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 2014 <br> BRANCH IV- CHEMISTRY <br> FIFTH SEMESTER

COURSE : MAJOR ELECTIVE
PAPER : COMPUTERS IN CHEMISTRY
TIME : 3 HOURS

## SECTION-A

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

1. a. What are the function keys used for the following functions:
(i) SAVE
(ii) RUN
(iii) CONTINUE
b. What is file infection?
2. a. What are the functions for the following special keys
(i)
(ii)
b. Find the errors in each of the following and label them as BASIC constants/ variables:
(i) $758+$
(ii) $2^{\text {nd }}$ DAY
(iii) CLS
3. a. Split $\frac{1}{(1-x)^{2}(1-2 x)}$ into partial fractions.
b. Solve the equation $15 x^{4}-8 x^{3}-14 x^{2}+8 x-1=0$.
4. Match the following:
(i) \&
A. String declaration
(ii) NOT
B. Circumflex
(iii) < >
C. Logical negation
(iv) **
D. Not equal to
(v) $\$$
E. Asterisk
F. Ampersand
5. A certain amount of ideal gas occupies a volume of $2.56 \mathrm{dm}^{3}$ at a pressure of 200 torr and temperature 40 C . the gas is compressed to a volume of $1.6 \mathrm{dm}^{3}$ by applying pressure 400 torr. Calculate the final temperature.

Where $p_{1}=200$ torr, $\mathrm{V}_{1}=2.56 \mathrm{dm}^{3}, \mathrm{~T}_{1}=313 \mathrm{~K}$ $p_{2}=400$ torr, $\mathrm{V}_{2}=1.6 \mathrm{dm}^{3}, \mathrm{~T}_{2}=$ ?
6. a. Find the name of the compound given using chemdraw:

b. Convert the given names of the compounds to structures using chemdraw.
(i) D-erythrose
(ii) potassium hexacyanoferrate(II)
(iii) 2-methyl-1-phenyl propene
7. Explain logical relational operators.
8. Find the bond angle of $\mathrm{O}-\mathrm{C}=\mathrm{O}$ for the following compounds:
(i)

ethyl 2-oxopropanoate
(ii)

dihydrofuran-2(3H)-one
9. a. Solve the system of equations $x+y+z=3 ; x+2 y+3 z=4 ; x+4 y+9 z=6$
b. Find the eigen values and eigen vectors of $\left(\begin{array}{ccc}2 & 2 & 0 \\ 2 & 1 & 1 \\ -7 & 2 & -3\end{array}\right)$.
10. Calcium was detected from different brands of green tea by complexometric titration method. The amount of calcium present in each sample in mg is given below:

| 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| 125 | 105 | 110 | 122 | 97 | 105 | 122 | 120 | 105 | 114 |

Find the mean, median, and standard deviation for the above data, using the formula bar in excel sheet.
11. a. Find the $4^{\text {th }}$ derivative of $\cos ^{4} x$
b. Evaluate $\int \frac{\left(x^{2}+4 x\right)(2 x-3)}{x^{3}} d x$
12. a. Convert the following into decimal numbers:
$(2 \times 1.5=3)$
(i) $(2 \mathrm{AF})_{16}$
(ii) $(6012)_{8}$
b. Give the rules for constructing string constants.

11CH/ME/CC53

## SECTION-B

## II. Answer any five from the following:

5x10=50 Marks
13. a. Using Chemdraw, draw the scheme of the reaction given below and copy it in the microsoft word document file:


b. Explain the following terms:
(3x2=6)
(i) Wild character
(ii) super computers
(iii) Firmware
14. Plot the curves $y=x^{2}$ and $y=\frac{8}{x^{2}+4}$ on the same graph with first curve in green color and second curve in brown color.
15. a. Give the BASIC expressions for the following algebraic expressions:
(i) $\quad E^{o}-\frac{R T}{n F} \ln \frac{a_{M^{+}} a_{X^{-}}}{a_{M X}}$
(ii) $\left[\frac{1}{\pi \eta}\left(\frac{k_{b} T m}{\pi}\right)^{1 / 2}\right]^{1 / 2}$
(iii) $\frac{a}{C_{V}}\left(\frac{1}{V_{2}}-\frac{1}{V_{1}}\right)$
(iv) $\frac{C_{1}}{n \sqrt{C_{2}}} \quad$ (v) $\frac{-2 \pi^{2} \mu \mathrm{Z}^{2} e^{4}}{n^{2} h^{2}\left(4 \pi \varepsilon_{o}\right)^{2}}$
b. Calculate the frequency $v$,required to excite proton from $m_{1}=1 / 2$ to $m_{2}=-1 / 2$, given $\mathrm{g}_{\mathrm{N}}=5.585$ and magnetic field applied $\mathrm{H}=14000 \mathrm{G}$

Where $\mathrm{g}_{\mathrm{N}}=5.585, \beta_{\mathrm{N}}=5.0508 \times 10^{-31} \mathrm{JG}^{-1}, \mathrm{H}=14000 \mathrm{G}$ and $\mathrm{h}=6.6262 \times 10^{-34} \mathrm{Js}$
16. a. Phosphorescence emission of Acetone-d6 $(0.05 \mathrm{M})$ in acetonitrile at $20 \square \mathrm{C}$ was measured at 450 nm . Calculate the rate constant for the emission and also calculate the average life time of triplet state of acetone from the following data:

| $\mathrm{t}(\mu \mathrm{s})$ | 20 | 32 | 40 | 60 | 80 | 100 | 120 | 140 |
| :--- | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| Intensity $(I)$ (arbitary units) | 5.5 | 4.6 | 4.0 | 2.9 | 2.1 | 1.5 | 1.05 | 0.75 |

(i) Find $\log I$ from the above data and plot a graph of $\log \mathrm{I}$ (y-axis) vs t (x-axis)
(ii) Determine the rate constant by using the formula $\mathrm{k}=-$ (slope)*2.303, to use the value of the slope obtained from the above plot.
(iii) Calculate the average life time of triplet state from the formula $1 / \mathrm{k}$.
b. Using chemdraw obtain the ${ }^{1} \mathrm{H}$ NMR spectra for the following compounds:
( $2 \times 2=4$ )
a) benzaldehyde
b) ethanol
17. Explain the following :
$(5 \times 2=10)$
(i) Formatting
(ii) Operating system
(iii) Byte
(iv) DOS
(v) CPU
18. a. Using chemdraw identify
A. close contact of -C[5]-H[9] in (i) and H[8], H[15] in (ii)
B. bond order and bond length of $-\mathrm{C}-\mathrm{N}$

In the following compounds after converting them to 3D structures
(i)

3-methylbutanenitrile
(ii)

cyclohexanamine
b. Draw the graph series in a single graph scale for the following data.

| Elements | Atomic <br> Weight <br> $(\mathbf{g} / \mathbf{m o l})$ | Ionization <br> energy <br> $(\mathbf{k J / m o l})$ |
| :--- | :--- | :--- |
| Boron | 10.81 | 801 |
| Aluminium | 26.98 | 578 |
| Gallium | 69.72 | 558 |
| Indium | 114.81 | 558 |
| Thallium | 204.38 | 589 |

19. a. Give the symbol and its purpose for the following.
(i) Annotation (ii) Decision box
b. What are real and string variables? Explain.
