

OCTOBER 2012

P/ID 40008/PPHH

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Time : Three hours

Maximum : 100 marks

PART A — (10 × 2 = 20 marks)

Answer ALL questions.

1. What are asymmetric top molecules?
2. Outline the effect of isotopic substitution on the rotational spectra of molecules.
3. What are group frequencies?
4. Give the selection rule for perpendicular vibrations.
5. Define polarizability of a molecule.
6. What is the condition for a molecular rotation or vibration to be Raman active?
7. Define electron spin angular momentum.
8. What is hyperfine structure?
9. State Franck-Condon principle.
10. Differentiate between the dissociation energies  $D_e$  and  $D_0$ .

PART B — (5 × 6 = 30 marks)

Answer ALL questions.

11. (a) Discuss about the instrumentation required for microwave spectroscopy.

Or

- (b) Obtain the expression for the rotational energy levels in terms of 'B' and 'J' for a symmetric top molecule.

12. (a) The fundamental and first overtone transition of  $^{14}\text{N}^{16}\text{O}$  are centered at  $1876.06 \text{ cm}^{-1}$  and  $3724.20 \text{ cm}^{-1}$ , respectively. Evaluate the zero point energy and the force constant of the molecule.

Or

- (b) Explain the construction of FTIR spectrometer with a schematic diagram.

13. (a) Give the quantum theory of Raman effect.

Or

- (b) Discuss about the Rotational Raman spectrum of a symmetric top molecule.

14. (a) Write about the atomic quantum numbers, their allowed values and function.

Or

- (b) Discuss about the building up rules which determine how electrons in large atoms occupy orbitals.

15. (a) Write in detail about predissociation.

Or

(b) Discuss about Born-Oppenheimer approximation.

PART C — (5 × 10 = 50 marks)

Answer ALL questions.

16. (a) Obtain the expression for energy of a rigid diatomic molecule.

Or

(b) Discuss about the spectrum of a non-rigid rotator.

17. (a) Discuss about skeletal and characteristic group vibrations in Infrared spectroscopy.

Or

(b) Explain the effect of anharmonicity on the vibrational spectra of diatomic molecules.

18. (a) Describe the techniques and instrumentation for Raman spectroscopy.

Or

(b) Explain the application of Raman spectroscopy in the molecular structural confirmation of water and carbon-di-oxide molecules.

19. (a) Explain about photoelectron spectroscopy. Also write about XPS and UPES spectra of argon.

Or

- (b) Discuss about the orbital and spin contribution of outer shell electrons to the total angular momentum.

20. (a) Write in detail about chemical analysis by electronic spectroscopy.

Or

- (b) Discuss about electronic angular momentum in diatomic molecules with classification of states.
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