

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

SUBJECT CODE: 19CH/ME/CC 45
B.Sc. DEGREE EXAMINATION, APRIL 2022
BRANCH IV – CHEMISTRY
SIXTH SEMESTER

COURSE : MAJOR ELECTIVE
TITLE OF PAPER : COMPUTERS IN CHEMISTRY
TIME : 3 HOURS

MAX. MARKS : 100

SECTION –A

Answer all the questions

(30 x 1 =30 Marks)

I. Choose the correct answers:

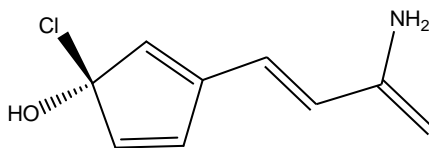
- In MS word _____ is used for quick access to commonly used commands and tools.
a) status bar b) tool bar c) title bar d) menu bar
- Ctrl + Right Arrow is used to move the cursor to _____.
a) end of the line b) end of the document c) one word right d) one paragraph down
- To copy a selected text _____
a) Ctrl + X b) Ctrl + V c) Ctrl + C d) Ctrl + Z
- To define a variable in Mathcad _____ is used.
a) Shift+. b) Ctrl+. c) Ctrl+; d) Shift+;
- A cell is in the fifth column and fifth row of the spreadsheet. It is defined as
a) D6 b) F4 c) E5 d) B6
- What type of chart is useful for comparing values over categories?
a) pie chart b) line chart c) scatter chart d) column chart
- To enter the range of variables in Mathcad _____ is operated
a) Ctrl + ; b) ; c) Ctrl + : d) :
- The chemical analysis window in chemdraw gives _____ of a molecule
a) dipole moment b) m/e c) polarizability d) boiling point
- To insert matrix the short cut key is _____
a) Ctrl + M b) Ctrl + \ c) Ctrl + d) Ctrl + -
- CHEMDB is a _____ online source
a) spectral database b) chemical database c) XRD database d) drug designing

II. Fill in the blanks :

11. The dipole moment of 3-chlorocyclohex-1-ene is _____

12. The 2nd derivative of $y = \log(x^2 + 1)$ is _____

13. The IUPAC name of



14. The O-H bond length

in ethanol is

15. A Excel file is called a _____

16. Ctrl + R is used _____

17. Functions in MS Excel must begin with _____

18. The applied magnetic field 107.85 G is _____ T

19. Convert 35.85 radians to _____ degrees

20. The equation of line in a graph using excel is found from _____

III. Match the following:

21. Query tool

A. MS Excel – Home tab

22. Symbolics

B. F4

23. Conditional formatting

C. Reaction map

24. Bond angles

D. Mathcad

25. Repeat last action

E. Analyse

IV. Answer in one or two lines:

26. What is place holder?

27. What is MOPAC ?

28. How to edit the active cell ?

29. How to obtain the chemical properties from chemdraw?

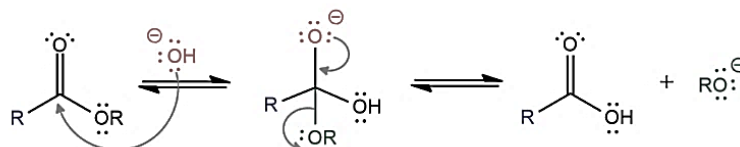
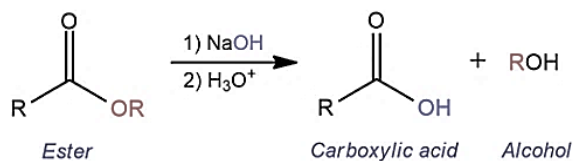
30. What is CAS registry?

SECTION -B**V. Answer any FIVE of the following:**

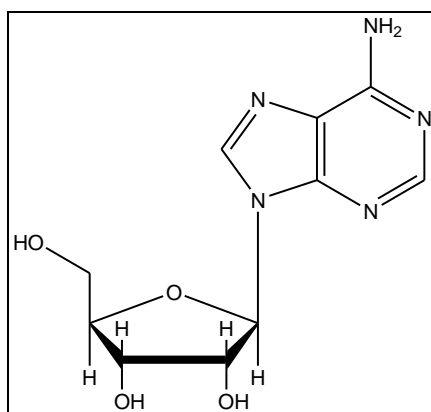
(5 x 6 = 30 Marks)

31. The following results were obtained for the analysis of Magnesium in a sample Volumetrically. 20.3, 20.4, 20.3, 20.4, 20.4, 20.2 and 20.4. Evaluate the following using MSEXCEL: Mean, Deviation, Absolute error, Standard deviation, Variance

32. a) Draw the following reaction scheme using chemdraw: (3 Marks)



b) Using the template in chemdraw, draw the following structure: (3 Marks)



33. a) Plot a graph on Atomic number Vs Ionisation Energy of 3d series of transition metals. (Mathcad) (3 Marks)

At. No.	21	22	23	24	25	26	27	28	29	30
IE kJ/mol	631	658	650	653	717	759	758	737	745	906

b) 1 mol of ideal gas at 300 K is compressed isothermally under the external pressure of 200 atm. Calculate W if the initial and final pressure of the gas is 2 atm and 100 atm.
 Ideal gas Equation : $V_1 = nRT/p_1$; $V_2 = nRT/p_2$; $W = p(V_2 - V_1)$ (Mathcad) (3 Marks)
 $n = 1 \text{ mol}$; $R = 8.2057 \times 10^{-5} \text{ atm m}^3 \text{ mol}^{-1} \text{ K}^{-1}$;
 $p_1 = 2 \text{ atm}$; $p_2 = 100 \text{ atm}$; $T = 300 \text{ K}$

34. a) Determine the % of C,H and O for the following compounds using chemdraw (3 Marks)

(i) Acetaldehyde (ii) 3-Methyloxiran-2-ol (iii) Methylbutyrate

b) From the above data plot a 3D bar graph of Compounds vs % of C,H and O using MS Excel sheet (3 Marks)

35. Determine the following parameters for (*1R*)-3-chlorocyclopentanol (2+1+1+1+1 Marks)
 (i) Bond distances of C-Cl, C-O and O-H (ii) Dihedral angles of Cl-C-C-H and O-C-C-H
 (iii) Non-bond distances of O,H and Cl,H (iv) Minimize energy of the molecule
 (v) Solvent accessible surface the molecule.

36. What is molinspiration software? Explain its applications ?

37. a) Determine the eigenvalues, eigenvectors and determinants for the given matrix.

(Mathcad) (3 Marks)

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

- b) An organic compound has been prepared by different methods. The actual and theoretical yield is given. Calculate the percentage yield and plot a pie chart.

(MS Excel) (3 Marks)

Methods	Actual yield(g)	Theoretical yield(g)
1	2.8	5
2	4.62	7.5
3	4.25	5
4	8.15	10
5	2.82	4

$$\text{Formula : Percentage yield} = \frac{\text{Actual yield}}{\text{Theoretical yield}} * 100$$

SECTION- C

38. a) In the experiment of study of kinetics of acid hydrolysis of methyl acetate the following result were obtained. The initial concentration in titration value $a = 28.4 \text{ cm}^3$. It was found that the at infinite time the reading was found to be 54.8 cm^3 . Find the mean K. (MS Excel) (6 Marks)

t (minutes)	x (cm ³)	a-x	$k = \frac{2.303}{t} \log \frac{a}{a-x}$ min ⁻¹
0	26.4		
10	26.9		
20	27.3		
30	27.7		
40	28.1		
50	28.5		
60	28.3		
70	28.6		

b) Find out the chemical properties of chloroacetone, N,N-dimethylformamide and lactic acid using chemdraw (3 x 2 = 6 Marks)

c) The wave function is given by $\psi = A \sin [n\pi x/a]$, where $A = 1/\sqrt{2}$ and $a = 1$ nm. For different values of x [in nm] = 0, 0.1, 0.2 -----, 0.8, 0.9, 1.0. Plot a graph of ψ versus x and ψ^2 versus x . (Mathcad) (8 Marks)

39. a) Calculate the relative populations including the degeneracy, of the rotational energy levels of a diatomic molecule. For the J values from 0 to 15. The rotational constant is $B = 5 \text{ cm}^{-1}$.

$$\text{Formula : } \frac{N_J}{N_0} = (2J + 1) \exp\left(\frac{-BJ(J+1)hc}{kT}\right)$$

Where, $h = 6.626 \times 10^{-34} \text{ Js}$; $c = 3 \times 10^{10} \text{ cm/s}$; $k = 1.381 \times 10^{-23} \text{ JK}^{-1}$; $T = 300 \text{ K}$ (MS Excel) (6 Marks)

b) Evaluate the following : (Mathcad) (3 x 2 = 6 Marks)

(i)
$$\int \frac{e^x}{1 + e^{2 \cdot x}} dx$$

(ii)
$$\int_0^{\frac{\pi}{2}} \sin(x) \cdot (4 \cdot \cos(x)) \cdot e^{2 \cdot \cos(x)+1} dx$$

(iii)
$$\int \sqrt{x} \cdot (x^2 + 1) \cdot \left[(2) \cdot \frac{4}{\sqrt{x}} + \frac{1}{\sqrt{x}} \right] dx$$

c) Plot a graph on Maxwell's Distribution of velocities at two different temperatures at 27°C and 227°C for Nitrogen molecule representing X axis as Velocity (c) and Y axis as Probable velocity (p) by using the below given data (Mathcad) (8 marks)

c x 10⁻² (m/s)	0	1	2	2.5	3	4	5	6	7	8	9	10	11	12
Probable velocity p(c) x 10⁻⁴	0	2.84	9.6	13.2	16.3	19.6	18.5	14.3	9.4	5.3	2.6	1.1	0.41	0.13

c x 10⁻² (m/s)	0	1	2	3	4	5	6	8	10	12	14
Probable velocity p(c) x 10⁻⁴	0	1.35	4.88	9.27	13.02	15.02	14.94	10.34	4.81	1.57	0.37

40. a) What is KEGG LIGAND database ? Explain its applications. (10 Marks)

b) Phosphorescence emission of Acetone-d₆ (0.05M) in Acetonitrile at 20°C was measured at 450 nm. Calculate the rate constant for the emission and also calculate the average life time of triplet state of acetone by plotting a graph on log I Vs time (μ sec) from the following data.

time (10⁻⁶ sec)	20	32	40	60	80	100	120	140
Intensity (I)	5.5	4.6	4.0	2.9	2.1	1.5	1.05	0.75

Obtain slope from the graph and substitute in $k = -\text{slope} \times 2.303$ to find the rate constant.

To obtain Average life of triplet state take the reciprocal of k. (Mathcad) (6 Marks)

c) Solve the following equations using matrix (4 Marks)

$$x + y - z = -3$$

$$2x - 3y + 4z = 23$$

$$-3x + y - 2z = -15$$
