

This question paper contains 4 printed pages]

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S. No. of Question Paper : **5899**

Unique Paper Code : **2173552004**

Name of the Paper : **DSE : Chemistry : IT Skills and Molecular Modelling**

Name of the Course : **Bachelor of Science in Industrial Chemistry**

Semester : **IV**

Duration : **2 Hours**

Maximum Marks : **60**

(Write your Roll No. on the top immediately on receipt of this question paper.)

Attempt 4 questions out of 6.

Each question carries equal marks.

Use of scientific calculator and logarithm table is allowed.

1. (i) What is the purpose of the following excel functions ?
 - (a) $\text{Cos}(x)$
 - (b) $\text{SGN}(x)$
 - (c) $\text{SUM}(C5:C10)$
- (ii) Why the following error messages appear while performing calculations using excel ?
 - (a) $\#DIV/0!$
 - (b) $\#NUM!$
 - (c) $\#N/A$

P.T.O.

- (iii) What is the significance of Molecular Orbitals ?
- (iv) Kohlrausch's law for the molar conductivity Λ_m of a strong electrolyte at low concentration c is given as

$$\Lambda_m = \Lambda_m^\circ - kc^{1/2}$$

where Λ_m° is the molar conductivity at infinite dilution and k is a constant. Explain how k and Λ_m° can be obtained graphically from results of measurements of Λ_m over a range of concentration c .

- (v) What is the relation between the following ?

- (a) Log_{10} and natural log
- (b) Variance and standard deviation
- (c) Slope and intercept.

5×3

2. (i) How the following function can be written in excel ?

(a)
$$F(v) = 4\pi v^2 \left(\frac{m}{2\pi kT} \right)^{1/2} \exp \left(-\frac{mv^2}{2kT} \right)$$

(b) $x^2 + y^2 = 4ax.$ 3

- (ii) Name any *three* softwares used for 3-D optimization and visualization of the molecules. 3

- (iii) Explain the use of trendline function in excel software. Can a trendline be drawn for a function ? If yes, explain with an example. 4

- (iv) Write short notes on the following (any *two*) :

- (a) Semi-Empirical Method
- (b) Global maxima and minima
- (c) Intrinsic reaction coordinate.

5

3. (i) The wavefunction of a 1s orbital of hydrogen atom as a function of distance from the nucleus (r) is given by :

$$\psi_{1s} = \left(\frac{1}{\pi a_0^3} \right)^{1/2} e^{-r/a_0}$$

where a_0 is a constant, Bohr's radius = 52.9 pm. Plot ψ as a function of r and indicate the nature of the graph. 3

- (ii) A particle is described by a wavefunction ψ , where ψ has the form : $\psi = a - ib$. Calculate the probability ($\psi \psi^*$) of finding this particle. 3

- (iii) Explain constants, dependent and independent variables with suitable example of an equation from chemistry discipline. 4

- (iv) Deabbreviate the following terms (any *five*) :

(a) PM3

(b) GUI

(c) CNDO

(d) HOMO

(e) PDB

(f) STO. 5

4. (i) Find the equation of the line passing through the point $(-2, -5)$ and $(1, 4)$. 3

- (ii) Give various methods of energy minimization. 3

- (iii) Solve a pair of the simultaneous equation : 4

$$x + y = 3$$

$$2x + 3y = 4.$$

- (iv) Write short notes on the following (any *two*) :
- (a) AB-initio methods
 - (b) DFT methods
 - (c) Advantages of Molecular Mechanics. 5
5. (i) For the equation $2y - 4x^2 + x = 0$, find slope, point of maxima/minima. 3
- (ii) What is a stationary point ? What kinds of stationary points are of interest to Chemists ? 3
- (iii) What is the function of the following in Excel :
- (a) $\leftarrow .0$
 .00
 - (b) Fill
 - (c) Font color
 - (d) Redo. 4
- (iv) (a) Simplify/Expand the following expressions :
- $$(x^3 + 4x^2 + x - 6)/(x - 1)^2$$
- $$(P + an^2/V^2) (V - nb) = nRT.$$
- (b) What will be the output of the functions in Excel :
- LEN(123456)
- RIGHT("IT SKILL", 5)
- ABS(-15) 5
6. (i) Name any *three* softwares used to draw posters/banners for an event. 3
- (ii) What is the difference between Quantum Mechanics and Molecular Mechanics ? 3
- (iii) Write steps to creating Charts in Excel. 4
- (iv) Give world-wide applications of MS-Excel. 5