

STELLA MARIS COLLEGE (AUTONOMOUS) CHENNAI-86
(For candidates admitted during the academic year 2004 -05 & thereafter)

SUBJECT CODE: CH/MO/CC34

B.Sc. DEGREE EXAMINATION, NOVEMBER 2007
BRANCH IV- CHEMISTRY
THIRD SEMESTER

COURSE : MAJOR OPTIONAL
PAPER : COMPUTATIONAL CHEMISTRY
TIME : 3 HOURS

MAX.MARKS : 100

SECTION – A

Answer ALL questions(15×2=30)

1. Solve the equation for the matrix A, $3A + \begin{pmatrix} 4 & -1 \\ -2 & 1 \end{pmatrix} = \begin{pmatrix} -2 & 2 \\ 1 & 4 \end{pmatrix}$.
2. Solve $(D^2 + 3D + 2)y = 0$.
3. State the Simpson's $3/8^{\text{th}}$ rule to find $\int_a^b y dx$.
4. Solve $\frac{dy}{dx} = \frac{e^x}{e^y}$.
5. What is the function in MathCAD to find Eigen vectors of a matrix.
6. Why the following integer constants are invalid

a. $590 * 2 + 5 =$

b. $234Vi 68$

7. Draw the graphical representation for the following data

Volume	20	20.3	20.6	20.9	21.3	21.5
Time	10	15	20	25	30	35

8. Pick out the following scalar and vector quantities

. Temperature., force, momentum, density

9. Draw the following structure in chem. Draw for the following molecules and compare their steric energy.



10. Give any two applications of computers in analytical chemistry
11. Give basic operator for exponentiation and not equal to
12. Give the correct constant \$ 350, 1,584E .5
13. What are string constants . Give any one valid string constants
14. Give the correct expression $N \cdot R \cdot T / V$ ii $XI(N_1 + N_2)$
15. What is the function for factorizing a given equation in MATLAB

SECTION – B

Answer any FIVE questions (5×6=30)

16. Find the eigen values of the matrix $\begin{pmatrix} 3 & -0 & 3 \\ -1 & 5 & 1 \\ 3 & 1 & 5 \end{pmatrix}$.

17. Solve $x^2 p^2 + 3xyp + 2y^2 = 0$.

18. Solve the simultaneous equation in MathCAD

$$x + 2y + 5z = 23$$

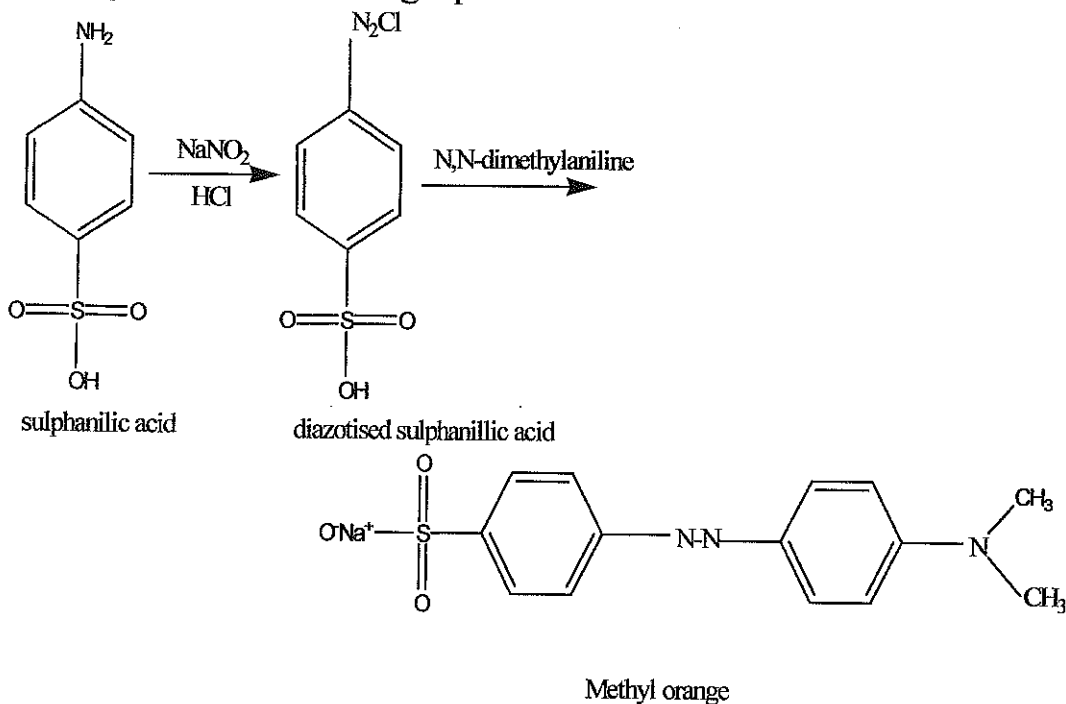
$$3x + y + 4z = 26$$

$$6x + y + 7z = 47$$

19. Find the sum up to 20 terms of the arithmetic progression whose first term is 2 and common difference is 3, using MathCAD.
20. Find the standard deviation of 46,59,66,74,83,88,99,36,47
21. Write the chemical equations for the following :

Benzaldehyde is condensed with acetophenone in presence of NaOH to give benzilideneacetphenone.

22. Represent the following equation in chem. Draw



Section – C

Answer any TWO questions: (2×20=40)

23.(a) The following table gives the various values of two variables:

X : 42 44 58 55 89 98 66

Y : 56 49 53 58 65 76 58

Determine the two regression lines.

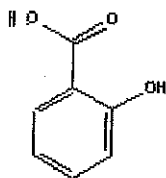
(b) Plot the graphs $y = x^3 + x + 1$ and $y = \frac{\sin x}{x}$ on the same graph in

MathCAD.

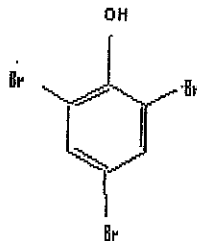
(c) Determine the second derivative of $e^{\sin x} x^2$ in MathCAD.

(8+8+4)

24. i Draw the following models on chem. 3D and deduce the minimized energy Calculate the length and breadth of the molecule

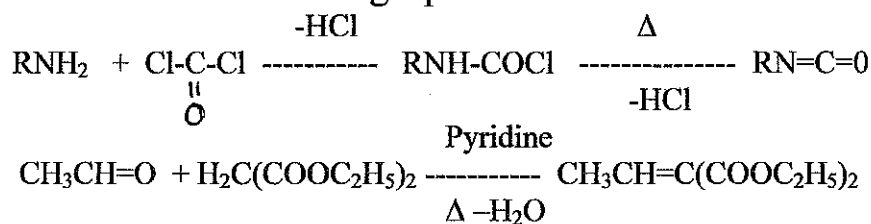


A



B

ii. Write the chemical following equations in chemdraw



25.a. Experimental data for the reaction between ethylacetate and sodium hydroxide at 25 C are recorded below find the k and average k $a = 0.04682$ mol/litre $b = 0.08712$ mol/lit

T (sec)	264	407	644	844
(a-x) mol/lit	0.01327	0.011086	0.008846	0.00669
(b-x) mol/lit	0.0484	0.04268	0.03892	0.03684

Use the equation $k = 2.303 \times (b/a) \times 1/t \times \log \{a (b-x/b (a-x))\}$

b. calculate the effective diameter of an argon molecule at 293 K. Given that its viscosity coefficient is 0.2217 millipoise. molecular mass of argon is 40.

$$\sigma^2 = \frac{2}{3 \Pi N_A \eta} \sqrt{\frac{RTM}{\Pi}} \quad (R = 8.314 \text{ KJ/mol})$$