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 2017
BRANCH IV- CHEMISTRY
FIFTH SEMESTER

COURSE   : MAJOR ELECTIVE
PAPER   : COMPUTERS IN CHEMISTRY
TIME   : 3 HOURS   MAX.MARKS : 100
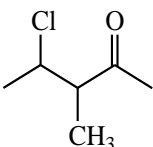
SECTION – A   (30x1=30)

ANSWER ALL THE QUESTIONS:
I. **Choose the correct answer:**

1. Paper spreadsheets can have all the same advantages as an electronic spreadsheet except which of the following?
    a) Rows and columns   b) Headings   c) Speed   d) None

2. What's a quick way to extend these numbers to a longer sequence, for instance 1 through 20?
    a) Select both cells, and then drag the fill handle over the range you want, for instance 18 more rows
    b) Select the range you want, include both cells, point to fill on the Edit menu, and then click down.
    c) Copy the second cell, click in the cell below it, on the standard toolbar click the down arrow on the Paste button, and then click Paste Special
    d) All of above

3. Which of the following is not a font style?
    a) Bold   b) Italics   c) Regular   d) Superscript

4. Using Find command in Word, we can search?
    a) Characters   b) formats   c) symbols   d) All of the above

5. What type of chart is good for single series of data?
    a) Column chart   b) line chart   c) pie chart   d) cone chart

6. The Matrix toolbar can be found in the _____ menu in Mathcad.
    a) File   b) Insert   c) View   d) Symbolics

7. The _____ command displays the output of a C program on the screen.
     a) scanf()   b) printf()   c) run ()   d) close ()

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

9. Page number in word document can be inserted at
    a) Header   b) footer   c) both A and B   d) none

10. The process of removing unwanted part of an image is called
    a) Hiding   b) bordering   c) cropping   d) cutting

II. Fill in the blanks:

11. Constants which are enclosed in a pair of double-quote marks is _____ constant.
12. Each statement in a C program ends with a _____ symbol.

13. The IUPAC name of the compound

is _____.

14. The C programming language was invented by _____.
15. In Mathcad, a: 1; 20 implies the values of a are _____.
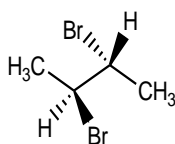
III. State whether True or False:

16. MS Office is application software
17. Any number of columns can be inserted in a word document
18. Cell is a basic unit of a worksheet
19. Line chart is useful for showing trends or changes over time
20. Pie chart is useful for comparing values over categories

IV. Match the following:

21. Ctrl + z   (i) copy/paste
22. Ctrl + k   (ii) save
23. Ctrl + =   (iii) hyperlink
24. Ctrl + y   (iv) undo
25. Ctrl + s   (v) superscript
                       (vi) Redo
                       (vii) subscript

V. Answer in one or two sentences:

26. Give the name of a data base used for XRD pattern.
27. Get the structure of 1H-phenalene using chem draw.
28. Draw the following structure using chem draw.

29. What is hyperlink?
30. Define relational operators in the C language.

SECTION B

ANSWER ANY FIVE QUESTIONS: **(5x6=30)**

31. . Using chemdraw obtain the ^{1}H and ^{13}C NMR spectrum of acetophenone   [3+3]
32. a] Find the inverse and determinant of the given matrix A.

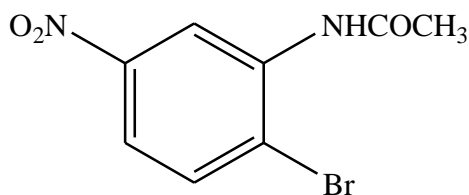$$A = \begin{bmatrix} 2 & -4 & -2 \\ 4 & 6 & 2 \\ 0 & 10 & -4 \end{bmatrix}$$

b] Find the transpose of A .

$$A = \begin{bmatrix} 1 & 2 & 4 \\ 6 & 8 & 1 \end{bmatrix}$$

[4+2]

..3

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

34. Using Matlab solve the following equations: [3+3]

(i) If $y = \dfrac{x-4}{2\sqrt{x}}$ find $\dfrac{dy}{dx}$ at $x = 4$ (ii) Evaluate: $\int \dfrac{1}{9-4x^2} dx$

35. The 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.

36. [a] Write a program to calculate the half-life $(t_{1/2})$ of a first order reaction.
Given formula: $(t_{1/2}) = 0.693/K$ [4]
   [b] Convert the name of the compound alpha-**pinene** to 3D- ball & stick labeled structure.   [2]

37. A compound has been prepared by four different methods. Calculate the % yield of the product in each method and draw a bar diagram by plotting different methods Vs % yield of the product
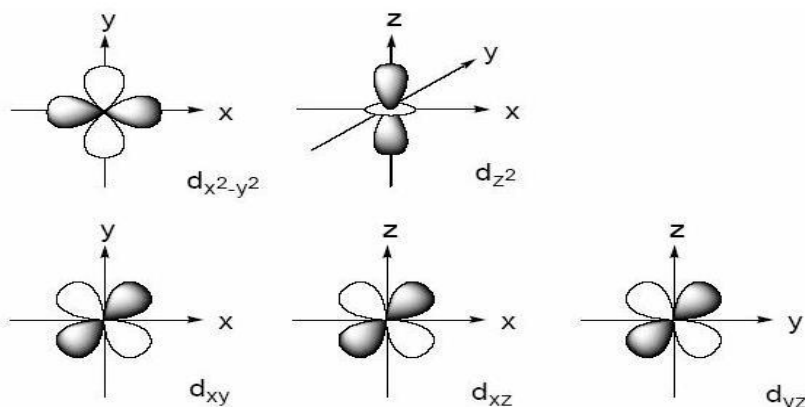
Formula = [Actual yield / Theoretical yield] **x** 100

Yield of the product	A	B	C	D
Theoretical yield	50	75	82	95
Actual yield	42	68	75	64
% yield of the product				

SECTION C
ANSWER ANY TWO QUESTIONS: **(2x20=40)**

38. [a] Draw the following orbital structures using chemdraw   [10]

[b] From the following data for the decomposition of ammonium nitrite in aqueous solution

i) Determine the rate constant of the reaction using the formula $k = (1/t) \ln (V\infty/(V\infty - Vt))$

ii) Plot a graph of time vs $\ln(V\infty/(V\infty - Vt)$

iii) Add the trendline

iv) Determine the slope and intercept.   [10]

Time (min)	10	15	20	25	∞
Volume of N_2 (ml)	6.25	9.00	11.40	13.65	35.05

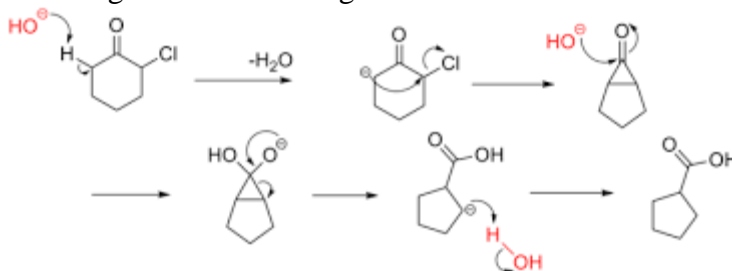39. [a] Define the following terms with an example: [5]

     (i) Keywords   (ii) constant   (iii) string   (iv) identifiers   (v) float
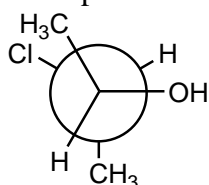
[b] If $A = \begin{pmatrix} 1 & 2 & -1 \\ 3 & 0 & 2 \\ 4 & 5 & 0 \end{pmatrix}$ and $B = \begin{pmatrix} 1 & 0 & 0 \\ 2 & 1 & 0 \\ 0 & 1 & 3 \end{pmatrix}$, verify if $(AB)^T = B^T . A^T$ [5]

[c] Draw the following mechanism using chemdraw   [6]

[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]

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

Sample	Amount of Nickel (%)
1	45
2	68
3	80
4	16
5	20

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

[c] Write a C program to check whether a given number is positive.   [6]

[d] Represent the equations f=-3 x+2 and g=2x-3 on the same graph as a function of x. [5]

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