M.Sc. - Chemistry
I Semester End Examination - May 2022
Physical Chemistry-I

Course Code: MCH103T **QP Code: 11009**
Time: 3 hours **Total Marks: 70**

Instruction: *Answer Question* ***No.1*** *and any* ***FIVE*** *of the remaining.*

1. Answer any ***TEN questions*** **(2×10 =20)**

a) Examine whether the operator d^2/dx^2 is Hermitian for the function e^{ix}

b) What is J-J coupling?

c) Evaluate [x^, P^$_x$]

d) State variation theorem.

e) What is term symbol? Write the term symbols for Na for ground and exited state.

f) Give a comparative account of spin and angular momenta.

g) The rate constant of first-order reaction was found to be 7.38×10^{-5} s^{-1} at 25^0c. Calculate Arrhenius pre-exponential factor. Given energy of activation of the reaction was 55.5 kJ/mol.

h) Explain the effect of activators on the enzyme activity.

i) Give reasons for the inadequacy of conventional techniques in the study of fast reactions

j) Explain the significance of Gibbs adsorption isotherm.

k) Give Laplace equation and mention the terms involved in it

l) Explain autocatalysis with an example.

2. a) Formulate time-dependent Schrondinger wave equation.
b) State the postulates of quantum mechanics.
c) Explain quantum mechanical tunneling. **(4+ 3+3=10)**

3. a) Formulate the Schrondinger equation for the hydrogen atom in spherical polar co- ordinates.
b) Demonstrate the Stern-Gerlach experiment **(6+4=10)**

4. a) Discuss the kinetics and mechanism of thermal reaction between H_2 and Br_2 molecules.

b) Obtain an equation for the relaxation time for the reversible reaction and explain the temperature - Jump method in the study of rapid reactions. **(5+5=10)**

5. a) Discuss the Lindemann theory of unimolecular reaction rates.

b) Obtain Michaelis-Menten equation for the single substrate-enzyme catalyzed reaction. **(5+5=10)**

6. a) Solve the Schrondinger equation for the simple harmonic oscillator.

b) Derive a general kinetic expression for the acid-base catalysis

c) Explain the quantum mechanical degeneracy. **(4+3+3=10)**

7. a) Apply pertubation theory to electron in a box and find its solution.

b) Explain in detail the transition state theory. How the theory is superior compared to collision theory. **(5+5=10)**

8. a) Obtain Kelvin's equation for the vapour pressure droplet and mention its significance

b) Write about slater determinates.

c) State the characteristics of chain reactions. **(4+3+3=10)**

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