STELLA MARIS COLLEGE (AUTONOMOUS) CHENNAI 600 086
(For candidates admitted during the academic year 2010 - 11)

SUBJECT CODE: CH/ME/CC24

B.Sc. DEGREE EXAMINATION, APRIL 2011
BRANCH IV - CHEMISTRY
SECOND SEMESTER

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

SECTION-A

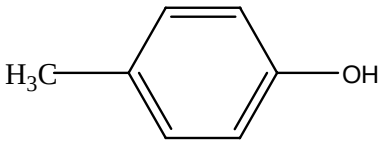
Answer all the Questions: **(10X 3 = 30)**

1. What are Analog computers?
2. Define string integer. Give any two valid string integers.
3. Draw a tabular form for the following data in MS word:

Samples,	He, Ne,	Ar, Kr, Xe
A	2, 10,	18, 36, 54
B	11.2, 0.68,	14.5, 0.66, 13.6
C	2.45, 5.9,	0.12, 0.89, 10.6

4. Find the determinant, Eigen values and Eigen vectors of the matrix
$$\begin{bmatrix} 2 & 2 & 2 & 2 \\ -1 & -3 & -5 & -6 \\ 0 & 0 & 1 & 5 \\ 10 & 11 & 12 & 13 \end{bmatrix}.$$

5. Find the bond length of O-H in the following compound.



6. Give any two applications of computers in chemistry.

7. Identify the error in the following:
   i) 234V6 (ii) 4.48E
8. Give the computer operator for the basic operator of division and logarithms
9. If $A = \begin{bmatrix} 2 & 5 & 10 & 5 \\ -2 & 1 & 2 & 3 \\ 6 & 0 & 6 & 6 \\ -9 & -1 & 8 & 6 \end{bmatrix}$, then find $A^2 - 5A + 2I$.
10. Evaluate $\lim_{x \to \infty} \left(\frac{x+3}{x-1} \right)^{x+3}$

..2

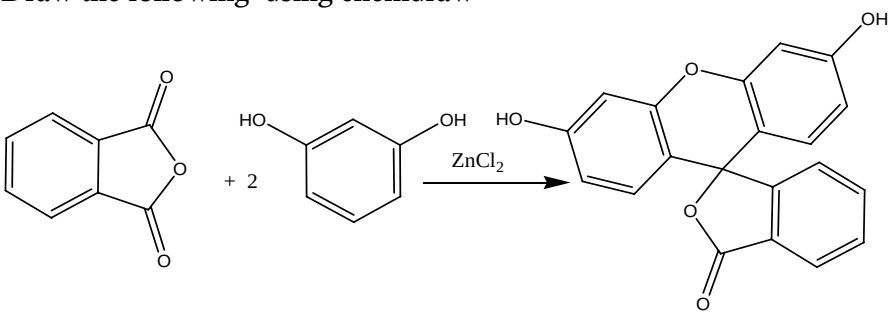
SECTION-B

(5*6=30)

Answer any five questions of the following:

11. Calculate (i) Average (ii) % of each value and average %
for the following values observed in the analytical data 13.09g, 17.25g, 14.9g,15.6g, 16.75g

12. Draw the following using chemdraw



13. Draw the structure of o-OH-C_6H_4-m-$CH(CH_3)_2$ in chemdraw and convert it into 3D and analyse the bond length and bond order of -OH , C=C and C-CH_3.

14. Solve the system of equations

$x-5y+6z+9w=10$

$4x+5y+6z+4w=20$

$4x+2y-2z+6w=30$

$5x+4y+5z+-8w=40$

15. Find the value of the function $f(x)=x^2-2x+5$

(i) At $x=4$.
(ii) At the range values 1 to 10
(iii) At the vector values $1,-2,0,4,10,9$.

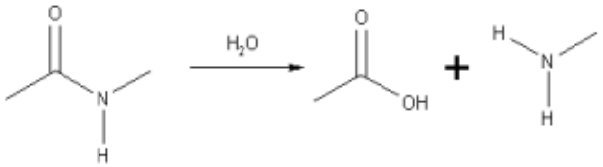
16. Write basic expressions corresponding to the following expressions

i) $E=n^2h^2/8ma^2$ ii) $4(3.14)(M/2)\exp(-MC^2/2RT)C^2$

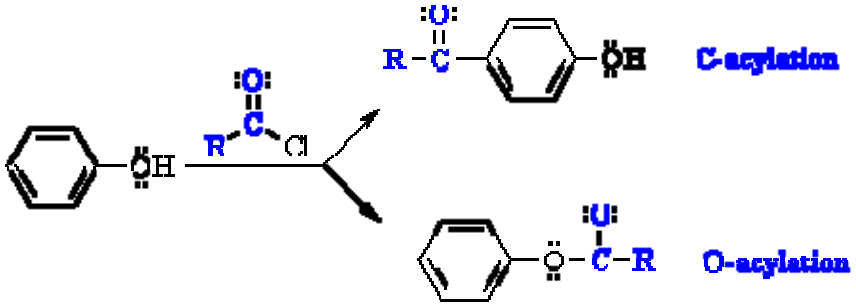
SECTION-C

Answer any Two (2*20=40)

17. i) Draw the equations by using chemdraw



(ii)



(iii) Plot the graph for time Vs log $V\alpha - Vt$ and obtain the slope from the equation by using the trend line. ($V\alpha - V_0 = 9.6$) .Calculate k by using the given equation

$K = 2.303/t \log(V\alpha - V_0)/(V\alpha - V_t)$

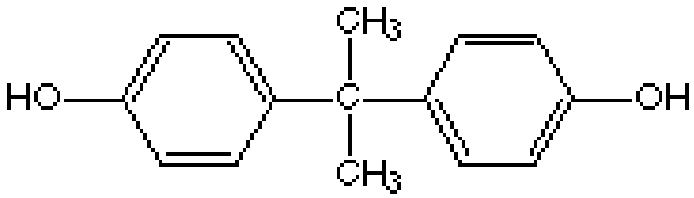
Time : 20, 25, 30, 35, 40, 45,

$V\alpha - V_t$: 4.9, 4.4. 2.8, 2.4, 1.7. 0.8 (4+8+8)

18. (a) Find the second derivative of $\frac{e^x \tan^{-1} x}{\sqrt{1+x^2}}$.

(b) Evaluate $\int \frac{x+1}{\sqrt{8+x-x^2}} dx$.

(c) Draw the following structure by using chemdraw and predict NMR



Bisphenol A

(5+5+10)

19. i) Create a plot that has the two curves $y = x \sin x$ and $y = \frac{16}{x^2+4}$ with the first curve in blue color and the second curve in green color. Also draw the axis as intersecting in the origin.

(ii) Plot the graph for ΔH vs number of moles and obtain the slope from the equation by using the trend line.

S.No.	No. of moles of KNO_3	Heat of Solution (ΔH)
1	1.25	20
2	2.50	23
3	3.75	26
4	4.00	32
5	5.50	50
6	6.20	53
7	7.10	58
8	7.40	61
9	7.60	63

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