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 2022

Subject: Energetics and Bonding ***Subject Code(s): CHS1101***
Full Marks: 50 ***Time Allotted: 3 h***

Answer any 10 questions

1. (a) Show that for an ideal gas $\frac{\partial H}{\partial P} = 0$ at constant temperature.

   (b) In a given change of state 40 joule of work is destroyed and the internal energy increases by 170 joule. If the temperature increases by 10 K, what is the heat capacity of the system? (3+2)

2. (a) At 25^0C the coefficient of thermal expansion of water is $2.07X10^{-4}$ *per degree K* and the density is 0.9970 gm/cc. If 200gm of water is raised from 25^0C *to* 50^0C under a pressure of 101 KPa, calculate W.

   (b) When one mole of an ideal gas, $C_v = \frac{5}{2}$R, molar heat capacity, is compressed adiabatically temperature rises from 20^0C to 50^0C. Calculate the change in internal energy ΔE and change in enthalpy ΔH. (2.5+2.5)

3. (a) Show that for a Carnot engine with $w_{cy} = q_1 + q_2$, where q_1 and q_2 refer to the heat flows across the two reservoirs at temperatures T_1 and T_2, respectively then q_1 *and* q_2 must bear opposite signs.

   (b) Derive an expression for Joule-Thomson inversion temperature. (3+2)

4. (a) Show that heat flows from high temperature to low temperature region in an isolated system spontaneously.

   (b) Show that $\frac{\partial T}{\partial P_S} = \frac{\partial V}{\partial S_P}$ (2.5+2.5)

5. (a) α fraction of gas molecules A dissociates at equilibrium to give molecules B as A = 2B.
   How do you determine α, K_P and ΔG^0 ?
   (b) At 300K one mole of liquid water (molar volume 18cc) is subjected to an isothermal increase in pressure from 100KPa to 1000KPa. Calculate ΔG. (3+2)

6. (a) Establish the Claperon equation.

   (b) Show how this equation can be used to construct phase diagram for solid-liquid, liquid-gas and solid –gas transition. (2.5+2.5)

7. Show that the quantum mechanical average value of position operator for a particle moving in a one-dimensional box of length L is L/2 while average over the linear momentum operator is zero. (5)

8. Show that a function $\psi(x) = x \exp(-\alpha x^2)$ can be an eigen-function of the Schrodinger equation for harmonic oscillator for a given value of α. What is the eigen-value ? Draw the function. (5)

9. (a) Normalize the 1s wave function of H-atom
(b) How do you recover Bohr radius from 1s wave function. (2.5+2.5)

10. (a) Show that $-ih\frac{\partial}{\partial\varphi}$ is an hermitian operator.
(b) Calculate the commutator of angular momentum operators $L_xL_y - L_yL_x$.

11. (a) Write down the total quantum mechanical Hamiltonian and electronic Hamiltonian for hydrogen molecule.
(b) Draw the Molecular orbital diagram for N_2 and NO. Calculate the bond orders. (2+3)

12. Establish the secular equations for constructing molecular orbitals of H_2^+ .
Draw the bonding and anti-bonding orbitals. (5)