Total number of printed pages–12

3 (Sem–5/CBCS) CHE HE 1/2

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 : 1×7=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 : 2×4=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 $A = \begin{matrix} 1{\cdot}0000 & -0{\cdot}3000 \\ -0{\cdot}2000 & 4{\cdot}0000 \end{matrix}$

Matrix $B = \begin{matrix} 0{\cdot}8000 & 4{\cdot}0000 \\ 3{\cdot}0 & 0{\cdot}7000 \end{matrix}$

Then find A*B.

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

(a) What are computer hardwares ? Explain the functions of the major computer hardwares.

(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 : 10×3=30

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

(ii) Write the following expression in BASIC : 4

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

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

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.

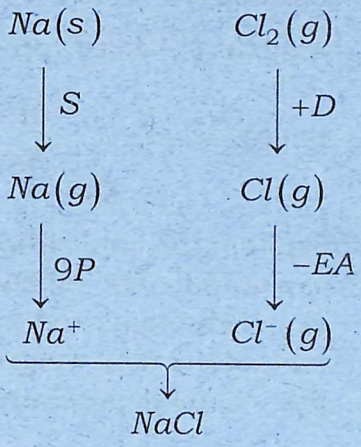
Given : $a = 0.4$, $b = 0.427$, $P = 80$, $T = 298$

(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

$Na(g) + Cl_2(g) \xrightarrow{-Q} NaCl$ 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 *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

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

Conc./M	Molar conductance/S m^2 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

Slope $= \left(N\sum x_i y_i - \sum x_i \sum y_i\right) / \left(N\sum x_i^2 - \left(\sum x_i\right)^2\right.$

intercept $= \left(\sum x_i^2 \sum y_i - \sum x_i y_i \sum x_i\right) / \left(N\sum x_i^2 - \left(\sum x_i\right)^2\right.$ 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 pKa 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 $145{\cdot}3mg$ to $115{\cdot}4mg$ between $500-900^{o}C$. Calculate the percentage of $CaCO_3$ in the sample. 5

(d) (i) Discuss the principle of colorimetric estimattion 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^{o}. If a sample of *A* contains 40% of the (+) enantiomer and 60% of the (–) enantiomer, what is the observed rotation value ? 2