2018

M.Sc.

1st Semester Examination

CHEMISTRY

PAPER—CEM-101

Full Marks : 40

Time : 2 Hours

The figures in the margin indicate full marks.

Candidates are required to give their answers in their own words as far as practicable.

Illustrate the answers wherever necessary.

(*Physical Chemistry*)

Group—A

Answer *four* questions taking *one* question from each of these pairs (Q1, Q2), (Q3, Q4), (Q5, Q6), (Q7, Q8) 4×2

1. Define Fourier series for an even periodic function, $f(x)$ in the interval $(-\pi, \pi)$.

2. Which of the following is not a suitable un-normalized wave function for the excited $1s'2s'$ electronic configuration of the Helium atom ?

   (a) $[1s(1)\ 2s(2) - 2s(1)\ 1s(2)]\ \beta(1)\ \beta(2)$

   (b) $[1s(1)\ 2s(2) + 2s(1)\ 1s(2)]\ [\alpha(1)\ \beta(2) - \beta(1)\ \alpha(2)]$

   (c) $[1s(1)\ 2s(2) + 2s(1)\ 1s(2)]\ [\alpha(1)\ \beta(2)]$

   (d) $[1s(1)\ 2s(2) - 2s(1)\ 1s(2)]\ [\alpha(1)\ \beta(2) + \beta(1)\ \alpha(2)]$

3. The letters 'PHILOSOPHY' are written separately one on each card. The ten cards are shuffled. Calculate the probability of obtaing the word 'Philosophy'.

4. Give one example each of Boson and Fermion.

5. What is fugacity co-effiicient ? What is it's utility ?

6. What is the degeneracy of the rotational energy level with $J=4$ for a hetero nuclear diatomic molecule ?

7. Graphically show the size dependence of a property on the number of atoms (X) in the nano dimension.

8. Why thiols are considered as better capping agent?

Group—B

Answer *four* questions taking
one question from each of these pairs
(Q9, Q10), (Q11, Q12), (Q13, Q14), (Q15, Q16) 4×4

9. Find the expression for angular momentum operators $\left(\hat{L}_x, \hat{L}_y, \hat{L}_z\right)$ in terms of linear momentum operators $\left(\hat{p}_x, \hat{p}_y, \hat{p}_z\right)$ and co-ordinator (x,y,z).

Evaluate the commutator, $\left[L_z, L_+\right]$.

10. A freely moving particle of mass, 'm' is confined in a one-dimensional box extending from $x = -2L$ to $x = 2L$. Write down the expression of energy and wave function for its ground state. Find the value of $\langle x \rangle$ in its ground state.

11. Use constrained extremum condition to find the dimension of a rectangular area for which the area is maximum and the circumference is minimum.

12. Calculate the translational partition function for $H_2(g)$ at $1000k$ and $1 atm.$ pressure.

13. Define partial molar quantity. Describe a suitable method to estimate partial molar volume for a binary system. 1+3

14. Calculate the force constant for a *Br–Br* bond, given that the harmonic vibrational wave number of the $^{79}Br^{81}Br$ isotopomer of the bromine molecule is $323{\cdot}2 cm^{-1}$.

15. Write down with explanation the order of increasing wave number of the stretching vibrations of (1) $C-H$ (Alkane), (2) $O-H$ (Alcohol), (3) $C=O$ (Ketone), and (4) $C \equiv C$ (Alkyne)

16. What is Ostwald Ripening process? Write down the expression to estimate the fraction of atoms only surface of the particle (P_s)? 2+2

Group—C

Answer *two* questions taking either odd (Q17, Q19) or even (Q18, Q20) pair of question. 2×8

17. Deduce Schwartz inequality relation. Use this relation to obtain Heisenburg Uncertainty relation for two non-commutating operator. 3+5

18. (a) Derive Sackur-Tetrode equation for molar entropy of a monoatomic gas.

(b) The rotational constant of gaseous *HCl*, determined from micro wave spectroscopy, is 10·59 cm^{-1}. Calculate the rotational partition function of *HCl* at 500*K*. 5+3

19. 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

20. (a) How many normal modes of vibrational are possible for a benzene molecule ? The A, rotational constant of a phosphorus pentafluoride, PF_5, molecule in 3·566 *Hz*. Calculate the lengths of the equatorial $P-F$ bonds. 1+3

(b) A free particle of mass 'm' is moving in a two dimensional square box having length in each side 'a'. How does the energy of its first excited state change upon small change (da) in the Y-direction. Comment on your result. 4