MANIPAL
ACADEMY of HIGHER EDUCATION
(Deemed to be University under Section 3 of the UGC Act, 1956)

Reg. No.										

DEPARTMENT OF SCIENCES, II SEMESTER M.Sc (CHEMISTRY)
END SEMESTER EXAMINATIONS, JUNE 2018

Subject: PHYSICAL CHEMISTRY II [CHM 4206]
(REVISED CREDIT SYSTEM-2017)

Time: 3 Hours Date:18-06-2018 MAX. MARKS: 50

Note: (i) Answer **ALL** questions
(ii) Draw diagrams, and write equations wherever necessary

1.A Explain with relevant equation and experimental evidences, wave nature of a particle. If the position of the electron (mass = 9.109×10^{-31} kg) in H-atom could be determined with an accuracy of 0.01 nm, what would be its uncertainty in its velocity? Comment on the result.

1.B Set up the Schrödinger wave equation for a particle rotating on a sphere of constant radius, separate the variables and solve for ϕ equation. **[5+5]**

2.A Write the solution for Schrödinger wave equation for a particle in a box of finite length and infinite barrier. Draw and explain the probability curves for particle in a box for n= 1 to n=3. Show that particle in a box satisfies the Heisenberg uncertainty principle.

2.B Apply molecular orbital theory and elucidate the structure of H_2^+ by quantum mechanical approach. **[5+5]**

3.A State and prove two assumptions of linear variation method. Explain the use of Iterative technique in solving the Schrödinger wave equation for atoms containing multi-electrons.

3 B Apply Huckel molecular orbital theory to elucidate the structure of allyl moiety. Give the graphical representation of Huckel molecular orbitals **[5+ 5]**

4.A Write explanatory note on the following:

(i) Born Oppenheimer Approximation and its application

(ii) Slater type orbitals and Slater Rules.

4.B (i) Calculate the liquid junction potential associated with the following cell :
Ag(s), AgCl(s), HCl ($m_1 = 1.0$, $\gamma_1 = 0.809$) : HCl ($m_2 = 0.05$, $\gamma_2 = 0.830$), AgCl(s), Ag(s), If the transference number of H^+ is 0.83.

(ii) Define emf of a cell. Explain the function of a salt bridge. **[5+5]**

5.A (i) Derive an expression for EMF of electrode concentration cell without transference for gas electrode and amalgam electrode.

(ii) List characteristics of a battery and requirements of a fuel cell.

5.B (i) Derive Nernst equation for measuring EMF of a cell

(ii) Give a brief description of a polymer electrolyte membrane fuel [PEMFC] cell **[5+5]**