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**3 (Sem-5/CBCS) CHE HE1/2**

**2024**

**CHEMISTRY**

**(Honours Elective)**

**Answer the Questions from any one Option.**

**OPTION - A**

***(Applications of Computers in Chemistry)***

Paper : CHE-HE-5016

**OPTION - B**

***(Analytical Method in Chemistry)***

Paper : CHE-HE-5026

*Full Marks : 60*

*Time : Three hours*

***The figures in the margin indicate  
full marks for the questions.***

*Contd.*



### OPTION - A

Paper : CHE-HE-5016

#### (Applications of Computers in Chemistry)

1. Answer **all** questions :  $1 \times 7 = 7$

- (a) Mention a software used in chemistry for drawing molecular structures.
- (b) What is the use of the GOSUB statement ?
- (c) Mention the difference between a variable and a constant.
- (d) What are data processing operations ?
- (e) Define the term ABS.
- (f) What is meant by syntax in BASIC ?
- (g) What is the function of an interpreter ?

2. Answer **all** questions :  $2 \times 4 = 8$

- (a) Convert the decimal number 102.132 to its binary equivalent up to four places of decimal.
- (b) Explain the meaning of the following error messages :  
overflow, syntax error

(c) What is the purpose of the following library functions ? (**any two**)

(i) SGN(X)

(ii) SQR(X)

(iii) RND(X)

(d) Matrix  $A = \begin{matrix} 1.0000 & -0.3000 \\ & -0.2000 & 4.0000 \end{matrix}$

Matrix  $B = \begin{matrix} 0.8000 & 4.0000 \\ 3.0 & 0.7000 \end{matrix}$

Then find  $A \cdot B$ .

3. Answer **any three** questions :  $5 \times 3 = 15$

- (a) What are computer hardware ? Explain the functions of the major computer hardware.
- (b) Write a program in BASIC (using user-defined functions) for finding roots of the following polynomial equation using iterative method using a tolerance of  $10^{-6}$  :  
$$x^3 - x^2 - 3x + 2 = 0$$
- (c) Differentiate between the following :
  - (i) RAM and ROM
  - (ii) Compiler and Interpreter
- (d) What is a search engine ? Explain different search engines with their specific features.



(e) Write short notes on the following : (any two)

(i) ASCII

(ii) DRAW in BASIC

(iii) The error message : Division by zero

4. Answer **any three** questions :  $10 \times 3 = 30$

(a) (i) Convert  $(2A.C1)_{16}$  to binary, decimal and octal numbers. 6

(ii) Write the following expression in BASIC : 4

$$a = \frac{27R^2 T^2}{64P}$$

(b) Make a flow chart for computing normality, molarity and molality of a solution as per the data given.

Normality,  $N = (1000 \times w) / (V \times E)$  ;

Molarity,  $M = (1000 \times w) / (V \times Mol)$  and

Molality,  $m = (1000 \times w) / (Mol \times W)$

where  $W$  is the weight of solvent,  $V$  is the volume of solution,  $E$  is the equivalent of solute and  $Mol$  is the molecular weight of solute.

**Or**

Systems of simultaneous equations are given as

$$A1X + B1Y = C1$$

$$A2X + B2Y = C2$$

Write a BASIC program to compute the values of  $X$  and  $Y$ .

(c) Write a general user-friendly program in BASIC to print the Maximum wavelength of electronic transition arising from HOMO of a conjugated linear polyene ( $-C=C-C=C-----$ ). The program requires only the number of carbon atoms in the molecule. Consider a polyene containing even number  $n$  of carbon atoms with average C—C bond length 140 pm. Assume the linear molecule as one-dimensional box of length  $(140 \times n)$  pm. Energy for  $n$ th

$$\text{energy level, } E_n = \frac{n^2 h^2}{8m l^2}$$

**Or**

Explain the applications of spreadsheets to estimate the following : (any two)

(i) Empirical and molecular formula

(ii) Molecular weight

(iii) Vapour pressure



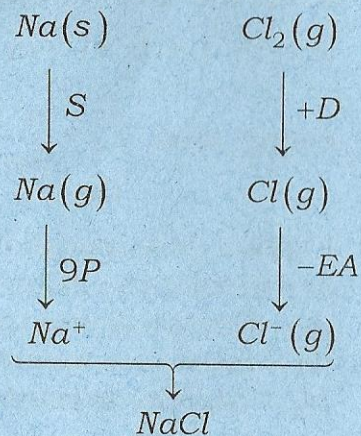
- (d) (i) Explain iteration method for solving a polynomial equation. Write a program using iteration method, to calculate the volume of van der Waals equation of state using BASIC.

Given :  $a = 0.4$ ,  $b = 0.427$ ,  $P = 80$ ,  
 $T = 298$

- (ii) Explain how amount of water in a sample can be determined using thermogravimetry.

- (e) Lattice energy on the basis of Born-Haber cycle can be calculated for a reaction as follows :  
 e.g., for the reaction

$\text{Na}(g) + \text{Cl}_2(g) \xrightarrow{-Q} \text{NaCl}$  this cycle is as follows :



So,  $-Q = S + IP + \frac{1}{2}D - EA - U$ , where  $S$  is the heat of sublimation,  $IP$  is the ionization potential of Na,  $D$  is the dissociation energy,  $EA$  is the electron affinity,  $U$  is the lattice energy and  $Q$  is the heat of formation. On rearranging it  
 $-U = -Q - S - IP - \frac{1}{2}D + EA$  or

$$U = Q + S + IP + \frac{1}{2}D - EA.$$

Draw a flowchart for calculating the lattice energy of  $\text{NaCl}$  on the basis of above Born-Haber cycle.

- (f) (i) Write a program in BASIC to plot the molar conductance  $\wedge_m$  vs  $\sqrt{c}$ . Fit the data to a straight line using the equation

$$\wedge_m = \wedge_m^0 - k\sqrt{c} \text{ and calculate } \wedge_m^0.$$

Conc./M	Molar conductance/ $\text{S m}^2 \text{ mol}^{-1}$
17.68	42.45
10.8	45.91
2.67	51.81
1.28	54.09
0.83	55.78
0.19	57.42

$$\text{Slope} = (N \sum x_i y_i - \sum x_i \sum y_i) / (N \sum x_i^2 - (\sum x_i)^2)$$

$$\text{intercept} = (\sum x_i^2 \sum y_i - \sum x_i y_i \sum x_i) / (N \sum x_i^2 - (\sum x_i)^2) \quad 6$$



- (ii) Explain the Newton-Raphson method for evaluating the roots of a real valued function. 4
- (g) (i) What is FTIR ? Explain how computer application is useful in recording FTIR of a chemical sample ? 6
- (ii) Explain the working of ChemDraw in brief. 4
- (h) (i) Identify and correct the error in the following BASIC statements : 6
- (i) For A\$ = N\$ TO 10
- (ii) DATA, "MONTH", "TIME", -7.12; 81
- (ii) Write the principle of UV-Vis spectroscopy. Explain the application of computers in this spectroscopic technique. 4

## OPTION - B

Paper : CHE-HE-5026

### (Analytical Method in Chemistry)

1. Answer the following questions : 1×7=7
- (a) Why is IR spectrum considered 'finger print' of a molecule ?
- (b) How is standard deviation related to accuracy ?
- (c) What is the relation between transmittance and absorbance ?
- (d) What is the applicability of F-test in data analysis ?
- (e) What are the key components of a thermal analysis system ?
- (f) What is meant by Nernstian behaviour in an indicator electrode ?
- (g) Give an example of lanthanide shift reagent.
2. Answer the following questions : 2×4=8
- (a) What is the function of the monochromator in a spectrophotometer ?
- (b) Describe the source of pH dependence in a glass membrane electrode.



(c) The following values were obtained for the determination of cadmium in a sample of dust : 4.3, 4.1, 4.0, 3.2 mg/g. Should the value 3.2 be rejected ? Given the value of  $Q$  critical is 0.831 for a sample size of four.

(d) What are the factors that determine the mobility of a sample in thin layer chromatography ?

3. Answer **any three** of the following questions :  
5×3=15

(a) Explain with a suitable example how  $pK_a$  values of an indicator can be determined by UV-visible spectroscopy.

(b) Define ion exchange chromatography. Explain the principle involved in it by taking a proper example.

(c) Discuss the factors on which conductance of an electrolytic solution depend.

(d) How does a silicone photodiode detector work ?

(e) Discuss with an example how the strength of an acid can be determined by pH metric titration against a standard base.

4. Answer **any three** of the following questions :  
10×3=30

(a) (i) Define systematic and random errors. How can we reduce systematic errors ?  
2+3=5

(ii) How can we determine enantiomeric composition using NMR spectroscopy ? Explain with a suitable example. 5

(b) (i) Discuss the working principle of atomic absorption spectrometer. 5

(ii) What are the different atomization processes commonly employed in the atomic absorption spectroscopy (AAS) ? 3

(iii) Among atomic emission and atomic absorption, which *one* is more sensitive to flame instability and why ? 2

(c) (i) What are the different mechanisms used in solvent extraction ? What is a chelating reagent ? Discuss its role in solvent extraction by considering a suitable example. 5

(ii) A mixture of  $CaCO_3$  and  $CaO$  is analysed using TGA technique. TG curve of the sample indicates that there is a mass change from 145.3mg to 115.4mg between 500–900°C. Calculate the percentage of  $CaCO_3$  in the sample. 5



- (d) (i) Discuss the principle of colorimetric estimation of a metal ion with an example. 5
- (ii) Discuss the methods for the preparation of solid sample in IR spectroscopy. 3
- (iii) How is a double-beam UV-visible spectrophotometer different from a single-beam instrument ? 2
- (e) What is potentiometric titration ? How one reveals the end point of a potentiometric titration ? Describe the features of a potentiometric titration curve. Discuss the use of potentiometry in food industry and pharmaceutical industry. 1+1+3+5=10
- (f) (i) Explain with an example how Job's method of continuous variation can be used to determine the composition of a metal complex. 5
- (ii) Define the term 'distribution ratio'. How is it different from distribution coefficient ? Explain with example. 3
- (iii) The (+) enantiomer of compound A has a specific rotation value of  $19^\circ$ . If a sample of A contains 40% of the (+) enantiomer and 60% of the (-) enantiomer, what is the observed rotation value ? 2