Registration no:

Total Number of Pages: 02 **MSC.I**
FCYC603

6th Semester Regular Examination 2016-17
QUANTUM THEORY
BRANCH(S): Applied Chemistry
Time: 3 Hour
Max marks: 70
Q Code:Z259
Question No.1 which is compulsory and any five from the rest
The figures in the right hand margin indicate marks.

Q1 Answer the following questions: (2 x 10)

a) Write the conditions for the two different wave functions Ψ_A and Ψ_B to be orthogonal and normalized.

b) How is the energy calculated from wave function using Hamiltonian operator?

c) Outline salient features of time independent non –degenerate perturbation theory. Give example of a perturbed and an unperturbed system.

d) What is zero point energy for simple harmonic oscillator? How is it in accordance with Heisenberg's uncertainty principle?

e) Write down the expression for energy of a particle in a three dimensional box of dimensions a ,b and c. Show that when the box becomes cubical the ground state energy becomes equal to three times the particle in one dimensional box.

f) What do you mean by linear operator? On which condition two operators A and B commute?

g) Write two postulates of quantum mechanics.

h) Draw molecular orbital energy level diagram of HF molecule.

i) What is meant by Born Openheimer Approximation?

j) What do you mean by a rigid rotator? Write the Schrodinger wave equation of such rotator.

Q2 a) Setup a wave equation for a particle of mass 'm' moving inside in a one-dimensional box, where the potential energy inside the box is zero and infinite outside and prove that wave functions corresponding to two different eigen states are orthogonal. (6+2)

b) Show that eigen values of Hermitian operator whether real or complex (2)

is always real.

Q3 Write Schrodinger equation for motion of an electron in a Hydrogen like atom in spherical coordinates. Separate the equation into three functions R(r),Y(θ) and Z(ϕ) solve the Z (ϕ)function. (1+5+4)

Q4 a) On the basis of variation theorem show that $\langle \Psi | H | \Psi \rangle \geq E_0$ (6)

b) Derive an expression for the ground state wave function of Helium atom. (4)

Q5 For the microscopic particle exhibiting simple harmonic oscillation set up Schrodinger wave equation and derive an expression $E_n=(n+1/2)h\upsilon$ for quantized energy levels. (4+6)

Q6 Calculate the energy value for hydrogen molecule ion by using LCAO—MO wave function. Draw potential energy curve. How does the calculated value agree with the observed value? (8+1+1)

Q7 Discuss Heitler- London treatment of Hydrogen molecule by VB method. (10)

Q8 a) Write the ground state electronic wave function for N_2 and NO molecule and draw their Molecular orbital energy level diagram. (6)

b) Calculate the bond order of the following species and arrange them in the increasing of bond strength. $O_2^{2-}, O_2, O_2^{+}, O_2$ (3)

c) On the basis of MO theory show that Helium is mono atomic. (1)