STELLA MARIS COLLEGE (AUTONOMOUS), CHENNAI - 600 086
(For candidates admitted from the academic year 2019 & thereafter)
SUBJECT CODE: 19CH/ME/CC45
B.Sc. DEGREE EXAMINATION, APRIL 2023
BRANCH IV – CHEMISTRY
SIXTH SEMESTER

COURSE: MAJOR ELECTIVE
PAPER: COMPUTERS IN CHEMISTRY
TIME : 3 HOURS   MAX. MARKS: 100

SECTION-A

Answer all the Questions   (30 x1 =30)
I. Choose the correct answers:

1. To obtain symbols from chemdraw _____ menu bar is used
    a) object   b) view   c) structure   d) text

2. The stereochemistry of a compound can be obtained from chemdraw from the tool bar option_____
    a) structure > structure tool > show stereochemistry
    b) structure > view tool > show stereochemistry
    c) structure > object tool > show stereochemistry
    d) structure > edit tool > show stereochemistry

3. The radical cation representation in a molecule can be represented by using _____
    a) query   b) structure   c) templates   d) chemical symbols

4. The shortcut key used to find and replace in a word document is _____
    a) Ctrl+S   b) Shift +S   c) Ctrl+H   d) Shift + H

5. To define a variable in Mathcad _____ is used.
    a) Shift+.   b) Ctrl+.   c) Shift+;   d) Ctrl+;

6. The tool used to label an atom in a molecule is_____

    a)   b)   c)   d)
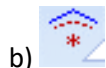
7. A cell is in the fourth column and sixth row of the spreadsheet. It is defined as
    a) D6   b) F4   c) A4   d) B6

8. Using Chemdraw 3D, the _____ in molecules can be determined.
    a) Bond length   b) bond order   c) close contacts   d) all the above

9. The equation of line in a graph using excel is found from _____
    a) Format horizontal axis   b) Title   c) Add Trendline   d) Add Gridlines

10. The elemental symbols for a molecule are obtained by _____
    a) Select the molecule → Analyze → Show elemental symbols
    b) Select the molecule → Tools → Show elemental symbols
    c) Select the molecule → Object → Show elemental symbols
    d) Select the molecule → View → Show elemental symbols

II. Fill in the blanks:

11. _____ tool is used for selecting a text or structure in chemdraw

12. The intercept for equation of line $y = mx$ graph is fixed at _____.
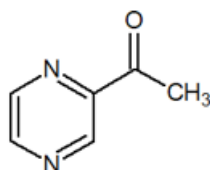
13. The IUPAC nomenclature of is _____.

14. The function used for standard deviation is _____.

15. The short key for inserting matrix is _____

16. The symbol is used for _____

17. In Mathcad, a: 1; 20 implies the values of a are _____.

18. The Gibbs energy of benzoic acid is found to be _____ from chemdraw.

19. A formula is introduced in a cell in MSEXCEL by starting with an _____.

20. The process of removing unwanted part of an image is called _____.

III. State True or False:

21. Cell is a basic unit of a worksheet

22. Pie chart is useful for comparing values over categories

23. Workbook is a collection of work sheets.

24. Line chart is useful for showing trends or changes over time

25. Error bars in a plot are not related to standard deviation.

IV. Answer in a line:

26. What is hyperlink?

27. Give any two uses of EXCEL

28. What is character map window?

29. What is MOPAC?

30. What are the tools present in Math?

SECTION B

V. Answer any five of the following: (5x6 = 30)

31. Using chemdraw (i) draw & name the compound (ii) Evaluate -C-Br, C-N, C-O and N-H bond lengths (iii) Find Minimize energy for the compound given below: [2+2 +2]
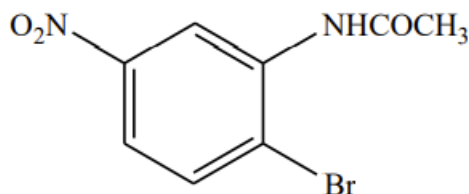
32. he following data were collected as part of a quality control study for the analysis of Na in serum; results are concentrations of Na^+ in mmol/L.140, 143, 141, 137, 132, 157, 143, 149, 118 & 145. Find the mean, median, mode, standard deviation and variance for the above data.

33. Using Mathlab solve the following equations: [3+3]

(i) If $y = \dfrac{x-4}{2\sqrt{x}}$ find $\dfrac{dy}{dx}$ at $x = 4$

(ii) Evaluate: $\displaystyle\int \dfrac{1}{9-4x^2}dx$

34. Calculate molar absorption coefficient by calculation for the following data. Plot a graph of absorbance versus concentration from the following data and calculate the molar absorption coefficient (ε) from slope. A = ε bC, where ε= Molar absorption coefficient Lmol⁻cm⁻, path length= 1 cm and A is absorbance. Graph of A verses C gives Slope = ε.
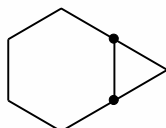
Concentration of Malachite green (molarity) $\times 10^{-4}$	Absorbance A (unitless)
0.2	0.145
0.4	0.254
0.6	0.376
0.8	0.452
1.0	0.559
1.2	0.662
1.4	0.770
1.6	0.818

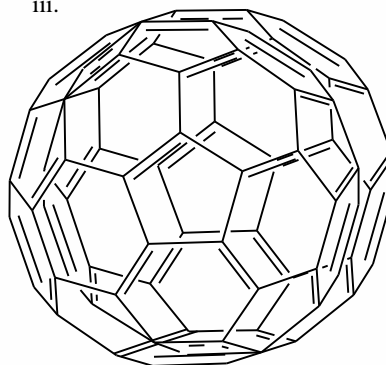35. Draw the following structures using the templates in chemdraw and give the name of template used.
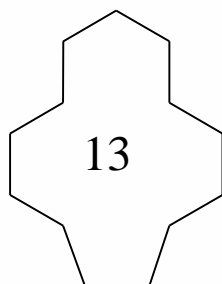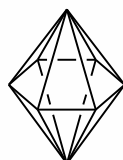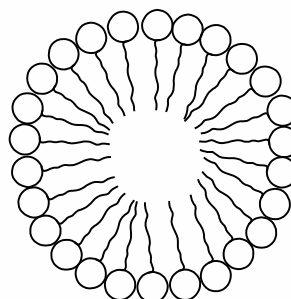
i.

ii.

iii.

iv.

13

v.

vi.

36. Find out the % composition of elements for the following using chemdraw. and plot a bar

H₅C₆——NH₂

aniline

acetamide

(1Z)-1-nitroprop-1-ene
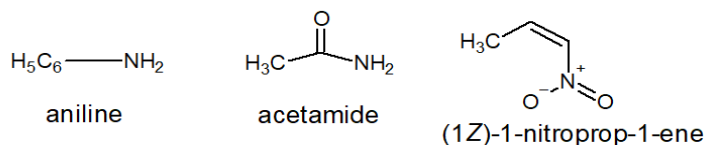
graph % composition of elements vs Compounds using **MS Excel**.

37. Convert the following SI units (Mathcad)   (6x1=6)

   (i) 4.1×10^{-5} mol/L to gal   (ii) 328.56 T to gauss   (iii) 425 atm to psi
   (iv) 178 kW to hp   (v) 785.28 F to pF   (vi) 20.35kW to ehp

SECTION C

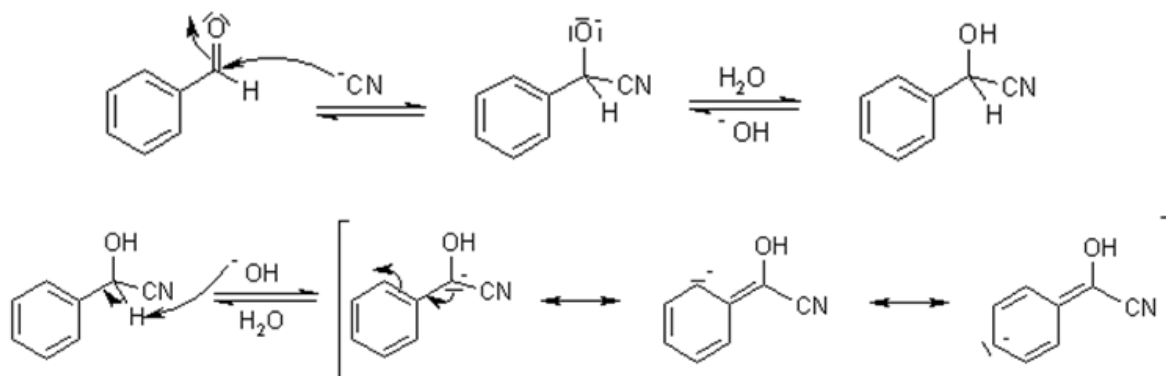**VI. Answer <u>any two</u> of the following:**

38. a. Complete the following table and plot a combined graph of ψ and ψ^2 verses x for n=1
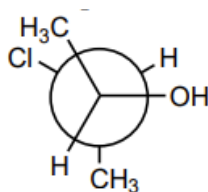   and n=2. Given a = 10nm. (10)
       plots to be plotted
       i. ψ vs x for (n=1, n=2)
       ii. ψ^2 vs x for (n=1, n=2)
       iii. ψ & ψ^2 vs x for n=1
       iv. ψ & ψ^2 vs x for n=2

x nm	$\psi = \sqrt{\dfrac{2}{a}} \sin(n\pi x/a)$		ψ^2	
	n=1	n=2	n=1	n=2
0				
2				
4				
5				
6				
8				
10				

   b. Draw the following mechanism using chemdraw [6]

c. Find dihedral angles of Cl-C-C-H, H-C-C-C, O-C-C-H and C-C-C-H in the given compound [4]

39. a. Using Excel draw the pie chart for the following data. [5]

Method of Analysis	% Chromium
1	36
2	45
3	20
4	7
5	65

b. Find the C-O bond length and bond order in diethyl ether and benzoic acid using Chemdraw 3D. [4]

c. Draw chem 3D for the following compounds and evaluate the solvent accessibility using chemdraw [6]
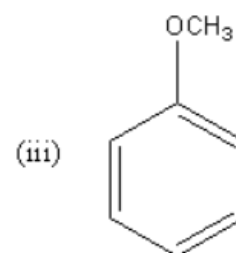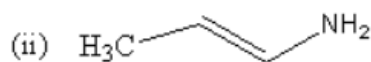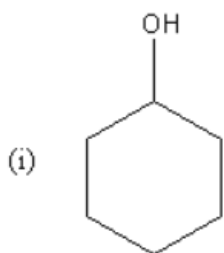
d. Evaluate determinant, inverse, transpose, eigenvalues and eigenvectors for the given matrix [5]

$$A = \begin{pmatrix} 4 & 5 & 9 \\ 1 & 10 & 7 \\ 8 & 15 & 3 \end{pmatrix}$$

40. a. The following data was obtained for the kinetic study of hydrolysis of methyl acetate. Given $T\infty = 49.5$mL. From the table $T_o = 23.2$ml, a = $(T\infty-T_o)$ mL

t in minutes	T_t mL	x= (Tt-To) mL	a-x	log (a/(a-x))	k
0	23.2				
10	23.7				
20	24.2				
30	24.1				
40	24.5				
50	24.9				
60	25.3				

Calculate $k = \frac{2.303}{t}\left[\log_{10}\frac{a}{a-x}\right]$ by calculation. Also evaluate k from a plot of log (a-x) verses t. slope $= -\frac{k}{2.303}$. Compare the k values from graph and calculation. (8)

..6

b. Plot Atomic number of elements vs Ionisation Energy graph from the given data
   using Mathcad   (6)

Atomic number of elements	1	2	3	4	5	6	7	8	9	10
Ionisation Energy of elements kJ/mol	1312	2372.1	520.1	899.3	800.1	1086.2	1402.1	1313.7	1680.8	2080.4

c. Following is the data (specific conductivity for each addition of sodium hydroxide) for
   conductometric titration of a HCl and NaOH. Evaluate the end point from graph from the
   graph. From the end point find the strength of given acid. (4)

Volume of 0.25M NaOH in mL	Specific conductance mS/cm
0	27.8
1	25.6
2	23.45
3	21.98
4	19.32
5	17.47
6	15.22
7	12.48
8	14.45
9	16.87
10	18.64
11	20.44
12	22.39
13	24.78
14	26.99
15	28.21

d. Find $2A-B^2+3C$ from the given matrices. (Mathcad)   (2)

$$A = \begin{pmatrix} 2.5 & 5 \\ 9 & 8.3 \end{pmatrix} \qquad B = \begin{pmatrix} 1.5 & 10 \\ -4.3 & 11 \end{pmatrix} \qquad C = \begin{pmatrix} 6.8 & 11 \\ 7 & 2.5 \end{pmatrix}$$

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