STELLA MARIS COLLEGE (AUTONOMOUS) CHENNAI-86
(For candidates admitted during the academic year 2011–12 & thereafter)

SUBJECT CODE: 11CH/ME/CC53

B.Sc. DEGREE EXAMINATION, NOVEMBER 2016
BRANCH IV- CHEMISTRY
FIFTH SEMESTER

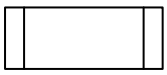
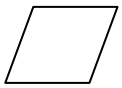
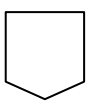
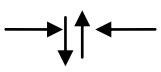
COURSE : MAJOR ELECTIVE
PAPER : COMPUTERS IN CHEMISTRY
TIME : 1 ½ HOURS **MAX.MARKS : 50**

THEORY

SECTION-A

I. Answer any ten from the following: (10x5=50 Marks)

1. What are the basic functions a computer can perform?
2. Expand the following:
   (i) TRON (ii) DOS (iii) RISC (iv) HDD (v) MIPS
3. Find out the type of errors in the following and give the valid constants / variables:
   (i) -26,53.296 (ii) 10^{th} day (iii) 10E3.5 (iv) AT. NO (v) 5$
4. What are micro computers? Explain in detail.
5. Distinguish between relational and logical operators.
6. Match the following:

(i) 	(A) flow lines
(ii) 	(B) off page connector
(iii) 	(C) on page connector
(iv) 	(D) decision box
(v) 	(E) predefined process
	(F) Input / Output box

7. Explain the following:
   (i) Hardware (ii) word (iii) byte (iv) Firmware (v) nibble

..2

8. a) What are the different types of viruses known? (3)

   b) Define force fields. (2)

9. a) Convert the following to decimal numbers :

   (i) $(7F4A)_{16}$ (ii) $(45)_8$ (iii) $(1011)_2$ (3)

   b) Give two applications of web source in determining the structure of a compounds. (2)

10. Give the basic expressions for the following algebraic expressions:

   i) $V = \frac{1}{(2a_0)^{n-1}}$ ii) $G = R\left[\frac{5}{2} + 2\frac{e^u}{(e^u-1)^2}\right]$ iii) $C = 4\pi\left(\frac{M}{2}\pi RT\right)^{3/2}\exp\left(-\frac{MC^2}{2RT}\right)C^2$

   iv) $E = \frac{n^2h^2}{8mc^2}$ v) $P = \frac{RT}{V-B} - \frac{A}{V^2}$

11. Give the application of the following BASIC functions:

   (i) RND (X) (ii) SGN (X) (iii) ABS (X) (iv) CINT (X) (v) INT (X)

12. Distinguish between analog, digital and hybrid computers.

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PRACTICAL

SECTION-B

II. Answer any five from the following: 5x10=50 Marks

1. The following data were obtained for the temperature – dependence of the equilibrium constant of an inhibitor binding an enzyme.

Temperature (K)	289	294.1	298	304.9	310.5
Equilibrium constant (K_C *10^7)	7.25	5.25	4.17	2.66	2.01

a. Plot a graph of ln K_C versus 1/T * 1000 , add trend line and find the slope.

b. From the above slope determine ΔH°, where ΔH° = - slope *R; R = 8.314*10^{-3} kJ/K mol

c. Determine also ΔG° and ΔS° . (5+2+3)

Formula

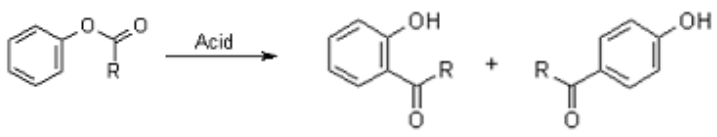
ΔG° = -RT ln K_C

ΔS° = $\frac{(\Delta H^\circ - \Delta G^\circ)}{T}$

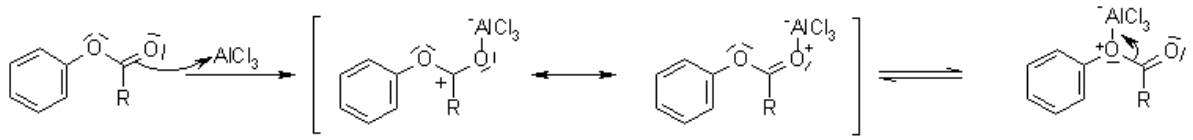
2. a. Using Matlab solve the following equations: (2+3)

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

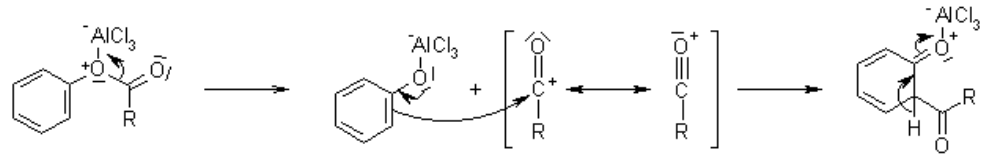
b. Draw the following Fries rearrangement mechanism using chem draw: (5)



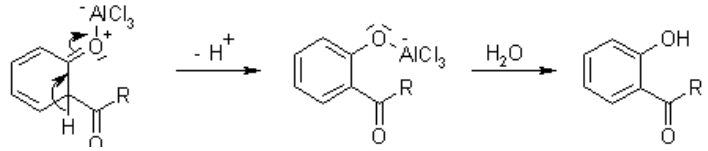
Step 1: Aromatic esters forms a complex with Lewis acid



Step 2: The above complex dissociates and forms acylium ion . The acylium ion acylates in the ortho position of the compound



Step 3: Removal of proton to stablize the aromatic ring and hydrolysis is done to obtain acylphenols



3. a. Draw the histogram for the following data (using Matlab): (3)
Amount of Oxalic acid (mg): 0.25, 0.25, 0.25, 0.30, 0.30, 0.30, 0.30, 0.30, 0.20, 0.20, 0.20, 0.20, 0.20, 0.15,0.10 and 0.10

b. For a two- component system, $\Delta H_{fus,A}$ = 500 cal/mol and $T_{fus,A}$ = 400°C. If the eutectic temperature is 350°C, calculate the solubility in terms of the fractions of B $(x_B)_e$ in A $(x_A)_e$ at 350°C. (2)

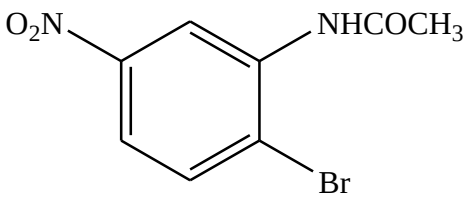
Formula:

$$\ln x_{A\ e} = \frac{\Delta H_{fus,A}}{R}\left(\frac{1}{T_{fus,A}} - \frac{1}{T_e}\right)$$

$$x_{B\ e} = 1 - x_{A\ e}$$

Where, R = 8.314J/Kmol; $\Delta H_{fus,A}$ = 500 cal/mol; $T_{fus,A}$ = 400°C= 673K; T_e= 350°C= 623K

c. Using chemdraw find (i) name of the compound (ii) C-Br, C-N, C-O and N-H bond lengths (iii) Minimize energy for the compound given below: (1+2 +2)



4. a. Draw the radius ratio plot for the alkali metal halides using Excel sheet for the following data and label the X – axis as Alkali metal halides ; Y- axis as Radius ratio (γ) and title the graph. (3)

Elements	F	Cl	Br	I
Li	0.57	0.42	0.39	0.35
Na	0.77	0.56	0.52	0.46
K	0.96	0.76	0.7	0.63
Rb	0.9	0.82	0.76	0.67
Cs	0.8	0.92	0.85	0.76

b. Different concentrations were made from (1/50M) $KMnO_4$ solution and its absorbance were analysed under colorimetric technique. The absorbance values are as follows:
Absorbance: 0.3, 0.4, 0.5, 0.45, 0.55 and 0.6 . Calculate, the average, median, Standard deviation and variance for the absorbance data. (4)

c. Create a table in microsoft word document for the given data:
Amount of Copper : 4.07, 4.09, 4.20, 4.22, 4.24, 4.11, 4.13, 3.99, 4.01,4.03, 4.05, 4.15, 4.17, 4.18, 4.26 and 4.28. Arrange them in (i) ascending and descending order (ii) find the maximum and minimum value from the data. (3)

5. a. Convert the name of the compound Camphene to 3D- ball & stick labeled structure. (4)

b. Find the dihedral angle of the following:
(i) -C-C-C-C- (ii) H-C-C-C (iii) H-C-C-H (2)
c. Find the bond angle: (i) Bridged and non bridged C-C-C (ii) H-C-H (2)
d. Find the close contact: (i) C, C (ii) C, H (iii) H, H (2)

6. a. Solve the system of linear equations: (2)

$-2x+3y=8$

$3x-y = -5$

b. Resolve into partial fractions: (2)

$$\frac{-2}{x-3}+\frac{3}{2x+5}$$

c. Find the inverse and determinant of the given matrix A. (4+2)

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

7. a. Using chemdraw obtain the ^{1}H and ^{13}C NMR spectrum of benzaldehyde. (4+4)

b. Find the transpose of $A=\begin{bmatrix} 1 & 2 & 4 \\ 6 & 8 & 1 \end{bmatrix}$. (2)

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