

Roll No.

DD-457

**M. Sc. (Second Semester)
EXAMINATION, May-June, 2020**

CHEMISTRY

Paper No. CH—9

**(Quantum Chemistry : Thermodynamics and Chemical
Dynamics—II)**

Time : Three Hours

Maximum Marks : 80

Note : Attempt all the *four* questions. *One* questions from each Unit is compulsory. All question carry equal marks.

Unit—I

1. (a) Write down the role of operators in quantum mechanics, with suitable examples. 10

(b) Prove that : 5

$$\left[x, \frac{d}{dx} \right] = -1$$

(c) Explain the operator ∇ and ∇^2 with suitable example. 5

(B-29) P. T. O.

Or

- (a) Write down the application of determinants in quantum chemistry. 10
- (b) Explain Ladder operators in brief. 5
- (c) The approximate energy of a system is given by $E = K^2 + 2K - 5$ where K is a variational parameter. What value of K leads to the lowest energy and what is the value of the minimum energy ? 5

Unit—II

2. (a) What is thermodynamic probability ? Explain its importance to statistical thermodynamics. 8
- (b) Define the term 'partition function' and discuss its physical significance. 8
- (c) What is statistical weight factor (g) ? Explain with example. 4

Or

- (a) Derive the mathematical form of Fermi-Dirac statistics. 8
- (b) Discuss Einstein models of equation for specific heat of solid at low temperature. Write down its limitations. 8
- (c) Explain permutation with example. 4

Unit—III

3. (a) Discuss the structure of electrified interfaces. 6
- (b) Discuss various theories of structure of electrical double layer. 14

Or

- (a) Derive Tafel equations for overpotential. Discuss its graphical plots. 8

- (b) Discuss Stern model for the electrified double layer. 8
- (c) Explain 'hydrogen electrode' with diagram. 4

Unit—IV

4. (a) What are fast reactions ? Discuss nuclear magnetic resonance method for study of fast reaction. 10
- (b) Derive an expression to calculate K with the help of modifications made by Marcus in the RRK theory. 10

Or

- (a) Give energetics of vary fast reactions. Explain with derivation the nature of relaxation method. 8
- (b) Discuss Riee-Ramsperger-Kassel-Marcus (RRKM) theories for uni-molecular reaction. 8
- (c) Write down the dynamics of molecular motion. 4