

B.Sc. DEGREE EXAMINATION, NOVEMBER 2014
BRANCH IV- CHEMISTRY
FIFTH SEMESTER

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

MAX.MARKS : 100

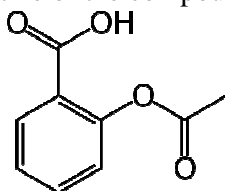
SECTION-A

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

1. a. What are the function keys used for the following functions:
(i) SAVE (ii) RUN (iii) CONTINUE (3)
b. What is file infection? (2)
2. a. What are the functions for the following special keys (2)
(i) (ii)
b. Find the errors in each of the following and label them as BASIC constants/
variables:
(i) 758+ (ii) 2nd DAY (iii) CLS (3)
3. a. Split $\frac{1}{(1-x)^2(1-2x)}$ into partial fractions.
b. Solve the equation $15x^4 - 8x^3 - 14x^2 + 8x - 1 = 0$.
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 2.56dm³ at a pressure of 200 torr and temperature 40°C. the gas is compressed to a volume of 1.6dm³ by applying pressure 400 torr. Calculate the final temperature.

Where $p_1 = 200$ torr, $V_1 = 2.56$ dm³, $T_1 = 313$ K
 $p_2 = 400$ torr, $V_2 = 1.6$ dm³, $T_2 = ?$

6. a. Find the name of the compound given using chemdraw: (2)



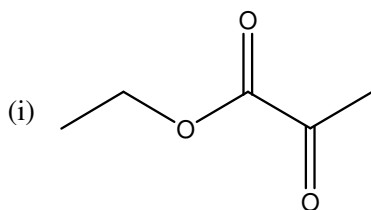
- b. Convert the given names of the compounds to structures using chemdraw.

- (i) D-erythrose
 (ii) potassium hexacyanoferrate(II)
 (iii) 2-methyl-1-phenyl propene

(3x1=3)

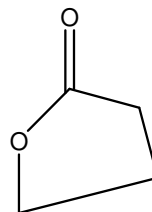
7. Explain logical relational operators.

8. Find the bond angle of O-C=O for the following compounds: (2x2.5=5)



ethyl 2-oxopropanoate

(ii)



dihydrofuran-2(3H)-one

9. a. Solve the system of equations $x + y + z = 3$; $x + 2y + 3z = 4$; $x + 4y + 9z = 6$

- b. Find the eigen values and eigen vectors of $\begin{pmatrix} 2 & 2 & 0 \\ 2 & 1 & 1 \\ -7 & 2 & -3 \end{pmatrix}$.

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 4th derivative of $\cos^4 x$

b. Evaluate $\int \frac{(x^2 + 4x)(2x - 3)}{x^3} dx$

12. a. Convert the following into decimal numbers: (2x1.5 =3)

- (i) $(2AF)_{16}$ (ii) $(6012)_8$

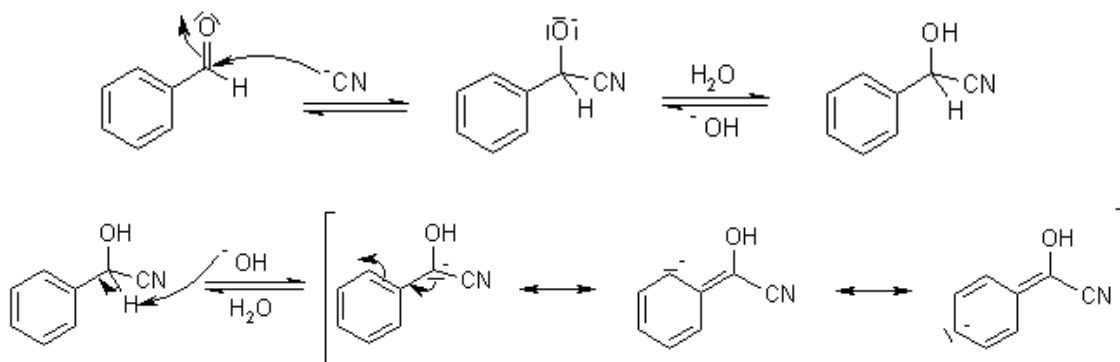
- b. Give the rules for constructing string constants. (2)

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: (4)



- 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: (5x1=5)

(i) $E^o - \frac{RT}{nF} \ln \frac{a_{M^+} a_{X^-}}{a_{MX}}$ (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) $\frac{C_1}{n\sqrt{C_2}}$ (v) $\frac{-2\pi^2 \mu Z^2 e^4}{n^2 h^2 (4\pi \epsilon_0)^2}$

- b. Calculate the frequency ν , required to excite proton from $m_1 = 1/2$ to $m_2 = -1/2$, given $g_N = 5.585$ and magnetic field applied $H = 14000$ G

Where $g_N = 5.585$, $\beta_N = 5.0508 \times 10^{-31} \text{ JG}^{-1}$, $H = 14000$ G and $h = 6.6262 \times 10^{-34} \text{ Js}$

16. a. Phosphorescence emission of Acetone-d6 (0.05M) in acetonitrile at 20°C was measured at 450nm. Calculate the rate constant for the emission and also calculate the average life time of triplet state of acetone from the following data:

t (μs)	20	32	40	60	80	100	120	140
Intensity (I) (arbitrary 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 $\log I$ (y-axis) vs t (x-axis)
 (ii) Determine the rate constant by using the formula $k = -(\text{slope}) \times 2.303$, to use the value of the slope obtained from the above plot.
 (iii) Calculate the average life time of triplet state from the formula $1/k$. (6)

