

Reg. No. :

Name :

Fourth Semester M.Sc. Degree Examination, May 2020

Chemistry

CH 242(c) – PHYSICAL CHEMISTRY IV

(2016 Admission onwards)

Time : 3 Hours

Max. Marks : 75

SECTION – A

Answer **any two** among (a), (b) and (c) from each question. Each sub question carries **2** marks.

1. (a) Write short note on polarizability transition moment operator?
(b) What is meant by overtones and combination bands?
(c) What is meant by complementarity principle of IR and Raman spectra.
2. (a) Explain the term 'degeneracy'. Give a sketch of the first three energy levels obtained in particle in 3-D cubic box indicating their degeneracy.
(b) Draw radial functions of 2s and 2p orbitals.
(c) What is space quantization? Take azimuthal quantum number $l = 2$ and explain.
3. (a) Set up the Hamiltonian operator for a one dimensional harmonic oscillator.
(b) Define variational parameters.
(c) Explain the term secular determinant.

4. (a) What is meant by trail function?
(b) Write down the time dependant wave equation and explain the terms.
(c) Describe selection rule for harmonic oscillator.
5. (a) What is meant by a force field?
(b) What is a PES (give two view points)?
(c) Construct the Z matrix of CO₂.

(10 × 2 = 20 Marks)

SECTION – B

Answer either (a) or (b) of each question. Each question carries **5** marks.

6. (a) Write down the symmetry selection rule for Raman spectra.
(b) Describe about the allowed and forbidden electronic transition in carbonyl groups.
7. (a) Write short note on angular momentum operator for rigid rotor.
(b) Show that harmonic oscillator wave functions are orthogonal.
8. (a) Solve the Shcrodinger wave equation for Helium atom.
(b) State and prove variation theorem.
9. (a) Discuss about the connection between time-independent perturbation theory and spectroscopic selection rules.
(b) Explain the terms :
- (i) Stark effect
 - (ii) Variational principle
 - (iii) Transition probability.

10. (a) Define polarised and diffused basic sets.
(b) Describe about Hohenberg-Kohn theorems.

(5 × 5 = 25 Marks)

SECTION – C

Answer **any three** questions. Each question carries **10** marks.

11. Find the IR and Raman active vibrations of C_{3V} and T_d point groups.
12. Derive the wave equation for one dimensional harmonic oscillator.
13. Describe and elaborate SCF and variation method.
14. Set up first order perturbation equation for a nondegenerate system and solve to get the expression for first order correction to energy.
15. Describe about strength and weakness of ab initio calculations.

(3 × 10 = 30 Marks)
