions and total energy of H_2 molecule using the LCAO method. What will be the wave functions of H_2 molecule if the two nuclei are at infinite distance? 12+2=14

UNIT—II

3. *(a)* Considering the molecule as a rigid rotator, discuss the rotational spectra of a diatomic molecule. 9

(b) The J 0 J 1 rotational absorption line occurs at 1 153 10^{11} cycles/sec in $^{12}C^{16}O$ and at 1 102 10^{11} cycles/sec in $^{?}C^{16}O$. Calculate the mass number of the unknown carbon isotope. 5

4. *(a)* Diatomic molecules such as CO and HF will show a rotational spectrum whereas N_2, O_2 and H_2 will not. Why? 2

(b) The intensity of J 0 J 1 is often not the most intense rotational line. Discuss why. 4

(c) What is Born-Oppenheimer approximation? 4

(d) Discuss isotopic effect on rotational spectra. 4

UNIT—III

5. (a) Write the salient features of vibrational spectra of a diatomic molecule. 5

(b) Discuss how the vibrational spectrum of a diatomic molecule enables us to determine the vibrational and anharmonicity constants. 9

6. (a) Explain Raman effect with the help of an energy-level diagram. 7

(b) Discuss the fine structure of infrared bands of diatomic molecules. 7

UNIT—IV

7. (a) Explain Franck-Condon principle. 7

(b) Discuss the vibrational structure of electronic band system in emission spectra. 7

8. Discuss the rotational structure of three branches in electronic transition. On the basis of fortrat parabola, explain the band-head formation. 14

UNIT—V

9. State and prove Hohenberg-Kohn theorems. 14

10. (a) What is electron correlation? 3

(b) What are the post HF methods? 3

(c) Write a note on density functional theory (DFT). 8

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