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M.Sc. (Chemistry) (Campus) (2015 to 2017) (Sem.-2) PHYSICAL CHEMISTRY-II(QUANTUM AND STATISTICAL CHEMISTRY)

Subject Code : CHL-413 M.Code : 51150

Time: 3 Hrs. Max. Marks: 70

INSTRUCTIONS TO CANDIDATES:

- SECTION-A is COMPULSORY consisting of TEN questions carrying TWO marks each.
- SECTION-B contains SIX questions carrying FIVE marks each and students have to attempt ALL questions.
- SECTION-C contains THREE questions carrying TEN marks each and students have to attempt any TWO questions.

SECTION-A

Determine whether the following operator is linear or nonlinear :

 d^2/dx^2

- Determine whether the following functions are normizable or not over the indicated intervals: e^x (0,∞)
- What is the complex conjugate of the wave function (ψ = 4 + 3i)?
- Write the conditions for two wavefunctions, ψ_i(x) and ψ_i(x) to be orthonormal.
- Arrange the following states (term symbols) for p² configuration in the increasing order of energy: ¹D, ³P and ¹S.
- 6. How many microstates are possible for d³ configuration?
- Write down time independent Schrodinger equation of one dimensional harmonic oscillator.
- Write down the relation between thermodynamic probability and entropy.
- Define the term partition function.
- What is Einstein characteristic temperature? Explain its significance.

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SECTION-B

- Normalise the wave function ψ = cos(nπx/L) over the interval -a<x<a.
- 12. The energy of particle in 3-d box is E = 25h²/8mL². How many degenerate states are possible and also write down the states?
- Write a short note on degenerate perturbation theory.
- 14. Calculate the Bond Orders (B.O.) of O₂⁺, O₂ and O₂⁻ using Molecular Orbital (MO) theory. Which one has the highest bond distance among the above three molecules?
- Define heat capacities at constant pressure and constant volume. Mention the relationship between them.
- Calculate the number of microstates for the distribution of three distinguishable particles in four boxes.

SECTION-C

- Derive the Hückel MO theory for ethylene. Draw simple schematics of the bonding and anti-bonding energy level diagrams.
- Show that if the linear operators A and B have common complete set of eigen functions, then A and B commute.
 - Calculate the probability that a particle in 1-D box of length L is found between 0 and L/2.
- Derive the Bose-Einstein distribution law.
 - Consider 40 molecules divided equally between 4 non-degenerate energy levels. Calculate the thermodynamic probability (W) for this distribution?

NOTE: Disclosure of Identity by writing Mobile No. or Making of passing request on any page of Answer Sheet will lead to UMC against the Student.

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