Indian Association for the Cultivation of Science

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

Integrated Bachelor's-Master's Program

End-Semester (Sem-I) Examination-Autumn 2024

Subject: Energetics and Bonding ***Subject Code(s): CHS 1101***

Full marks: 50 ***Time allotted: 3 h***

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1. (i) Show that molar entropy change on mixing of gases at constant temperature and pressure is given by:

$$\Delta S_m = -\sum_i X_i R \ln X_i$$

(ii) Calculate ΔS_m per litre when pure N_2, H_2 and NH_3 gases are mixed with the final composition 15 % N_2; 55 % H_2 and 30 % NH_3 (all at S.T.P). Given: R= 1.987 $cal\ mol^{-1}K^{-1}$ **[3+3=6]**

2. (i) Show that for 1 mole of Van-der Waal's gas:

$$\mu_{JT} = \left(\frac{\partial T}{\partial p}\right)_H = -\frac{1}{C_{p,m}}\left[b - \frac{2a}{RT}\right]$$

Use the relations: $\left(p + \frac{a}{V^2}\right)\left(V - b\right) = RT$ and $\left(\frac{\partial H}{\partial p}\right)_T = V - T\left(\frac{\partial V}{\partial T}\right)_p$

(ii) Briefly explain under what conditions heating and cooling effects will be observed for real gases except helium and hydrogen. **[4+1=5]**

3. Derive the first and second Thermodynamic Equations of State using Maxwell's relations **[2+2=4]**

4. (i) Derive expressions for work done during isothermal reversible and irreversible expansion of an ideal gas from volume V_1 to V_2 and pressure p_1 to p_2 [where $V_1 < V_2$ and $p_1 > p_2$].

(ii) Explain graphically which work is greater. **[3+2=5]**

5. (i) State the assumptions of Bohr theory.

(ii) Show that the energy of an electron in the n^{th} Bohr orbital can be expressed as

$$E_n = -\frac{\mu Z^2 e^4}{8\varepsilon_0^2 n^2 h^2}$$

where the potential between the electron and the nucleus is defined as, $V(r) = -\frac{Ze^2}{4\pi\varepsilon_0 r}$. **[1+4=5]**

6. When X-ray is scattered by the electrons in a graphite target, derive the shift in the wavelength, $\delta\lambda = \lambda_f - \lambda_i = 2\lambda_c\, sin^2(\frac{\theta}{2})$, where $\lambda_c = \dfrac{h}{m_e c}$ **[5]**

7. (i) What are the basic requirements of an acceptable wavefunction (ψ) in quantum mechanics?

(ii) Using the above requirements, show that the wavefunction for a particle confined in a one-dimensional box of length, a is:

$$\psi(x) = \left(\frac{2}{a}\right)^{1/2} \sin\left(\frac{n\pi x}{a}\right)$$

[2+3=5]

8. Show that the wavefunction for the ground state of a simple harmonic oscillator $\left[\frac{1}{(\pi a)^{1/4}} e^{-\frac{x^2}{2a}}\right]$ leads to an uncertainty in position and momentum equal to $\hbar/2$. Given: $\int_{-\infty}^{\infty} x^2 e^{-ax^2} dx = 1/2a \cdot (\pi/a)^{1/2}$ and $\int_{-\infty}^{\infty} e^{-ax^2} dx = (\pi/a)^{1/2}$ **[5]**

9. Derive the commutator relation of the angular momentum operators, $[\widehat{L}_x, \widehat{L}_y] = i\hbar\widehat{L}_z$. **[5]**

10. (i) Determine with reasons, whether the following are the acceptable wavefunctions in the given intervals:

(a) $1/x$, [-1,1]

(b) e^{-x}, $[0,\infty]$

(c) $\sin^{-1} x$, [-1,1]

(ii) Examine whether the function, $f(x,y,z) = \cos ax.\cos by.\cos cz$ is an eigenfunction of $-\nabla^2$. If it is, find the eigenvalue. **[3+2=5]**