Chemistry (P.G.)
[CBCS]
M.Sc. First Semester End Examination-2023
(Regular & Supplementary Paper)
PAPER- CEM-101

Full Marks: 40 ***Time: 02 Hrs***

The figures in the right-hand margin indicate marks.
Candidates are required to give their answers in their own words as far as practicable.
Illustrate the answers wherever necessary.

Group-A

1. **Answer any four questions.** **4×2=8**

a. From the molecules listed below, find out which one will give rotational spectrum. Mention the reason. (i) N_2 (ii) CCl_4 (iii) CH_3Cl and (iv) SF_6.

b. Existence of zero point energy is a consequence of Heisenberg Uncertainty Principle.

c. The most intense line in the rotational spectrum of $^{79}Br^{19}F$ at 300K is from $J=17\rightarrow18$ transition. Calculate the rotational constant.

d. How does fugacity relate to the chemical potential of a real gas? How can fugacity be estimated graphically?

e. Write the partition function for a two level system where the lower state (ε = 0) is non-degenerate and the upper state (ε) is doubly degenerate.

f. Write down time independent Schrödinger equation for He atom.

g. Find the commutators$[x, p_x]$ and $[x, p_y]$ where p_x and p_y are the linear momentum operators along x and y directions respectively.

Group-B

Answer any four questions. **4×8=32**

2. a) Prove that $(f_2/p_2) = \int_0^{p_2}(\frac{Z-1}{p})\,dp$, Where the terms have their usual meaning. Give the interpretation of the value of fugacity for a vander Waals gas using the above equation.

b) What are the different scales with respect to which the activities of electrolytes are defined for non-ideal solutions? 6+2=8

3. A solution of a free particle Schrodinger equation $(-h^2/8\pi^2 m)\, d^2\Psi(x)/dx^2 = E\, \Psi(x)$ is $\Psi(x) = e^{ikx} = Cos(kx) + iSin(kx)$

a) Derive the expression for energy 'E' and momentum 'p' of the particle.

b) Using the above relations, show that the wave length (λ) is h/p. 4+4=8

4. a) Number of spectral lines are observed in the rotational spectrum of $^1H^{127}I$ and the gap between the successive lines is 13.10 cm^{-1}. Calculate its (i) the rotational constant, B (ii) moment of inertia (iii) bond length (iv) wavelength of J=9 →10 transition.

b) (i) What is Born-Oppenheimer approximation? (ii) Using this, write down the energy expression for combined rotational-vibrational spectroscopy and mention the relevant terms. (iii) What are P, Q and R branches in combined rotational-vibrational spectra? 4+4=8

5. a) Write the ISO definition of nanomaterials. Give classification of nanomaterials on the basis of dimensions. Why do nanomaterials show properties in between that of molecules and bulk materials?

b) Give example of one top down and one bottom up approach for the synthesis of nanomaterials.

c) Write two biomedical applications of electro-spun nanofiber. 4+2+2=8

6. a) Derive the Gibbs-Duhem equation.

b) Show mathematically and graphically that $\Delta_{mix}G$ will have a minimum value and $\Delta_{mix}S$ will have a maximum value at $x = \frac{1}{2}$ when two gases are mixed together. 3+5=8

7. a) What is phase space? Show that number of energy levels in range E to E + dE is given by $g(E)dE = \frac{2\pi V}{h^3}(2m)^{\frac{3}{2}}.E^{\frac{1}{2}}.dE$

b) Four distinguishable molecules are distributed in the energy levels E_1 and E_2 with degeneracy 2 and 3 respectively. Find the number of microstates with 3 molecules in energy level E_1 and one in energy level E_2.

c) The population of proton spin in the highest energy level of a sample at 273k in magnetic field of 1.5 Tesla and 7.0 Tesla are N' and N respectively. Find out the value of $\frac{N'}{N}$. 4+2+2

8. a) For any arbitrary Hermitian operator A, write Heisenberg's equation of motion and hence, find an expression for the force acting on a particle (also known as Ehrenfest's relation). 1+3

b) Check whether $\psi(x,y) = \sin(n_x \pi x / L)\cos(n_y \pi x / L)$ is an eigen function of the 2-dimensional operator $H = -(\hbar^2 / 2m)(\partial^2 / \partial x^2 + \partial^2 / \partial y^2)$ 4