Indian Association for the Cultivation of Science

(Deemed to be University under *de novo* Category)

Integrated Bachelor's-Master's Program

End-Semester Examination-Autumn 2023

Subject: Energetics and Bonding | *Subject Code(s): CHS1101*

Full Marks: 50 | *Time Allotted: 3 hrs*

Answer any EIGHT questionsμ

All questions carry equal marks (8X6 +2)

1(a) Elucidate a method for determination of the standard entropy change ΔS^0 of a chemical reaction.

(b) Use μ (chemical potential) vs T (temperature) plot for phase equilibrium to explain sublimation temperature.

2. (a) One mole of an ideal monoatomic gas is compressed adiabatically. The temperature rises from 10^0C to 50^0C. Calculate w, ΔE and ΔH. $C_V = \frac{5}{2}R$

(b) Use two laws of thermodynamics to prove $\frac{\partial T}{\partial P_S} = \frac{\partial V}{\partial S_P}$

3. (a) Show that the total adiabatic work in a Carnot cycle is zero.

(b) Show that the Joule -Thomson expansion is iso-enthalpic.

4. (a) Derive Claperon equation.

(b) Use this equation to illustrate a phase diagram and explain triple point.

5. One mole of a gas obeying the equation of state $P(V - b) = RT$ undergoes free expansion. Calculate the change in entropy ΔS.

6. (a) Write down stationary Schrodinger equation for the particle-in- a -box and the boundary conditions for its solution. Solve the equation.

(b) Show that the wave function for the ground state is orthogonal to that for the first excited state.

7. (a) Write down the Hamiltonian for a simple harmonic oscillator and express the corresponding Schrodinger equation in dimensionless form.

(b) Draw and normalize the ground state wave function.

8. (a) Transform L_Z (Z- component of the angular momentum) from cartesian to polar coordinates.

(b) Determine the eigenvalues and eigenfunctions of L_Z under appropriate boundary condition.

9. (a) Draw the radial part of the orbitals 1s and 2s of hydrogen atom. Normalize 1s wave function.

(b)What is the relation between 1s orbital and first Bohr orbit.

10. (a) Use variational method to construct the secular equations for the molecular orbitals for a homonuclear diatomic molecule.

(b) Write down the expressions and draw the contours for the bonding and anti-bonding orbitals obtained from two 1s orbitals.