STELLA MARIS COLLEGE (AUTONOMOUS) CHENNAI-86
(For candidates admitted during the academic year 2015–16 & thereafter)

SUBJECT CODE: 15CH/ME/CC55

B.Sc. DEGREE EXAMINATION, NOVEMBER 2019
BRANCH IV- CHEMISTRY
FIFTH SEMESTER

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

SECTION – A (30x1=30)

ANSWER ALL THE QUESTIONS:

I. Choose the correct answer:

1. _____ is the correct function name to print today's date and time in Excel
   a) TODAY() b) DATE() c) NOW() d) TIME()
2. _____ is the short cut key to change caseof a word / paragraph / a line in Word Document
   a) SHIFT+F3 b) ALT+SHIFT+F3 c) CTRL+SHIFT+F3 d) CTRL+ F3
3. What punctuation is used to signal the beginning and end of code blocks?
   a) { } b) -> and <- c) BEGIN and END d) (and)
4. What is the short cut key to find the meaning of a selected word in Word Document
   a) CTRL+F3 b) SHIFT+F7 c) SHIFT+F2 d) SHIFT+F5
5. Which of the following is a correct comment?
   a) */ Comments */ b) ** Comment ** c) /* Comment */ d) { Comment }
6. To define a variable in Mathcad _____ key is used
   a) SHIFT +. b) CTRL+. c) SHIFT +; d) CTRL+;
7. To obtain a matrix _____ must be typed
   a) SHIFT+M b) CTRL+M c) MAT() d) SHIFT+Matrix
8. To determine the % of elements in a compound _____ tool is used
   a) Object → Analysis window b) View → Analysis window
   c) Structure → Analysis window d) Edit → Analysis window
9. Solvent accessible surface of a molecule is obtained from _____ tool bar
   a) View b) Analyse c) MM2 d) MOPAC
10. For unit conversions _____ short cut key is used in Mathcad
    a) CTRL+L b) CTRL+C c) CTRL+U d) CTRL+X

II. Fill in the blanks:

11. _____is the function to find out maximum among the numbers in Excel.
12. The correct syntax for an if statement _____.
13. _____ is the menu option to sort the table in Excel.
14. _____is the short cut key to open a file in Word or Excel.
15. _____ is the boolean operator for logical-and.
16. _____ punctuation ends most lines of C code.
17. _____ template is used to draw in Chemdraw 
18. MOPACis _____.
19. To replace a word in a whole of the document by another word _____ shortcut key is used.
20. _____ is used to open the **Save As** dialog box.

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III. State whether True or False:

21. The correct value to return to the operating system upon the successful completion of a program is -1.
22. To select the whole document in Word Document CTRL+A is used.
23. The correct operator to compare two variables is **==.**
24. Trend line is added in scatter diagrams to fit the line.
25. ALT+N open a new tab.

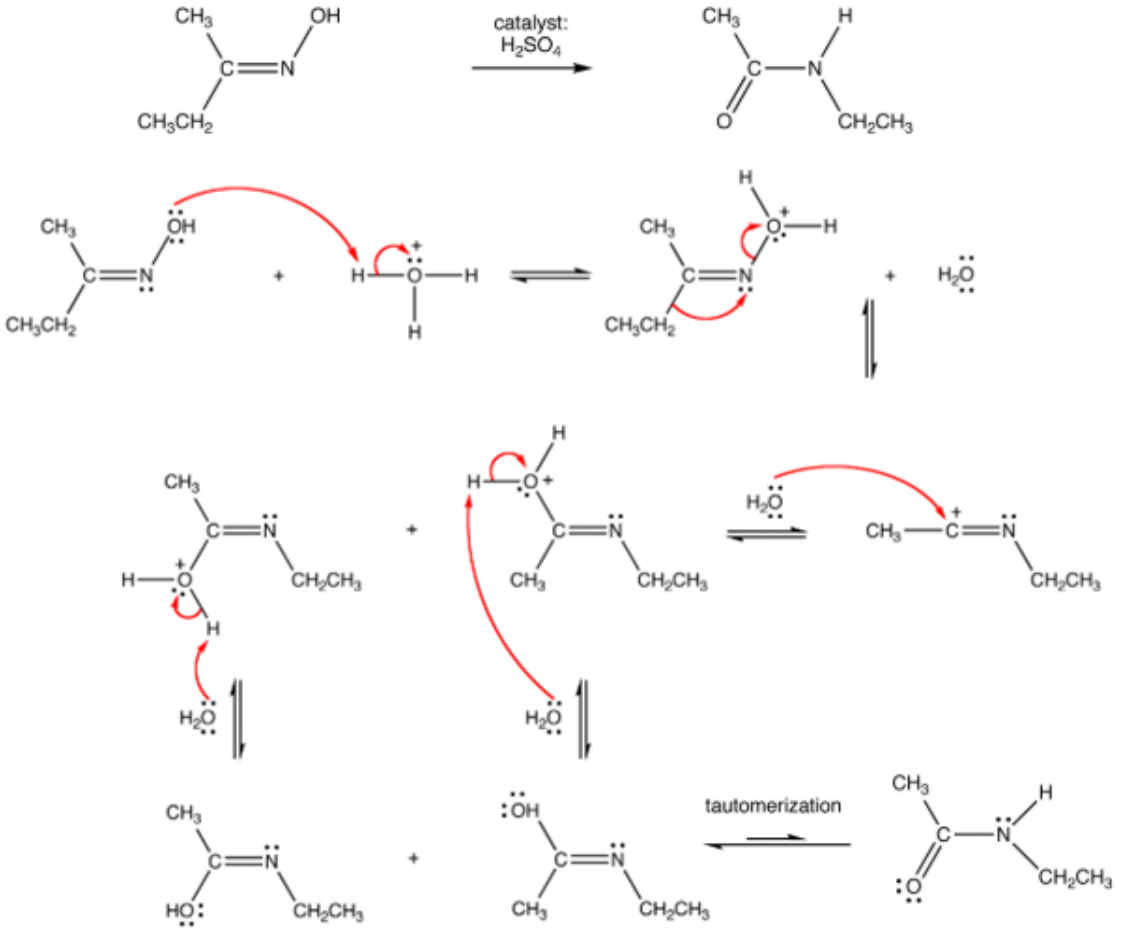
IV. Answer in one or two sentences:

26. What is the use of Format Painter?
27. What is the only function of all C programs must contain?
28. Write a formula to sum up the values of cell A1 and cell B1 and result in cell C1 ?
29. What is the menu option to insert a new table in Word document?
30. Give one application of surface plot in Mathcad.

SECTION B

ANSWER ANY FIVE QUESTIONS: (5x6=30)

31. Draw the reaction scheme and mechanism which is given below using **chemdraw**: (2+4 = 6)



32. Evaluate the following expressions using **Mathcad**: (2x3 = 6)

(i) $I(x) = \int \frac{x^3}{1+x^8}\,dx$ (ii) $f(x) = \int \frac{4\cdot\sin^{-1}\cdot x}{\sqrt{1-x^2}}\,dx$ (iii) $y(x) = \int \sin^4\cdot x\cdot\cos(x)\,dx$

33. Construct a vapour pressure curve for naphthalene at different temperatures from the following data given below using **Mathcad**. (Label the axes and title the plot)

Temp (K)	**273**	**285**	**300**	**325**	**340**	**350**	**353**	**375**	**400**	**450**	**475**	**500**	**550**	**575**
log *p*(mm)	**-2.2103**	**-1.6352**	**-0.9809**	**-0.0247**	**0.4815**	**0.7949**	**0.8825**	**1.33**	**1.74**	**2.43**	**2.72**	**2.98**	**3.43**	**3.61**

34. a. Obtain $C_2H_5^{\bullet}$ and $C_2H_3O^{\bullet}$radical species from butyraldehyde using mass fragmentation tool in **Chemdraw.** (3)

b. Determine the chemical properties of benzene and carbontetrachloride using **chemdraw**. (3)

35. a. Amount of Nickel present in different steel materials was estimated and the data is given below. (4)

Samples	S1	S2	S3	S4	S5	S6	S7	S8
Wt. of Ni in different steel materials (µg)	1.58	0.89	2.31	1.98	4.65	0.75	1.55	2.76

Find (i) Average (ii) Standard deviation (iii) Variance
(iv) Median from the above data using **MS Excel sheet**

b. Calculate the energy of a photon associated with light of wavelength 230nm. **(MS Excel sheet)** (2)

Formula : $\nu = \frac{c}{\lambda}$; **E = hν**

λ= 230 nm ; c = 3.0 x 10^8 m/s ; h = 6.63 x 10^{-34}Js

36. a. Calculate the magnetic moment (BM) for the given metal ions using excel sheet. **(MS Excel sheet)** (2)

Metal ions in complexes	Ti^{3+}	V^{3+}	Cr^{3+}	Cr^{2+}	Mn^{2+}	Co^{2+}	Fe^{3+}	Mn^{3+}	Cu^{2+}
Number of spin free electrons (*n*)	1	2	3	4	5	3	5	4	1

Formula:**Magnetic moment (BM) =** $\sqrt{n(n+1)}$

b. Construct a pie chart for the product yield of ethylbenzoate by different methods. **(MS Excel sheet)** (4)

Methods	Actual Yield	Theoretical yield
M1	5.8	6.0
M2	20.5	22.5
M3	43.4	40.5
M4	17.5	18.0
M5	12.5	13.0

Formula:**Percentage Yield=** $\frac{Actual\ yield}{Theoretical\ yield}$ **x 100%**

37. a. (i) If $y = x^2 \log x$, find $\frac{d^3y}{dx^3}$ (ii) If $y = \frac{x}{a^2+x^2}$, find $\frac{dy}{dx}$ **(Mathcad)** (2x1.5 = 3)

b. Convert the following using **Mathcad**: (3)
(i) 15Pa to torr (ii) 20 Faraday to pico Faraday (iii) 105 pounds to kg

SECTION C

ANSWER ANY TWO QUESTIONS: (2x20=40)

38. a. The following data obtained for the temperature-dependence of the equilibrium constant of an inhibitor binding an enzyme. Plot a graph of **ln *Kc* vs (1/T) x 1000** and determine the slope. From the slope calculate the values of $\Delta H°$, $\Delta G°$ and $\Delta S°$ for this process at 298 K (**MS Excel sheet**) (10)

T (K)	289	294.1	298	304.9	310.5
Kc $x10^7$	7.25	5.25	4.17	2.66	2.01

Formulas: $\Delta H° = -$ slope $x10^3$ x R (R = 8.314 x 10^{-3} kJ/K/mol)

$\Delta G° = -RT\ln Kc$ (R = 8.314 x 10^{-3} kJ/K/mol ; T =298 K ; lnKc = 17.5460)

$\Delta S° = (\Delta H° - \Delta G°) / T$ (T = 298 K)

b. Write a C-program to find the molecular weight for a compound containing C, N, H and O. Given molar mass of C = 12, H = 1, O =16.0, N = 14. (5)

c. Draw the Histogram for the particle size distribution of nanoporous of Pd-Ptdata using **Mathcad**. (5)

Particle size of nanoporous of Pd-Pt		
80	5	15
60	15	25
45	25	30
75	5	20
90	5	5

Frequency %	5	15	25	35	45	55	65	75	85

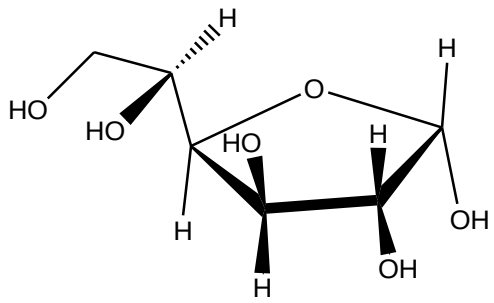
39. a. **Using Chemdraw:**

(i) Convert name to structure of the given compounds: (2x1.5 = 3 Marks)

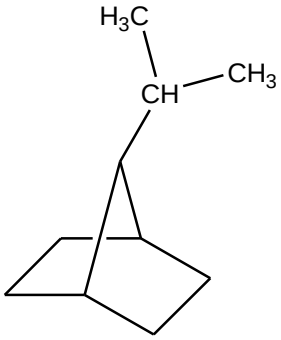
a) pyrrolidine-2-carboxylicacid b) 3H-indene-4-carbaldehyde

(ii) Convert structure to name for the given compounds: (2x1.5= 3 Marks)

a)



b)



(iii) Convert 2D structure of phenylacetate to 3D ball and stick structure, label, number the elements and find the dipole moment of the molecule. (2+2+2)

b. If $A = \begin{pmatrix} 1 & 2 & 3 \\ 0 & 5 & 7 \\ 6 & 8 & 9 \end{pmatrix}$ $B = \begin{pmatrix} 2 & 0 & 3 \\ 3 & 0 & 5 \\ 5 & 7 & 0 \end{pmatrix}$

Apply Mathcadto (i) Evaluate 2A-3B (2)
(ii) Find the determinant of matrix A and B , inverse of matrix B and transpose of matrix A. (4)
(iii) Determine the eigenvalues and eigenvectors of 2A-3B. (2)

40. a. Find (i) the bond length of enol OH , carboxyl OH , C-O of benzene and C-O of carbonyl (ii) bond angle of Carbonyl O-C-O of carboxylgroup (iii) dihedral angle of O-C-C-C (iv) Close contacts of C-O-H of carboxyl group**using chemdraw** (4+2+2+2)

b. Obtain ^{1}H NMR spectrum of furan-2-carbaldehyde from **Chemdraw**(3)

c. Phosphorescence emission of Acetone-d_6(0.05M) in acetonitrile at 20°C was measured at 450 nm.

t (μ sec)	20	32	40	60	80	100	120	140
log *I*	0.74	0.66	0.60	0.46	0.33	0.18	0.025	0.12

(i) Plot a graph of **log *I* vs *t(μ sec)*** and obtain the slope by **Curve Fitting method from Mathcad.** Label the graph and the axes. (4)
(ii) From the slope calculate the rate constant of the reaction using the formula: k = -slope x 2.303 . (2)
(iii) Calculate the average life of triplet state of acetone = 1/k . (1)

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