

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

SUBJECT CODE: 11CH/ME/CC53

B.Sc. DEGREE EXAMINATION, NOVEMBER 2013
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)

- a. What are special keys in computer? Give any five examples. (3)
b. Expand the following: (2)
(i) EDSAC (ii) VLSI
- a. What are hybrid computers? (2)
b. Convert the following hexadecimal number to decimal number:
(i) 2AF (ii) A56 (1x1.5 = 3)
- a. Give the application of Super computers. (2)
b. What is the usage of the following short cut keys in word document?
(i) Ctrl+Z (ii) Ctrl+C (iii) Ctrl+S (1x3=3)
- Match the following:

(i) (A) Off page connector

(ii) (B) Predefined process

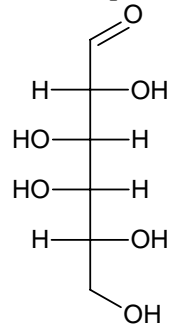
(iii) (C) Decision box

(iv) (D) Input / Output box

(v) (E) Annotation symbol

- 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 above data, using the formula bar in excel sheet.
- 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\$

7. a. Convert the given names of the compounds to structures using chemdraw.
 (i) 2-methyl-1-phenylpropene (ii) 5-methylcyclopent-1,3-diene
 (iii) Lithium diisopropylamide (1x3=3)
 b. Find the name of the compound given using chemdraw: (2)



8. Calculate the heat of sublimation (ΔH_{sub}) of solid CO_2 , by the given formula in excel sheet.

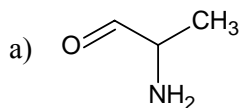
Where $R = 8.316 \text{ J K}^{-1} \text{ mol}^{-1}$; $T_1 = 153.5 \text{ K}$; $T_2 = 174.4 \text{ K}$; $P_1 = 10 \text{ mm}$; $P_2 = 40 \text{ mm}$

9. (a) Solve the equation $4x^4 + 3x^3 + 2x^2 + x + 1 = 0$.
 $x + y + z = 14$
 (b) Solve the system of equations $2x + 3y - 2z = 3$.
 $x - y + 2z = 1$

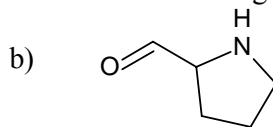
10. Resolve into partial fraction $\frac{x^2 + x + 1}{(x^2 - 1)(x + 3)}$.

11. Evaluate $\int_0^1 \int_0^{(x-x^2)^{1/2}} \frac{4xy}{x^2+y^2} e^{-x^2-y^2} dy dx$.

12. Find the bond angle of H-N-C- in the following compounds using chemdraw:



2-aminopropanal



pyrrolidine-2-carbaldehyde

SECTION-B

II. Answer any five from the following:

(5x10=50 Marks)

13. a. Give the BASIC expressions for the algebraic expressions:

(1x5=5)

(i) $\frac{RT}{V-b} - \frac{a}{V^2}$ (ii) $\frac{1}{2\pi} \sqrt{\frac{k}{\mu}}$ (iii) $\left(\frac{1}{\pi a_0^3}\right)^{\frac{1}{2}} e^{\frac{-r}{a_0}}$
 (iv) $w \left(\frac{KV_1}{KV_1 + V_2}\right)^n$ (v) $\frac{1}{1 - \exp\left(\frac{-\theta_{vib}}{T}\right)}$

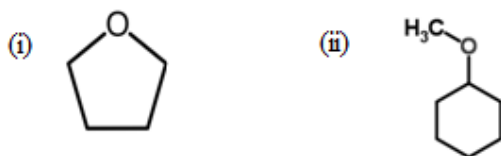
- b. Explain the following terms:

(2½ x 2 = 5)

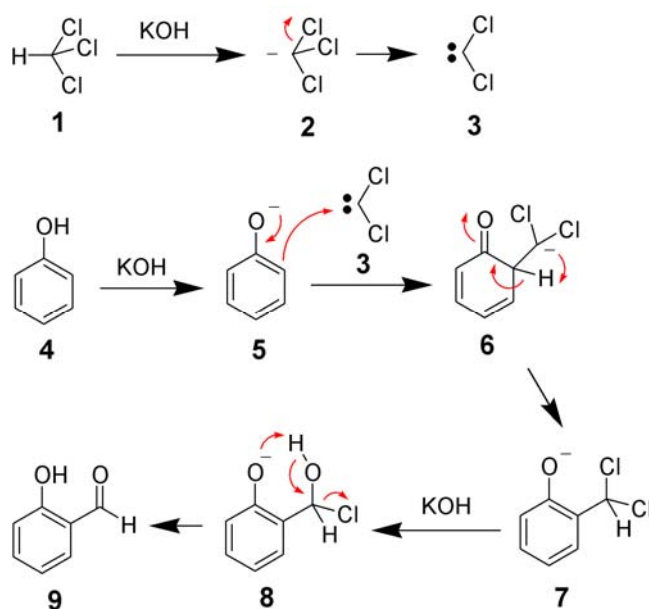
- (i) Debugging (ii) Relational operators

14. a. Find the -C-O bond length of the following compounds using 3D-Chem.

(2½ x 2 = 5)



b. Using Chemdraw, draw the scheme of the reaction given below and copy it in the microsoft word document file:



15. The optical rotations of sucrose in 0.5M HCl at 35°C at various time intervals are given below. (Use Microsoft excel spread sheets)

Time(minutes)	0	10	20	30	40	∞
Rotation(degrees)	+32.4	+28.8	+25.5	+22.4	+19.6	-11.1

- (i) Calculate the rate constant using the formula $k_1 = \frac{2.303}{t} \log \frac{r_0 - r_\infty}{r_t - r_\infty}$
- (ii) Plot a graph $\log \frac{r_0 - r_\infty}{r_t - r_\infty}$ vs t
- (iii) Add trendline for the above graph and find the equation & slope

16. a. Convert the density of water 1000 kg/m^3 to pounds per gallons.

b. Find the limit of $\frac{\sin 2x - 2\sin x}{x^3}$ as x tend to 0.

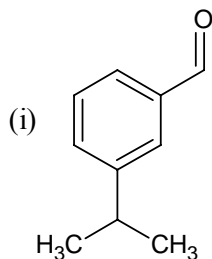
c. Find the second derivative of $e^{\sqrt{x}} \sin^2 2x$.

17. Find the inverse, determinant, maximum element, minimum element, eigen values and

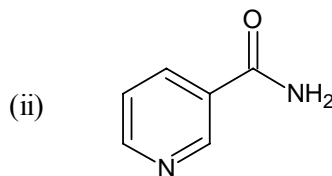
eigen vectors of the matrix
$$\begin{pmatrix} 1 & 2 & 0 & -1 \\ 9 & 8 & 6 & 5 \\ 9 & 11 & -2 & 3 \\ 4 & 5 & 6 & 9 \end{pmatrix}$$
.

18. 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. (2x2=4)



3-(propan-2-yl)benzaldehyde



Niacinamide

b. Draw Lother Meyer curve(Atomic Volume vs Atomic Weight) for the following data: (6)

Elements	Atomic Weight (g/mol)	Atomic Volume (mL/mol)
Lithium	6.941	13.10
Sodium	22.9897	23.7
Potassium	39.0983	45.46
Rubidium	85.4678	55.9
Cesium	132.91	71.07
Francium	223.00	101.35

19. a. Calculate the pressure exerted by 2 dm³ mol⁻¹ of ethane at 27⁰ C using van der Waals equation. (5)

where $a = 5.489 \text{ dm}^6 \text{ atm mol}^{-2}$; $b = 0.0638 \text{ dm}^3 \text{ mol}^{-1}$; $\bar{V} = 2.0 \text{ dm}^3 \text{ mol}^{-1}$
 $R = 0.0821 \text{ dm}^3 \text{ atm mol}^{-1}$; $T = 300\text{K}$

b. Explain logical operators in detail. (5)
