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 2015
BRANCH IV- CHEMISTRY
FIFTH SEMESTER

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

SECTION-A

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

1. Convert the following algebraic expressions into BASIC expressions:

$$a)U = -\frac{Mq^2}{4\pi\varepsilon_0 r_0}\left(1-\frac{1}{n}\right) \qquad b)q_{tr} = \left(\frac{(2\pi mkt)^{\frac{3}{2}}}{h^3}V\right) \qquad c)Y = \frac{A(1+r)^n}{(1+r)^n - 1}$$

$$d)x^2 + 2hx + h^2 = (x+h)^2 \qquad e)x = \frac{p}{2} + \sqrt{\left(\frac{p}{2}\right)^2 - q}$$

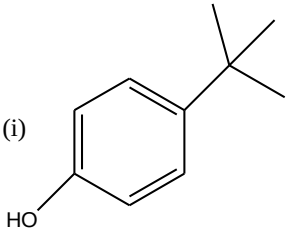
2. Expand the abbreviations that is given below:
   a) GEM b) DOS c) MM2 d) ROM

3. Differentiate between computer viruses, bug and worm.

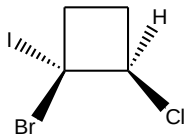
4. a. Convert the given names of the compounds to structures using chemdraw. (1x3=3)
   (i) potassiumferrocyanide (ii) 4-ethynylphenanthrene (iii) piperidone

   b. Find the name of the compounds given below using chemdraw: (1x2)

(i)



(ii)



5. The pre-exponential terms for two bimolecular gas reactions occurring at 300°C are (i) 7.4×10^{10} dm^3 mol^{-1} s^{-1} and (ii) 8.6×10^{11} dm^3 mol^{-1} s^{-1}. Calculate the entropy of activation in each case. (using the formula bar in Microsoft Excel sheet)

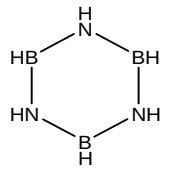
Formula :

$$k_\infty = \frac{k_B T}{h}\exp\left(\frac{\Delta S^*}{R}\right)\exp(1-\Delta n)$$

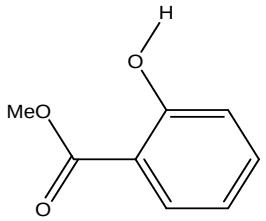
Where k_∞ = (i) 7.4×10^{10} dm^3 mol^{-1} s^{-1} (ii) 8.6×10^{11} dm^3 mol^{-1} s^{-1}; $\Delta n = -1$;
$k_B = 1.37\times10^{-23}$ J/K; T = 573K

..2

6. Find the specified bond lengths for each of the following compounds using chemdraw:

a) 

N(1)-B(3), B(7)-N(9), N(9)-H(10) & B(11)-H(12)

b) 

C(1)-C(2), C(1)-O(9), C(1)-O(10), O(4)-H(15), C(5)-C(6) & C(5)-H(18)

7. Match the following

i) CTRL + H	A) select all
ii) CTRL +A	B) shows paragraph marks & other hidden formatting symbols
iii) CTRL + E	C) Find and replace
iv) CTRL + Home	D) Center text
v) CTRL + *	E) Beginning of the document
	F) Create small letters above the line of text

8. Resolve into partial fraction :

$$\frac{3x^2+6x+5}{(x+2)^2(x-3)}$$

9. a. Solve the system of equations: (3)

$4x-3y = 25$

$-3x+8y= 10$

b. Find the determinant for the given matrix: (2)

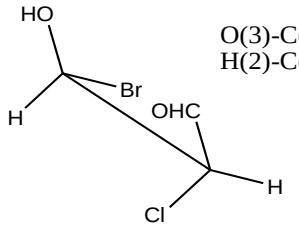
$$\begin{pmatrix} 5 & 3 & 7 \\ 2 & 4 & 9 \\ 3 & 6 & 4 \end{pmatrix}$$

10. Draw a cosine wave function for a particle in 1D box by plotting ψ_n against x, label the axes title and chart title. (Microsoft Excel sheet)

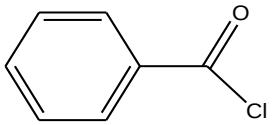
Formula : $\psi_n = A\cos(n\pi x)/L$

Where A= $\sqrt{2}$; n= 1; L=1; x= -0.5, -0.25, 0, 0.25, 0.5

11. Find the specified dihedral angles in the following compounds using chemdraw:

(a) 

O(3)-C(1)-C(4)-C(9) ; H(2)-C(1)-C(4)-Cl(5);
H(2)-C(1)-C(4)-C(9); C(1)-C(4)-C(9)-O(7) & Cl(5)-C(4)-C(9)-O(7)

(b) 

C(1)-C(6)-C(7)-O(8); H(11)-C(4)-C(5)-C(6);
H(14)-C(1)-C(2)-H(13) & C(5)-C(6)-C(7)-O(8)

12. Evaluate (i) $\int_0^{\pi} \sin^2 x dx$ (ii) Obtain $\frac{dy}{dx}$ for $y = e^{3x-2}$

SECTION-B

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

13. The following reaction was carried out under conditions

$C_6H_5COCl + 2\ C_6H_5NH_2 \longrightarrow C_6H_5CONHC_6H_5 + C_6H_5NH_2HCl$

Where benzoyl chloride was taken in excess. The pseudo first order rate constant when the concentration of benzoyl chloride was 0.015 mol dm^{-3} is 0.1356.
(x = [acetanilide]); [C_6H_5COCl] = a = 0.01; [$C_6H_5NH_2$] = b = 0.0005x10^4 = 5.0

t (min)	0	5	10	15	20	25	30
$10^4 x$ (mol dm^{-3})	0	1.038	1.488	1.856	2.090	2.239	2.339

(i) From the data calculate the value of the rate constant

$$k_2 m a^n = k_1 = \frac{2.303}{t} \log\left[\frac{b}{(b-mx)}\right]$$

m = 2; (4 marks)

(ii) Plot $\log\left[\frac{b}{(b-mx)}\right]$ vs *t(min)* , add trend line and determine the slope from the graph

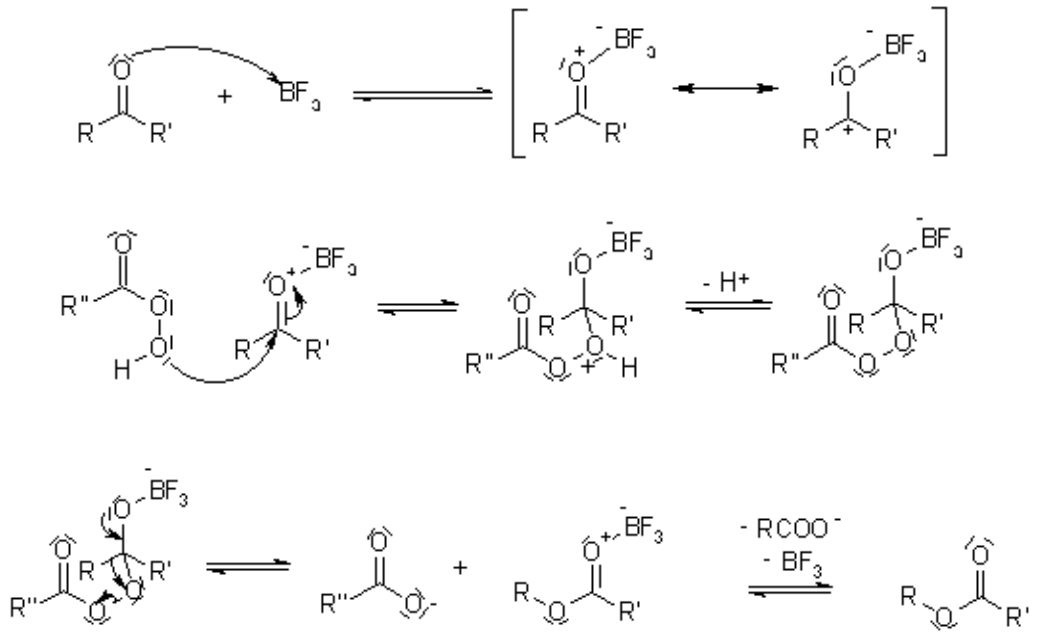
Slope = $k_1/2.303$ (3 marks)

(iii) For a_1 = 0.01 mol dm^{-3} ; k_1= slope *2.303 min^{-1}
a_2 = 0.015 mol dm^{-3} ; k_1= 0.1356 min^{-1}

Determine the order of the reaction (n) from the equation $\frac{2.303 * slope}{0.1356} = \left(\frac{a_1}{a_2}\right)^n$

(3 marks)

14. Draw the Bayer- Villiger oxidation reaction mechanism using chem draw:



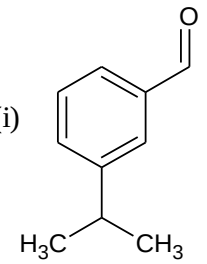
15. Find the determinant, maximum element, minimum element, transpose, eigen values and eigen vectors for

$$A = \begin{pmatrix} 4 & 6 & 10 \\ 3 & 10 & 13 \\ -2 & -6 & -8 \end{pmatrix}$$

16. a. Using chemdraw identify the close contact of the –C-O group and bond order of –C-O and for the following compounds and convert them to 3D structures.

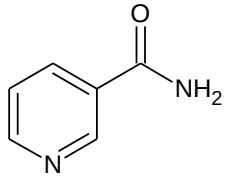
(5marks)

(i)



3-(propan-2-yl)benzaldehyde

(ii)



Niacinamide

b. Find the errors in each of the following and label them as BASIC constants/ variables:
(i) 2A6 (ii) "Symbol of nitrogen "N" (iii) 5.88-E (iv) 6th WEEK% (v) 2A$
(5 marks)

17. a. The following data were collected as part of a quality control study for the analysis of sodium in serum; results are concentrations of Na^+ in mmol/L= 140, 143, 141, 137, 132, 157, 143, 149, 118 & 145, Find the mean, median, and standard deviation for the given data, using the formula bar in excel sheet. (5 marks)

b. The solid A is heated at 1000K. The vapours are allowed to effuse through a pin hole of radius 4 mm and the amount collected is 1.70×10^{-4} kg in 40 min. Calculate the vapour pressure if M_A = 24 g/mol.

Formula : $$p = \frac{W}{\pi A t}\left(\frac{2\pi RT}{M}\right)^{\frac{1}{2}}$$

Where A = $(4 \times 10^{-3}\ m)^2$; W= 1.7 x 10-4 kg; t= 40x60 s; R =8.314 JK/mol;
T= 1000K; M= 24 x 10^{-3} kg/mol (5 marks)

18. a. Convert the following (i) 90 J to watts (ii) 55.23 liter to mL (2x1 =2 marks)

b. Evaluate $\int_0^{\pi/2} \sin^3(2x)\,dx.$ (4 marks)

c. Find the second derivative of $w = 3z^7 - 7z^3 + 21z^2$. (4 marks)

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