

10. (a) Write the limitation of Hartree Fock theory. 2
- (b) What is electron-correlation? 3
- (c) Write the usefulness of DFT. 5
- (d) What molecular properties can be calculated using DFT? 4

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**PG (CBCS) EVEN SEMESTER EXAMINATION, 2023**

**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) Derive the energy and wave function of  $H_2$  molecule using LCAO method. 12
- (b) Define bond order. Calculate bond order of  $H_2$  molecule. 2
2. (a) Write the conditions for generating an effective molecular orbital under LCAO method. 2
- (b) Write the electronic configuration of  $N_2$  molecule and  $N_2^+$  ions and (i) explain the type of bonding in them (ii) which one has the longer equilibrium bond length? (iii) which one has the larger dissociation energy? 12

(2)

UNIT - II

3. (a) Write a note on Born-oppenheimer approximation. 7
- (b) The  $J = 0$  to  $J = 1$  rotational absorption line occurs at  $1.102 \times 10^{11}$  cycles/s in  $^{13}\text{C}^{16}\text{O}$  and at  $1.153 \times 10^{11}$  cycles/s in  $^{12}\text{C}^{16}\text{O}$ . Calculate the mass number of the unknown carbon isotope. 5
- (c) What is the main difference between the fluorescence and phosphorescence phenomena? 2
4. (a) Write the salient features of the pure rotational spectra. 5
- (b) The transition  $J = 6$  to  $J = 5$  in OH-radical occurs at  $227 \text{ cm}^{-1}$ . Regarding the molecule to be a rigid rotator, calculate the wavelength of the transition  $J = 17$  to  $J = 18$  4
- (c) Discuss isotope effect on rotational spectra. 5

UNIT - III

5. (a) Show that the vibrational rotational bands are always degraded toward the red. 10

(3)

- (b) The fundamental band and the first overtone of AB molecule is at  $2143 \text{ cm}^{-1}$  and  $4259.7 \text{ cm}^{-1}$ . Calculate  $\omega_e$ ,  $\omega_e x_e$  and vibrational frequency. 4
6. (a) Discuss how the study of vibrational spectrum of a diatomic molecule enables us to determine anharmonicity constant and equilibrium frequency of vibration. 10
- (b) What is Raman effect? What is the condition for a molecule to be Raman active. 4

UNIT - IV

7. (a) Both the red and violet degraded bands are observed in electronic band system. Why? 7
- (b) Discuss vibrational structure of electronic band-system in emission. 7
8. The band head of Q-branch lies always at  $J = -\frac{1}{2}$ , while that of the P - or R - branch may be anywhere. Explain. 14

UNIT - V

9. (a) State and prove Hohenberg-Kohn theorems. 14

( Turn Over )