2022

1st Semester Examination CHEMISTRY

Paper: CHEM 101

Full Marks: 40

Time: Two Hours

The figures in the margin indicate full marks. Candidates are required to give their answers in their own words as far as practicable.

Group - A

Answer any *four* of the following questions: $2 \times 4 = 8$

- Classify the following molecules according to their moment of inertia along the three perpendicular directions.
 - (i) SF_6
 - (ii) Allene
- 2. How do you obtain the fundamental vibrational frequency of a diatomic molecule from the microwave spectral data?
- Show the different modes of vibration of an AB₂ type linear molecule and assign the modes of vibrations which are IR active.

- 4. Write down the Cartesian form for \hat{L} using rxp vector.
- 5. Explain the term fugacity. How is it related to the chemical potential?
- 6. Write down the conditions at which Bose-Einstein distribution reduces to Boltzmann distribution.

Group - B

Answer any four of the following questions: $4 \times 4 = 16$

- 7. Write down the rotational Hamiltonian and hence obtain the energy of the following class of molecules.
 - (i) prolate symmetric top, (ii) oblate symmetric top.

Give a comparison of their energy levels.

- 8. Find the degeneracy of the level having energy $\frac{6h^2}{8ma^2}$ for a particle confined in a cubical box whose length of each side is 'a'. If the length of the box along the x-axis is distorted by 'da', then find the fate of the above energy levels.
- 9. What is the energy difference between P_1 and R_0 branches of lines in vibration-rotation spectra? The fundamental and first overtone transitions of $^{14}N^{16}O$ are centred at 1876.06 cm $^{-1}$ and 3724.20 cm $^{-1}$ respectively. Evaluate the equilibrium vibration frequency and the zero-point energy. 1+3=4
- 10. Find out the best composition of a binary mixture.

- 11. Derive the expression which shows the rotational contribution to the molar entropy.
- 12. Calculate the translational partition function for toluene in a volume of 1 m³ at 25°C. (Assuming ideal behaviour of toluene)

Group - C

Answer any *two* of the following questions: $8 \times 2 = 16$

 Use rigid rotator approximation to determine the selection rules and the essential criteria for a molecule to be microwave active.

Recursion relation for Spherical Harmonics is given below:

$$(2J+1)xP_{J}^{M}(x) = (J-|M|+1)P_{J+1}^{M}(x) + (J+|M|)P_{J-1}^{M}(x)$$

14. For any dynamic variable of a quantum mechanical system, deduce the expression of Heisenberg equation of motion. Hence obtain the following expression for particle (mass, 'm') in 1-D box problem.

$$\frac{d < x >}{dt} = \frac{< p_x >}{m}$$

15. Obtain an expression for the thermodynamic probability distribution of particles described by antisymmetric wave functions and arrive at the appropriate quantum statistical distribution law.
8

16. Either

Explain the term activity. Discuss the principles of determination of the activity of a nonvolatile solute by measuring the freezing point depression. 2+6

Or

Using the Maxwell relations derive the thermodynamic equations of state.