

STELLA MARIS COLLEGE (AUTONOMOUS), CHENNAI - 600 086
(For candidates admitted from the academic year 2019 & thereafter)

B.Sc. DEGREE EXAMINATION, APRIL 2024
BRANCH IV – CHEMISTRY
SIXTH SEMESTER





COURSE : MAJOR ELECTIVE
PAPER : COMPUTERS IN CHEMISTRY
SUBJECT CODE : 19CH/ME/CC45
TIME : 3 HOURS

MAX. MARKS: 100


SECTION-A

Answer all the Questions (30 x1 =30)

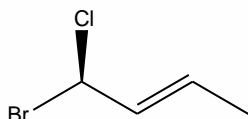
I. Choose the correct answers:

- To define a variable in Mathcad _____ is used.
a) Shift+. b) Ctrl+. c) Shift+; d) Ctrl+;
- The tool used to label an atom in a molecule is _____
a)  b)  c)  d) 
- MS Excel file can NOT be directly exported as _____
a) PDF b) TXT c) PPT d) CSV
- To obtain symbols from chemdraw _____ menu bar is used
a) object b) view c) structure d) text
- The stereochemistry of an 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
- The radical cation representation in a molecule can be represented by using _____ tool
a) query b) structure c) templates d) chemical symbols
- 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
- Steps to introduce a reciprocal of a number in a cell,
a) cell, equal to, formula, math&Trig, Minverse, select number
b) select number, formula, math&Trig, Minverse, cell, equal to,
c) Minverse, select number, cell, equal to,
d) math&Trig, Minverse, cell, equal to, select number, formula
- To copy a selected text _____
a) Ctrl + X b) Ctrl + V c) Ctrl + C d) Ctrl + Z
- In Microsoft Excel spreadsheets, rows are labelled as _____
a) 1,2,3,... b) A,B,C,... c) A1,B1,C1.... d) I,II,III,....

II. Fill in the blanks:

11. The symbol  is used for _____ .

12. In Mathcad, a: 1; 10 implies the values of a are _____.
13. The Gibbs energy of benzoic acid is found to be _____ from chemdraw.
14. A formula is introduced in a cell in MSEXCEL by starting with an _____.
15. The 5th root of 14563 is _____
16. The function used for standard deviation is _____.
17. The IUPAC name of the following compound using chemdraw is _____.



18. The short cut key to obtain a matrix is _____.
19. The intercept for equation of line $y=mx$ graph is fixed at _____.
20. The most common graph used in chemistry is _____.

III. Match the following:

S.No.	A		B
21.	A collection of cells organized in rows and columns where you keep and manipulate the data	a.	Saving data
22.	In MS Excel spreadsheet, Data can be sorted using	b.	1,048,576
23.	In MS Excel, Ctrl+S can be used for	c.	Filter
24.	The best alternative to MS Excel offered by Google Inc.	d.	Worksheet
25.	Row limit of MS Excel 2019	e.	Google sheet
		f.	1,57,648

IV. Answer in a line:

26. Draw the given structure using orbital tool in chemdraw.



27. Give any one use of EXCEL.
28. Find out the % of C, H, N in p-nitro benzoic acid.
29. Mention any four tools in Mathcad?
30. If $A = \begin{pmatrix} 2 & 4 \\ 6 & 8 \end{pmatrix}$ find its determinant.

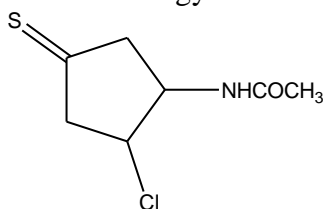
SECTION B

V. Answer any five of the following:

(5x6 = 30)

31. The following data were collected as part of a quality control study for the analysis of iron in serum; results are concentrations of iron in mmol/L.- 236, 237, 265, 243, 254, 244, 237, 240, 248, 242. Find the mean, median, mode, standard deviation and variance for the above data.

32. Using chemdraw (i) draw & name the compound (ii) Evaluate -C-Cl, C-N, C-S, C-O and N-H bond lengths (iii) Find Minimize energy for the compound given below: [2+2 +2]



33. Calculate molar absorption coefficient by calculation for the following data. Plot a graph of absorbance versus concentration using the data and calculate the molar absorption coefficient (ϵ) from slope. $A = \epsilon bC$, where ϵ = Molar absorption coefficient $\text{Lmol}^{-1}\text{cm}^{-1}$, path length = 1 cm and A is absorbance. Graph of A versus C gives Slope = ϵ .

Concentration of Congo red (molarity) $\times 10^{-4}$	Absorbance A (unitless)
0.2	0.164
0.4	0.272
0.6	0.365
0.8	0.459
1.0	0.566
1.2	0.653
1.4	0.751
1.6	0.853

34. Using chemdraw obtain the ^1H and ^{13}C NMR spectrum of benzophenone and malonic acid.

35. Convert the following SI units (Mathcad)

(6x1=6)

(i) 56.23kW to ehp

(ii) 356.2 T to gauss

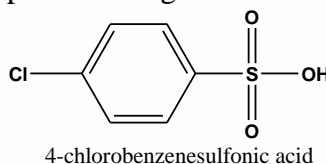
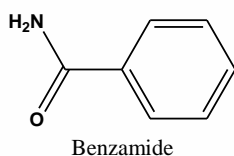
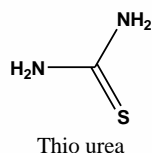
(iii) 5 atm to psi

(iv) 52 kW to hp

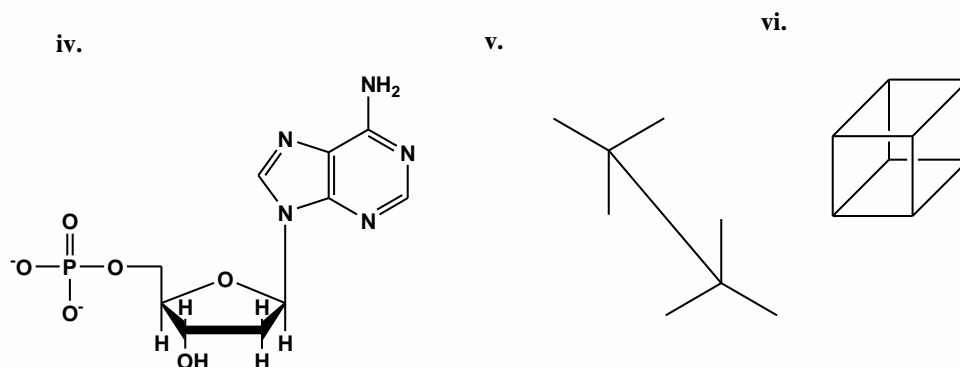
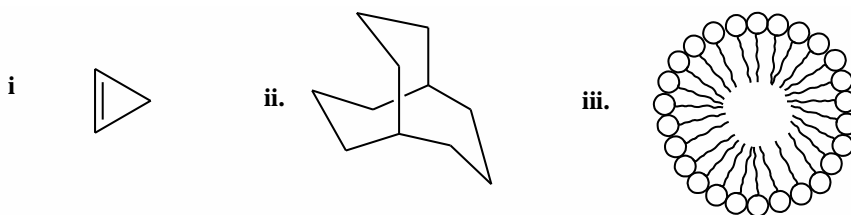
(v) 978 F to pF

(vi) 6.25×10^{-3} mol/L to gal

36. Find out the % composition of elements for the following using chemdraw. and plot a bar graph % composition of elements vs Compounds using **MS Excel**.



37. Draw the following structures using the templates in chemdraw and give the name of template used. (6)



SECTION C

VI. Answer any two of the following:

(2x20=40)

38. a. Find the C-O bond length and bond order in ethyl methyl ketone and Cinnamic acid using Chemdraw 3D. [5]

b. For the organic compound camphor

i) Obtain the solvent accessibility with solvent radius 1.4 and wire mesh surface type.

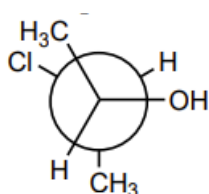
ii) Convert to 3D- ball & stick labeled structure.

iii) Find the dihedral angle of the following: (I) C-C-C-C (II) C-C-C-O (III) Find the close contact: C, O and C, H (6)

c. Using Excel, draw a pie chart for % of C,H,N, O with the given data . [5]

Elements	%
C	33
H	45
O	10
N	7
S	8

d. 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]



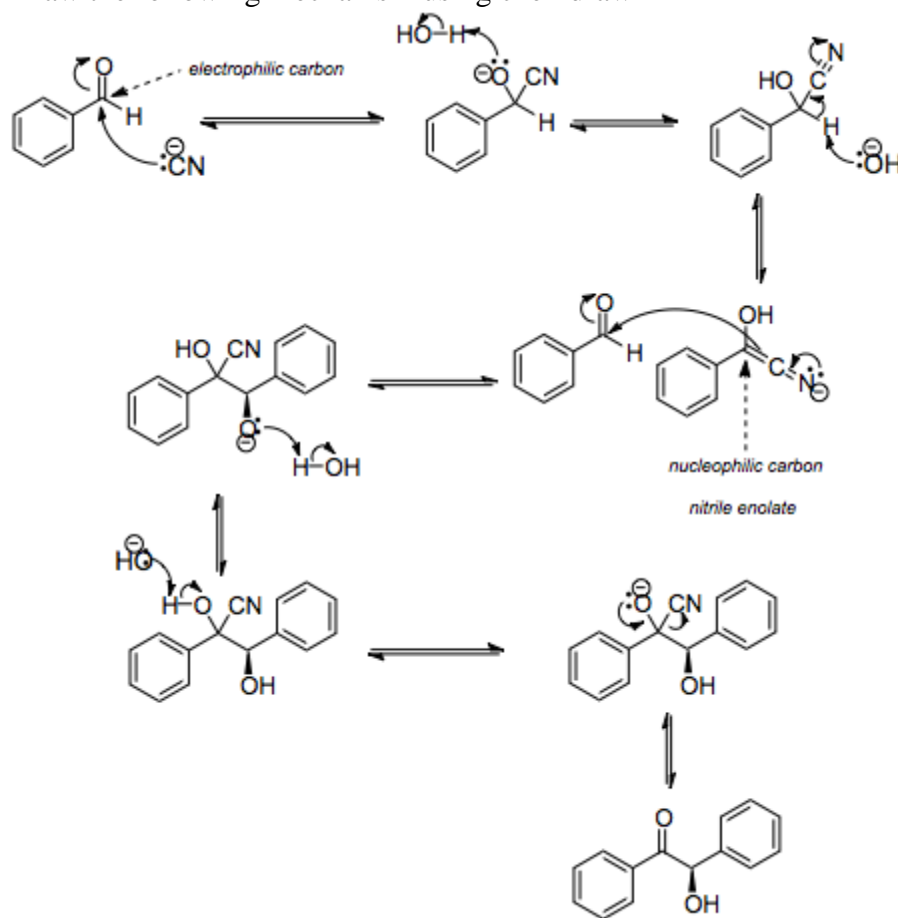
39. a. Complete the following table and plot a combined graph of ψ and ψ^2 verses x for n=1 and n=2. Given a = 100nm. (10)

plots to be plotted - ψ vs x for (n=1, n=2), ψ^2 vs x for (n=1, n=2), ψ & ψ^2 vs x for (n=1) and ψ & ψ^2 vs x for (n=2)

x nm	$\psi = \sqrt{\frac{2}{a}} \text{Sin}(n\pi x/a)$		ψ^2	
	n=1	n=2	n=1	n=2
0				
1				
2				
3				
4				
5				
6				
7				
8				
9				
10				

b. Draw the following mechanism using chemdraw

(10)



40. a. Evaluate determinant, inverse, transpose, eigenvalues and eigenvectors for the given matrix (5)

$$A = \begin{pmatrix} 2 & 3 & 6 \\ 1 & 3 & 5 \\ 2 & 3 & 3 \end{pmatrix}$$

b. From the given data of conductivities at various concentrations of benzoic acid verify Oswald's dilution law. Given: λ_∞ for benzoic acid = 380Scm^2 (5)

Concentration C	Conductivity (k)S/cm $\times 10^{-3}$	$\lambda = \frac{1000 \times k}{C}$	$\alpha = \frac{\lambda}{\lambda_\infty}$	$K_a = \frac{\alpha^2}{(1-\alpha)}C$
0.001	72.4×10^{-3}			
0.002	81.4×10^{-3}			
0.003	93.2×10^{-3}			
0.004	107.2×10^{-3}			
0.005	0.325			
0.006	0.775			
0.007	0.932			
0.008	1.346			
0.009	4.323			
0.010	6.730			

c. Plot Ionisation enthalpies verses Atomic number of elements using Mathcad. (5)

Atomic number of elements	3	4	5	6	7	8	9	10
Ionisation Enthalpies of elements kJ/mol	520	899	801	1086	1402	1314	1681	2080

d. 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. (5)

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
