CLASS: IMSc   SEMESTER : VIII
BRANCH: CHEMISTRY   SESSION : SP/19

SUBJECT: SAC2001 THEORETICAL CHEMISTRY

TIME: 3.00 Hrs   FULL MARKS: 60

INSTRUCTIONS:
1. The question paper contains 7 questions each of 12 marks and total 84 marks.
2. Candidates may attempt any 5 questions maximum of 60 marks.
3. The missing data, if any, may be assumed suitably.
4. Before attempting the question paper, be sure that you have got the correct question paper.
5. Tables/Data hand book/Graph paper etc. to be supplied to the candidates in the examination hall.

Q.1(a)   Calculate the energies and wave functions for a particle of mass 'm' in one-dimensional box of length   [6]
         L (determination of value of A is not required).

Q.1(b)   Treating the π electrons in a conjugated system particle moving in a one-dimensional box, calculate   [6]
         the lowest absorption frequency (in cm^{-1}) and the wavelength (in nm) of absorbed light for the molecule
         of butadiene; the length of the molecule is 0.56 nm. What is the total ground state energy of the
         molecule?

Q.2(a)   Derive the equations for wave function and energy for a particle in a rectangular box of dimensions L_x,   [6]
         L_y and L_z, along the three coordinates.

Q.2(b)   Show that breakdown of degeneracy occurs after distortion along x-axis, in energy in the 2, 1, 1 state.   [6]

Q.3(a)   Derive the equations for wave function and energy of a Harmonic Oscillator (derivation of classical   [6]
         treatment is not required).

Q.3(b)   Compare the results of classical and quantum mechanical treatment of Harmonic Oscillator.   [6]

Q.4(a)   Identify the symmetry elements and point group of NH_3 molecule and then form the group multiplication   [6]
         table of the determined point group.

Q.4(b)   What is great orthogonality theorem? Prove it with respect to irreducible representations deduced for   [6]
         C_{2v} point group.

Q.5(a)   List the various transport processes and write their phenomenolized equations.   [6]
Q.5(b)   Derive an expression for entropy production due to heat flow.   [6]

Q.6(a)   Define and explain: [6]
         (i)   Degeneracy, Macro and microstate, Ensemble
         (ii)   Canonical, Granal canonical and microcanonical ensemble

Q.6(b)   Derive an expression for thermodynamic probability in accordance with Maxwell – Boltzmann statistics.   [6]

Q.7(a)   What is molecular partition function explain with limitations, the multiplication theorem.   [6]
Q.7(b)   Derive the expression for translational partition function.   [6]

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