COMPUTER APPLICATIONS IN CHEMISTRY-Part - I

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Topics covered

- Introduction to Computers
- General Information
- Some related terminology
- Flow Charting- Concept
- Some flow charts- examples
- Concept of Programming- BASIC language
- Some Programmes in BASIC

Computer

1. perform millions of arithmetic operations in a very short time with almost accuracy.
2. machine that gets input data with set of instructions process it and give us the results/output as processed data.
3. can store the information, million of words both in the memory on the hard disk and by means of off line devices such as disks, magnetic tapes etc.

Characteristics:

1. It is a fast electronic device.
2. more accurate.
3. quick as compared to man
4. perform arithmetic and logical operations
5. has high memory
6. does not feel exhausted or bored

In spite of all these advantages it is a machine and has no intelligence. It perform the operations as per given set of instruction.

Classification:

1. General purpose computers for general applications. Used in the offices for general requirements as financial accounting , management information
2. Special computer for special functions as used in researches, space stations, meteorological stations etc.
3. Analog computers chiefly used for scientific and engineering applications.
4. Digital computers are general purpose computers that represent and store data in discrete numbers. Stores information in terms of binary digits (0,1) . Each single entry has specified ASCII code
5. Hybrid computers involves technology of both analogue and digital computers. Can work as digital to analog and analog to digital computer.
6. Micro computers are small computers consists of microprocessor and associated input/ output devices.
7. Minicomputers :- fast , small and expensive computers which have limited input and output capabilities.
8. Main frame computers:- large systems with powerful peripheral devices.
9. Supercomputers: Example:- PARAM 10000

Modes of Computer operations:-

1. Batch mode: in this mode programs are processed one by one in a sequential manner. Generally the program and associated data are entered through any input device. Once a program is read by the computer, the user can't make alterations in any program. As the execution of program takes place at a fast speed, the batch mode is most suited for long programs.
2. Time-shared mode: In this mode the user communicated with the computer via a terminal which may be far away from the main computer. A modern time shared computer can have a large number of terminals. Several users can use the computer simultaneously independent of each other an d computer system can attend each of them periodically at a faster rate. Time shared computers can also be operated in batch mode by giving certain commands of the operating system which may be complicated set of programs.

Hardware and software: The physical portion of the system. This term is used to describe the electrical and mechanical parts of computer as well as peripheral devices.

Software is a general purpose term which describes all the written procedures and rules that controls computer operations. Software includes operating systems, user developed programs, compilers etc.

A compiler is a translating program that translates the instruction of a high level language into machine language. A compiler can translate only those source programs which have been written in the language for which the computer is meant.

An interpreter is another type of language translator which differs from compiler. Compiler convert whole high level language program into machine language at a time but interpreter takes one statement of high level language at a time and translates into a machine code and which is immediately executed.

Assembler is one of the translator program that translate a high level language to machine language program. It is a system program which is written by the system programmers.

Computer language: Can be classified into three categories: Machine language, assembly language and procedure oriented languages

BASIC COBOL etc.
FORTRAN
C C++

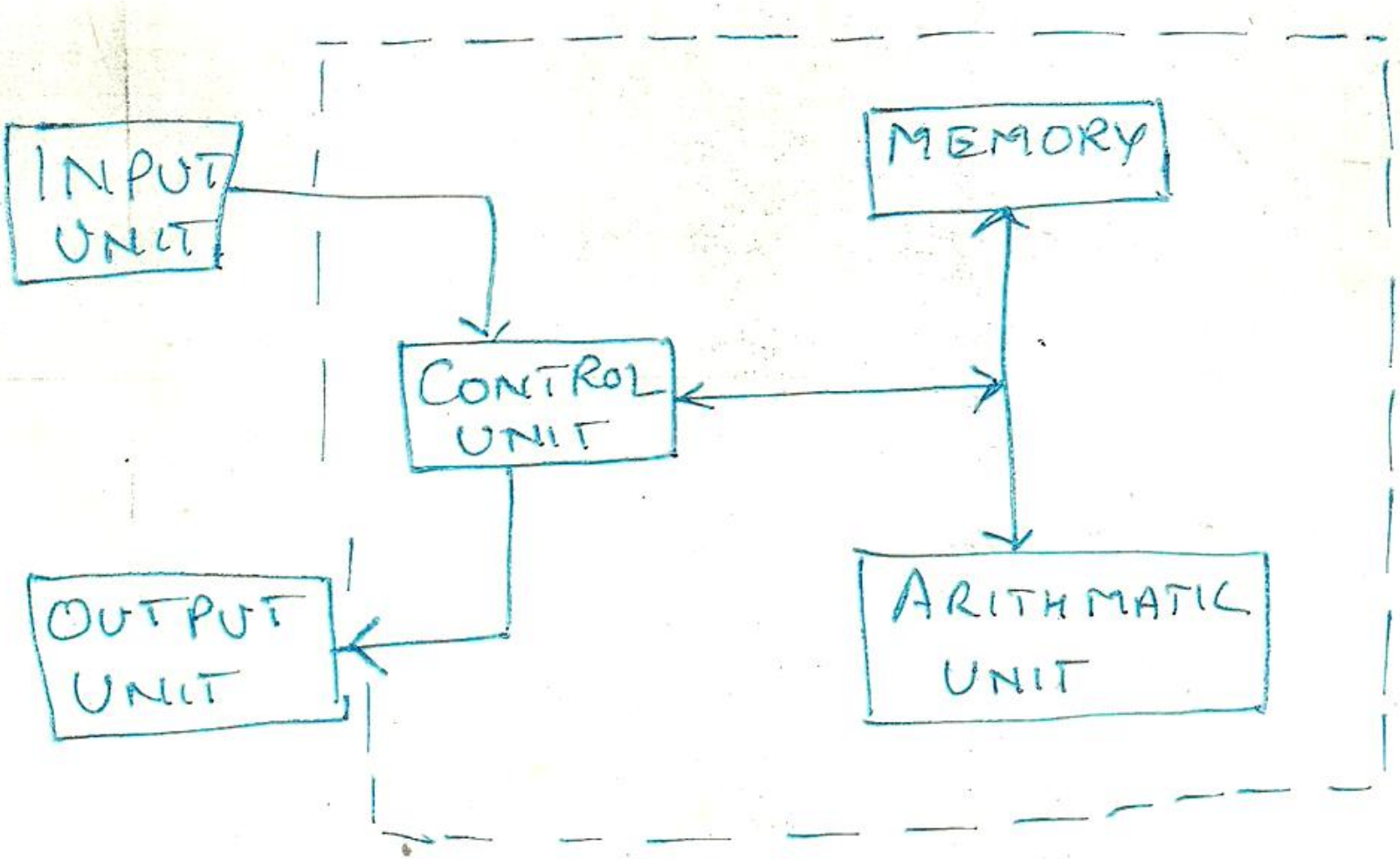
Input devices:
Magnetic tapes, floppy, CD, Punched Cards, Key boards, Mouse, Teletypewriters etc.

Output devices:
Magnetic tapes, Floppies, CD, VDU, Printers etc, Graph plotter, etc.

Memory unit: Computer can perform arithmetic operations on the data automatically as per set of instructions which is known as PROGRAM. It is necessary to store PROGRAM and processed data results These operation can be performed by memory unit. A memory location can be accessed by specified address.

Arithmetic unit Arithmetic operations are carried out by this unit. Numbers are stored in registers which are small but fats memories. The magnitudes of numbers that can be operated upon depends on the size of registers. The size of register depends on its function. It can be typically 1,2,3,4,16,32 bits. Most of the computers have word size 8 to 64 bits.

Control unit: This unit selects, interprets and executes the program instructions. It performs the function of overall supervision in the arithmetic, memory, input and output devices and supplies the appropriate data and control signals to these units. It basically coordinates the activities by timing and directing the flow of information form one unit to another.


INPUT UNIT
MEMORY
CONTROL UNIT
OUTPUT UNIT
ARITHMATIC UNIT

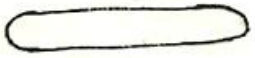
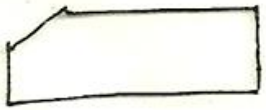
FUNDAMENTAL CONCEPTS OF PROGRAMING

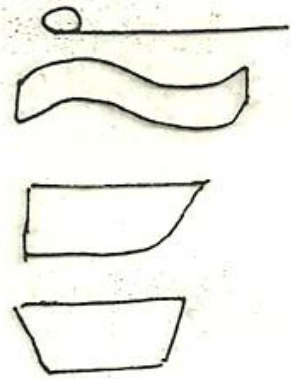
In the previous chapter (Ref. Section 1.6) it is mentioned that there are four steps involved for execution of a program of any problem. Out of these four steps one important step is development of logic for the solution of any problem which help in making flow charts. The process of showing diagrammatically the method of solution is referred to as flowcharting. It is desirable to draw flowchart for any problem before developing a program. Flow chart can proved to be useful in writing the program for the problem in any language, if one knows the syntax of that language. Therefore developing of programming logic and drawing of flowchart is necessary to write any program. In this chapter, Let's discuss the symbols used in drawing a flowchart with some flow charts related to problems of chemistry and of simple or numerical analysis. Any flow chart can be tested before actually writing of program, according to the logic i.e. developed by the data/ information flow lines. This step is known as dry run for the problem.

SECTION- 2.1
FLOW CHART SYMBOLS

There are some symbols which are used to draw a flowchart. These symbols have specific meanings. These symbols are given in table 2.1.

Table 2.1 : Flow Chart Symbols

Symbol	Meaning
	Start, Stop
	Input, Output
	Processing program Instruction
	Decision box
	Flow directions
	Connector
	Instruction that Change the program
	Punch Card



Magnetic Tape

Punch paper tape

Paper document

Manual Task

Discussion for some specific symbols which are in common use for drawing a flowchart is as under:

Oval: The oval is used for two purposes i.e. to define the beginning of a flow chart and to show the termination of a flowchart.

Parallelogram : The parallelogram symbol in any flowchart is used for operations involving input and output i.e. for INPUT, READ or PRINT statement.

Rectangle: The rectangle is used in connection with let statement and for any processing operation.

Arrows: An arrow (→, ←, ↑ , ↓) is used to indicate the direction of flow of data or information.

Decision Box : A decision box  is used to show decision making step in a program. It is used to decide alternate courses of action e.g. decision box asks question. It is the box which has one entering and two exit arrows.

Connector : The connector symbol ○ is used to eliminate lines between one part of flow chart to another. Connector symbols may also be used to connect a flow chart from one page to another.

Some of the flowcharts of some problems of mathematical analysis and of chemistry are given in section 2.2.

SECTION –2.2
FLOWCHARTS FOR SIMPLE PROBLEMS

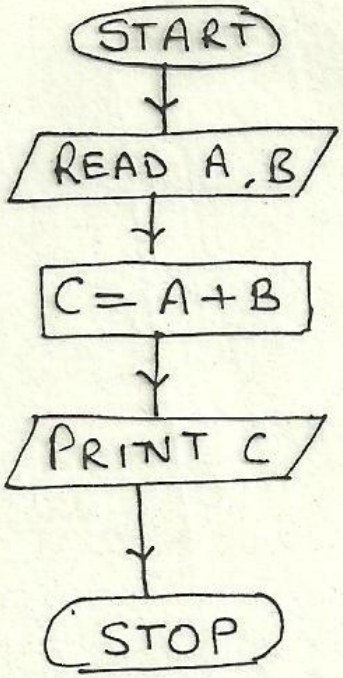
1.Addition of numbers

It involves following steps

a) Read the numbers

b) Add them and
c) Store into a new variable
d) Print the result in the form of that variable.

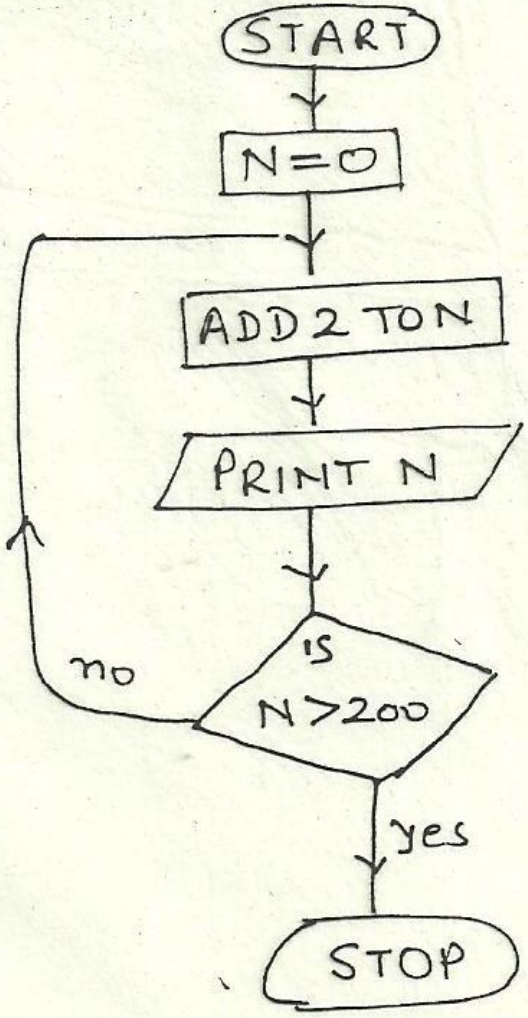
Its flow chart is



Like wise flow charts for subtraction and multiplication can be drawn.

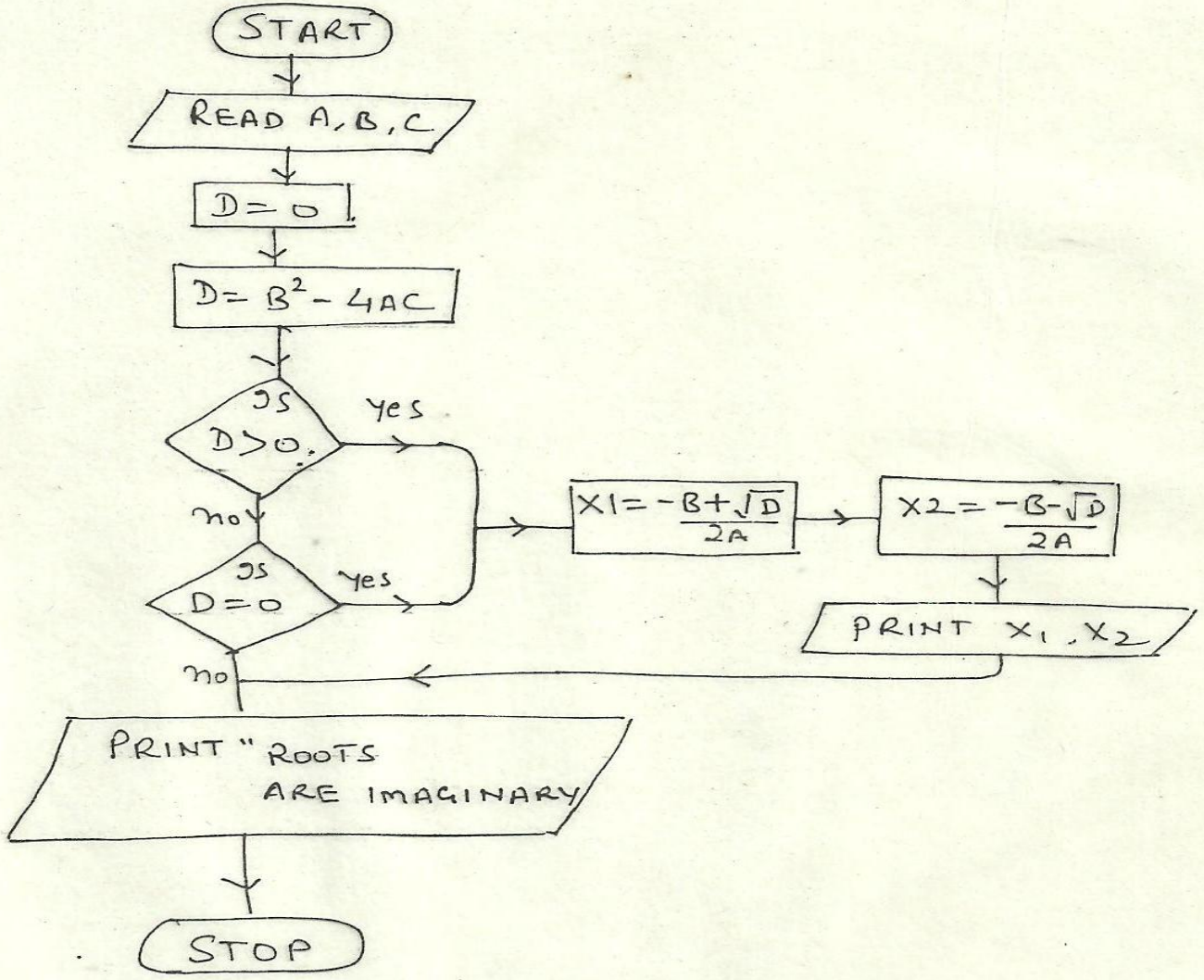
2. *To print even numbers (say upto 200)*

Flow chart for this problem is shown below:

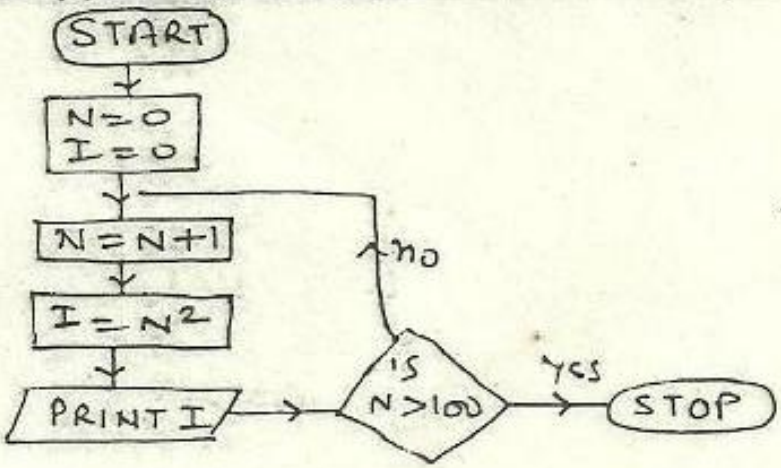


7. To compute the roots of quadratic equation $AX^2 + BX + C = 0$

In order to solve a quadratic equation we have to first find out discriminant D which is equal to $D = B^2 - 4AC$ and if $D > 0$ then only roots are real and can be calculated otherwise roots are imaginary. Roots are $(-B \pm \sqrt{B^2 - 4AC})/2A$. So, the flow chart for this problem is :



8. To print the squares of first 100 natural numbers the flow chart is :



9. To compute the value of X and Y variables in the solution of simultaneous equations :

As system of simultaneous equations are

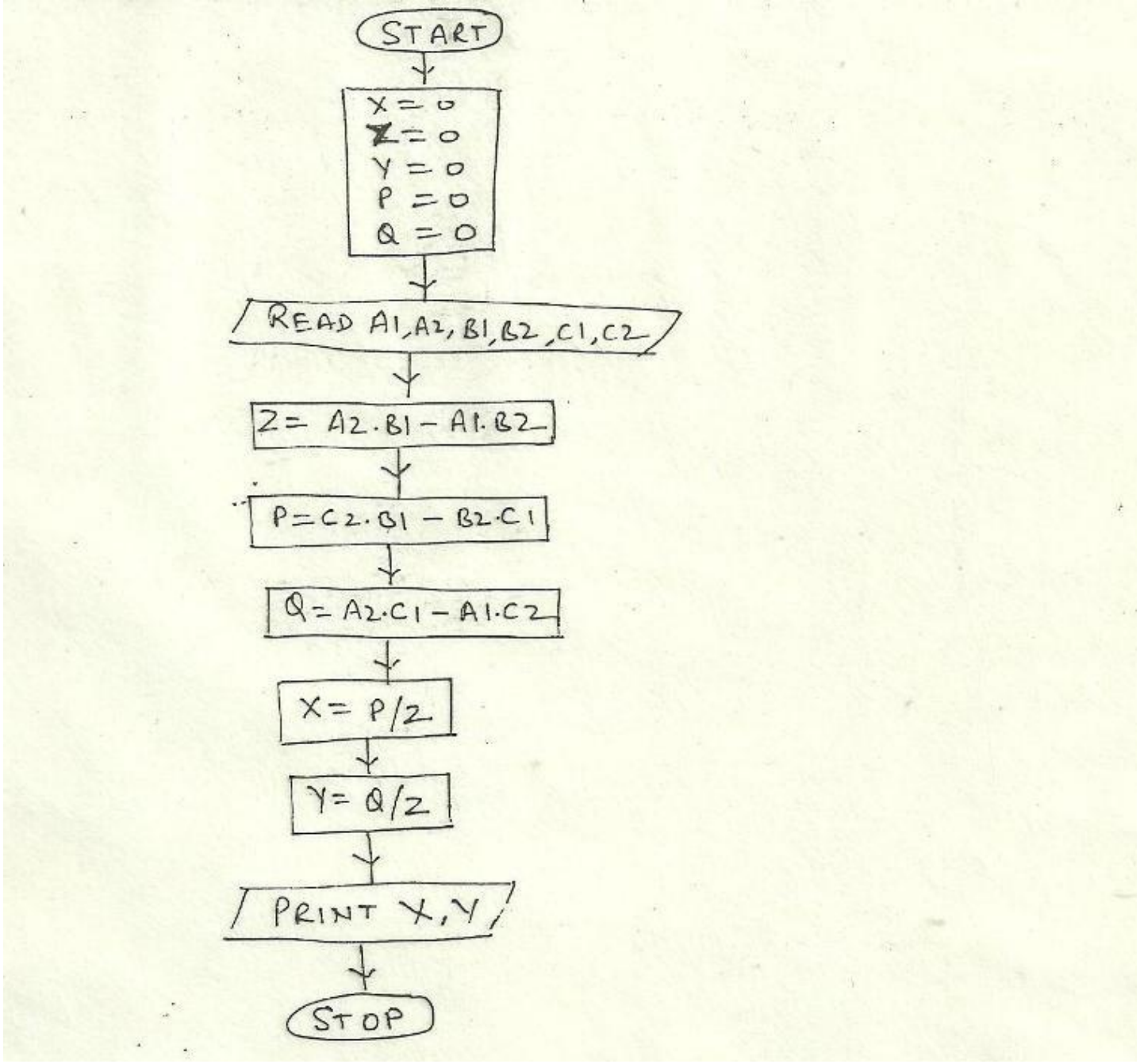
A1X + B1Y = C1

A2 X+ B2 Y = C2

These equations on solution gives

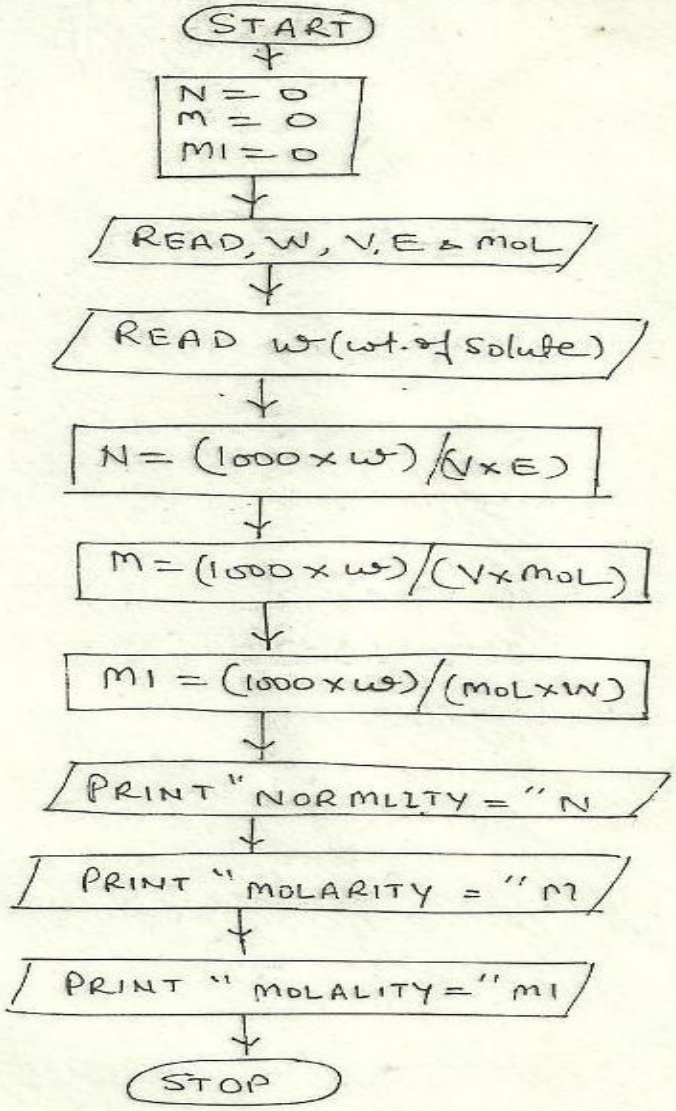
X = (B1C2 – B2C1)/(A2B1-A1B2) and Y = (A2C1 – A1 C2)/(A2B1- A1 B2).

So, flow chart for this problem.is


START
X = 0
Z = 0
Y = 0
P = 0
Q = 0
READ A1, A2, B1, B2, C1, C2
Z = A2 · B1 − A1 · B2
P = C2 · B1 − B2 · C1
Q = A2 · C1 − A1 · C2
X = P/Z
Y = Q/Z
PRINT X, Y
STOP

14. To compute normality, molarity and molality values for a given solution:

As normality is N = (1000×w)/ (V×E) ; molarity is M = (1000×w)/(V×Mol) and molality is m = (1000×w)/ (Mol×W) where W is the weight of solvent, V is the volume of solution, E is the equivalent weight of solute and Mol is the molecular weight of solute. Flow chart for computing these quantities is:

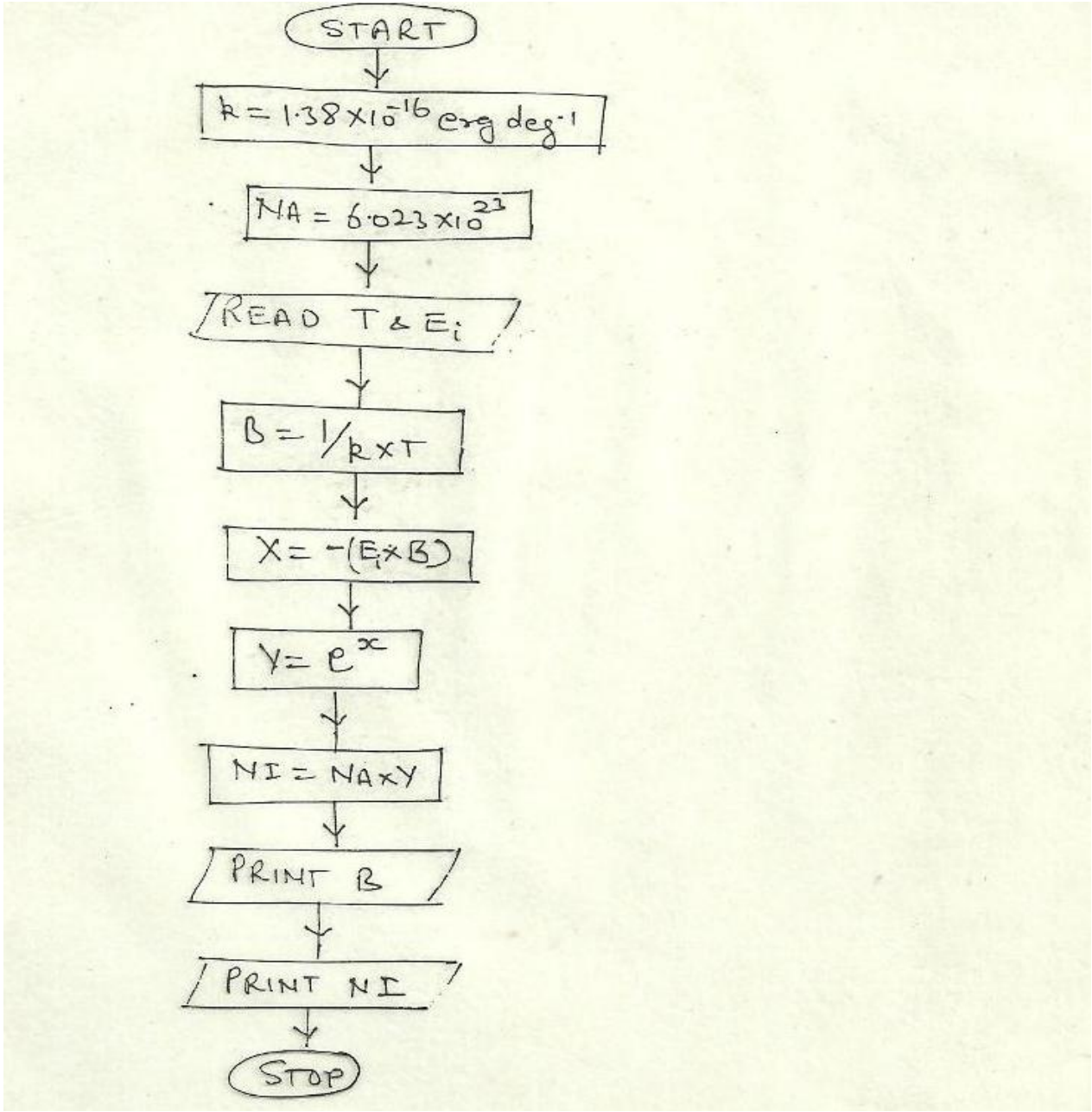


31 To compute the value of and hence to find out the value of n_i on the basis of Boltzmann Statistics

According to the Boltzmann Statistics number of particles in the I[th] level is given by

$$n_i = n_0 e^{-\beta \epsilon_i}$$

Where n_0 is the number of particles in the ground state or in the zeroth state and β is a constant equal to 1/kT and ϵ_i is the energy of i^{th} level. Flow chart for this computation can be drawn as follows, considering n_0 as N_A (the Avogadro's number)

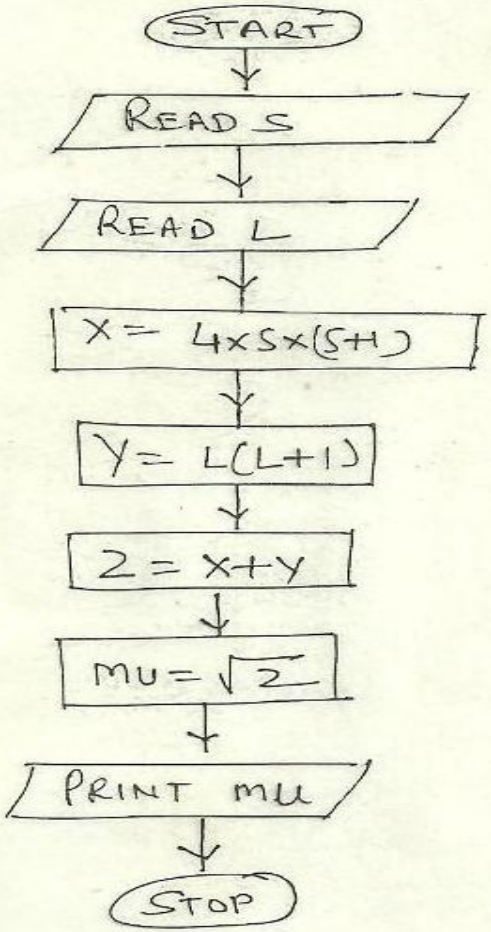

START
k = 1.38 x 10^-16 erg deg^-1
NA = 6.023 x 10^23
READ T & Ei
B = 1/k x T
X = -(Ei x B)
Y = e^x
NI = NA x Y
PRINT B
PRINT NI
STOP

34. To compute the value of magnetic moment of a substance on the basis of μ_{s+l} formula:

Magnetic moment of a substance can be calculated on the basis of μ_{s+l} formula as

$$\mu_{s+l} = \sqrt{4s(s+1) + l(l+1)} \text{ BM}$$

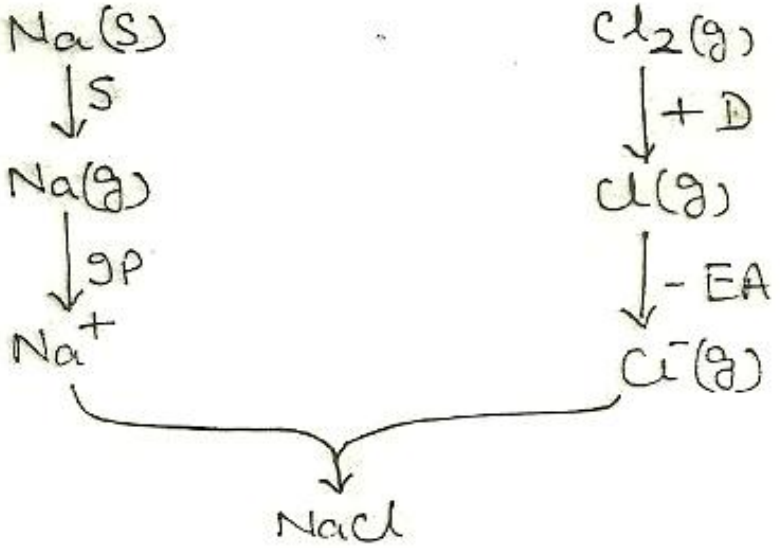
Its flow chart can be drawn as follows:



46 To compute the value of Lattice Energy on the basis of Born Haber's Cycle:

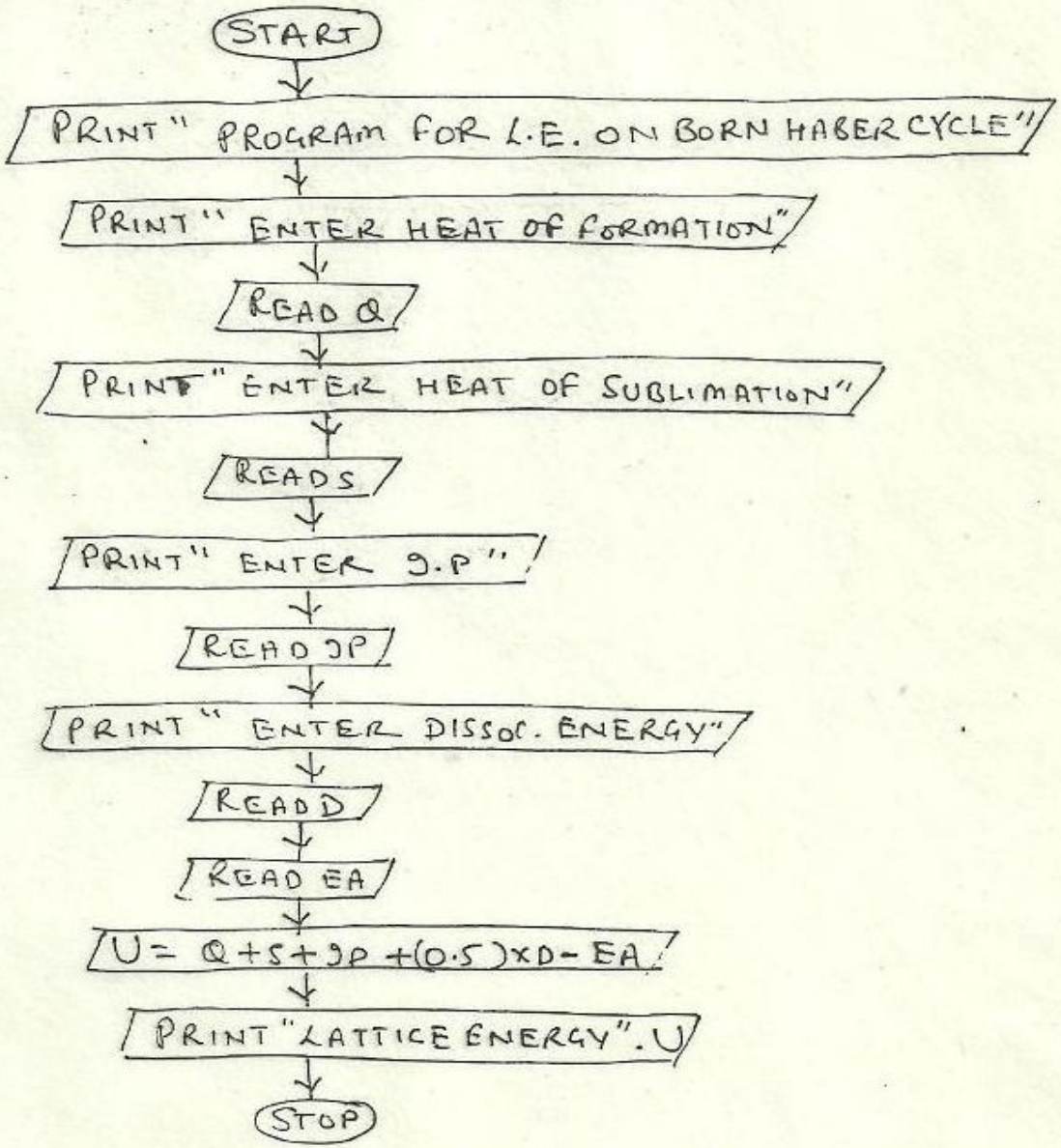
Lattice energy on the basis of Born Haber's Cycle can be calculated for a reaction as follows :

e.g. for the reaction $Na(g) + Cl_2(g) \xrightarrow{-Q} NaCl$ this cycle is as follows



So, $-Q = S + IP + \frac{1}{2}D - EA - U$, where S is the heat of sublimation, IP is the ionization potential of Na, D is the dissociation energy, EA is the electron affinity, U is the lattice energy and Q is the heat of formation. On rearranging it

$-U = -Q - S - IP - \frac{1}{2}D + EA$ or $U = Q + S + IP + \frac{1}{2}D - EA$. Its flow chart is :

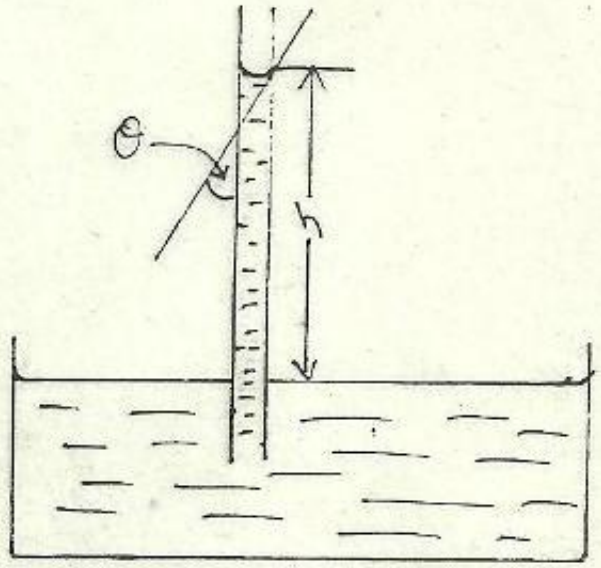


48 To calculate the value of surface tension on the basis of capillary action

For capillary action

$$\gamma = \frac{r h \rho g}{2 \cos\theta}$$

Where r is the radius of capillary, h is the height ρ is the density of the liquid, g is the acceleration due to gravity and θ is the angle that the liquid makes with the walls of capillary.

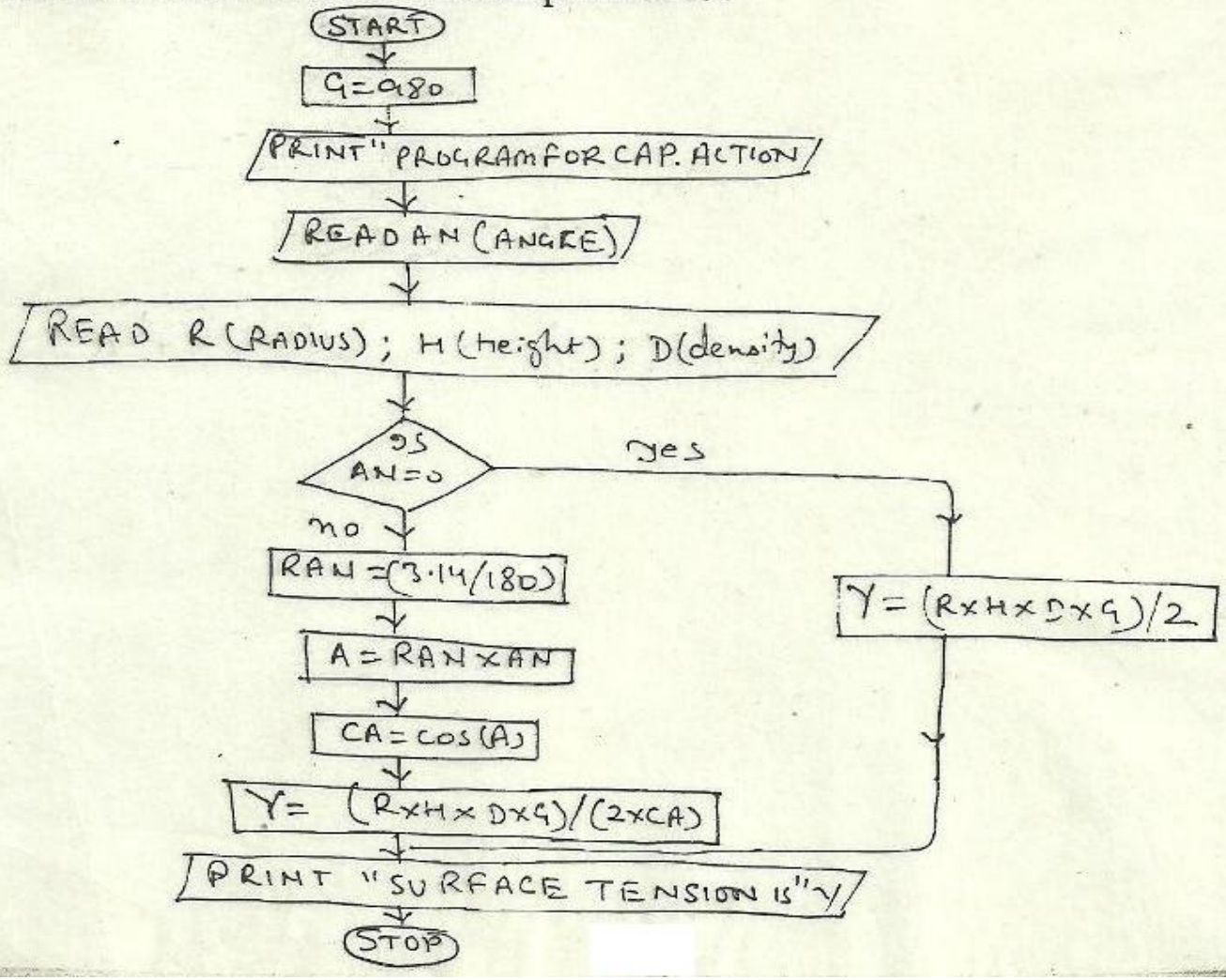


Figure

For $\theta = 0^{\circ}$ i.e. for $\cos\theta = 1$

$$\gamma = \frac{rh\rho g}{2}$$

Therefore the flow chart for this computation is :

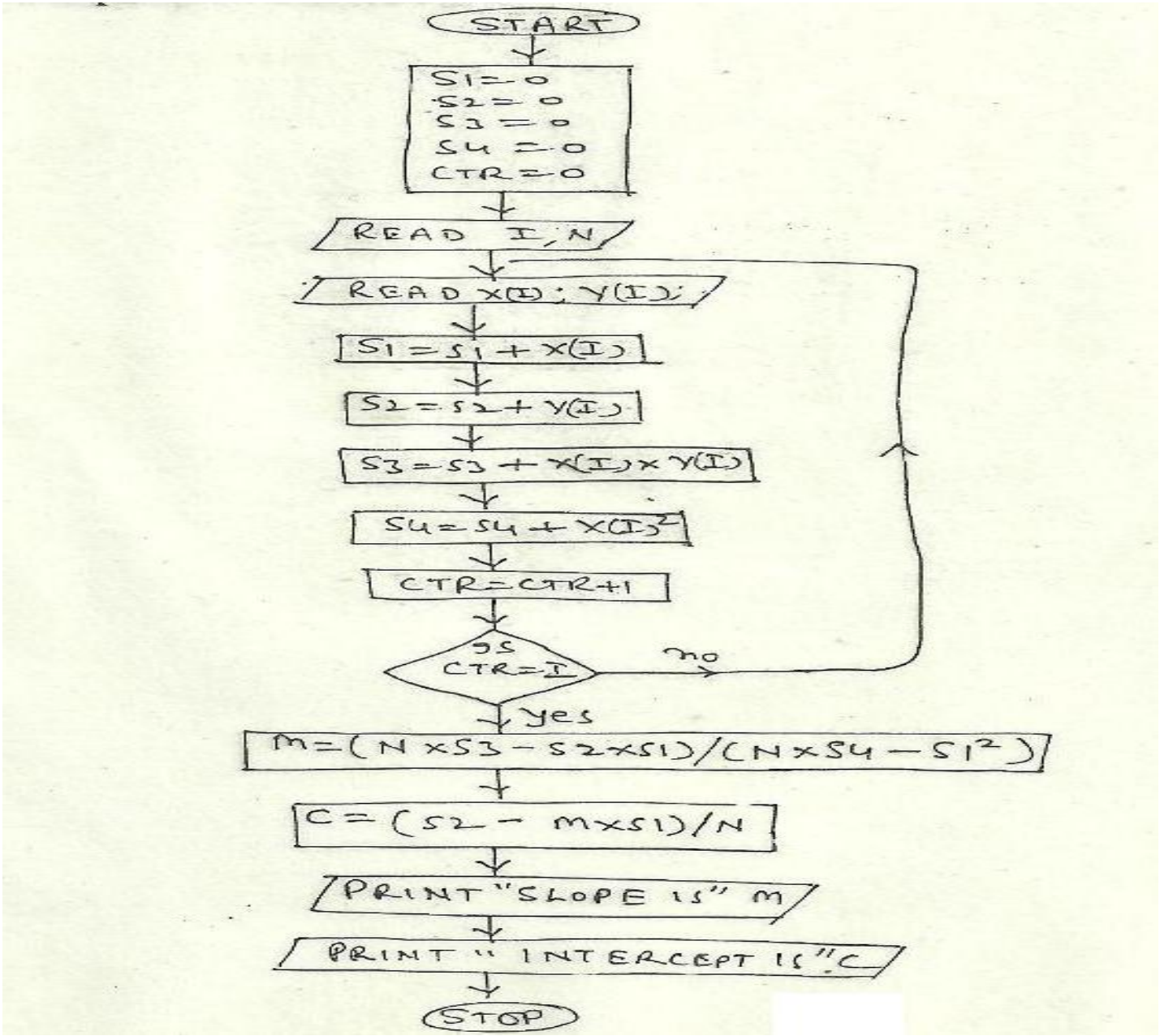


53. *To compute the slope and the intercept for the given set of data of straight line:*

As for computation of slope and intercept for a best fit straight line on the basis method of least squares, formulae are

$$m(\text{slope}) = \frac{(n \times \Sigma x_i y_i) - (\Sigma x_i)(\Sigma y_i)}{(n \times \Sigma x_i^2) - (\Sigma x_i)^2} \quad \& \quad C(\text{intercept}) = \frac{1}{n}\left(\Sigma y_i - m \times \Sigma x_i\right)$$

For x_i, y_i set of points. These two parameters for the best fit line can e computed using computer. In most of the experiments in the analytical and physical chemistry straight line graphs are to be plotted. Therefore, this computation is useful and beneficial for chemists. Flow chart for this computation is as follows:


START
S1 = 0
S2 = 0
S3 = 0
S4 = 0
CTR = 0
READ I, N
READ X(I); Y(I);
S1 = S1 + X(I)
S2 = S2 + Y(I)
S3 = S3 + X(I) x Y(I)
S4 = S4 + X(I)²
CTR = CTR + 1
IS CTR = I
no
yes
M = (N x S3 - S2 x S1) / (N x S4 - S1²)
C = (S2 - M x S1) / N
PRINT "SLOPE IS" M
PRINT "INTERCEPT IS" C
STOP

Program for COL or Normality & Molarity

molecular wt of solute. Flow chart for this computation has been included in chapter 2 (section 2.2). Its program listing in BASIC is given below:

```
10 N = 0
20 M = 0
30 M1 = 0
40 PRINT "GIVE WT OF SOLUTE"
50 INPUT W
60 PRINT "GIVE VOLUME OF SOLUTION"
70 INPUT V
80 PRINT "ENTER EQ WT OF SOLUTE"
90 INPUT E
100 PRINT "ENTER MOL WT OF SOLUTE"
110 INPUT MOL
120 PRINT "ENTER WT OF SOLVENT"
130 INPUT WT
140 N = (1000*W)/(V*E)
150 M = (1000*W)/(V*MOL)
160 M1 = (1000*W)/(MOL*WT)
170 PRINT "NORMALITY OF THE SOLUTION IS "N
180 PRINT "MOLARITY OF THE SOLUTION IS "M
190 PRINT "MOLALITY OF THE SOLUTION IS "M1
200 END
Ok_
```

Its output is :

```
RUN
GIVE WT OF SOLUTE
? 6.3
GIVE VOLUME OF SOLUTION
? 1000
ENTER EQ WT OF SOLUTE
? 63
ENTER MOL WT OF SOLUTE
? 126
ENTER WT OF SOLVENT
? 1000
NORMALITY OF THE SOLUTION IS  .1
MOLARITY OF THE SOLUTION IS  .05
MOLALITY OF THE SOLUTION IS  .05
Ok_
```

PROGRAM FOR AV & SD OF DATA

```
10 DIM X(100)
20 S = 0
30 S1 = 0
35 INPUT N
40 FOR I = 1 TO N
50 READ X(I)
60 S = S+X(I)
70 NEXT I
80 A = S/N
90 FOR I = 1 TO N
100 S1 = S1+(X(I)-A)^2
110 NEXT I
120 V = S1/(N-1)
130 SD = SQR(V)
140 PRINT A,V,SD
150 DATA 2,3,4,4,4,5,6,7,8,9
160 END
Ok_
```

Out put is

```
RUN
? 5
 3.4         .8          .8944272
Ok_
```

7. Program to compute and print the roots of quadratic equation

As quadratic equation is $AX^2 + BX + C = 0$ for which roots can be computed when D , the discriminant is greater than zero. Flow chart for this computation is given in chapter 2 (ref. 2.2). Its program in BASIC is given below:

```
5 REM PROGRAM FOR COMPUTING ROOTS OF QUADRATIC
EQUATION
10 D = 0
20 S = 0
25 PRINT " ENTER A,B,C"
30 INPUT A,B,C
40 D = (B^2)-(4*A*C)
50 IF D > 0 THEN 60 ELSE 100
60 S = SQR(D)
70 X1 = (-B+S)/(2*A)
80 X2 = (-B-S)/(2*A)
90 PRINT "ROOTS ARE "X1,X2
95 GOTO 110
100 PRINT "ROOTS ARE IMAGINARY"
```

```
110 END
Ok_
```

Output is

```
RUN
 ENTER A,B,C
? 1,3,2
ROOTS ARE -1  -2
Ok_
```

8. Program for printing squares of first 100 natural numbers:

Program listing for this computation is given below in BASIC and its flow chart has already given in chapter2.

```
5 REM PROGRAM FOR PRINTING SQUARES OF FIRST 100 NATURAL
NUMBERS
10 N = 0
20 I = 0
30 N = N+1
40 I = N^2
50 PRINT I
60 IF N > 100 THEN 70 ELSE 30
70 END
Ok_
```

Output is :

This program on execution will print the squares of first 100 natural numbers.

9. Program to compute the values of X and Y variables in the solution of system of simultaneous equations:

As system of simultaneous equations are

A1X + B1Y = C1

A2X + B2Y = C2

Flow chart for computation of the values of X and Y has already been given in chapter 2 and its program in BASIC is given below:

```
5 REM PROGRAM FOR SYSTEM OF SIMULTANEOUS EQUATION
10 X = 0
20 Y = 0
30 Z = 0
40 P = 0
50 Q = 0
60 PRINT "GIVE THE VALUES FOR A1,A2,B1,B2,C1,C2"
```

```
70 INPUT A1,A1,B1,B2,C1,C2
80 Z = (A2*B1)-(A1*B2)
90 P = (C2*B1)-(B2*C1)
100 Q = (C1*A2)-(A1*C2)
110 X = P/Z
120 Y = Q/Z
130 PRINT " THE VALUE OF X IS ";X
135 PRINT "THE VALUE OF Y IS " ;Y
140 END
Ok_
```

Out put is

```
RUN
GIVE THE VALUES FOR A1,A2,B1,B2,C1,C2
? 2,3,4,4,3,5
 THE VALUE OF X IS -.6666667
THE VALUE OF Y IS  1.25
Ok_
```

10. To print the factorial of a number N:

As factorial for a number is N(N-1)(N-2).....1. For this computation flow chart has already been given in chapter 2 and here program listing for this computation in BASIC is given.

```
5 REM PROGRAM FOR COMPUTING FACTORIAL OF A NUMBER
10 F = 1
20 INPUT N
30 F = F*N
40 N = N-1
50 IF N = 0 THEN 60 ELSE 30
60 PRINT " FACTORIAL OF THIS NUMBER IS " F
70 END
Ok_
```

Output is

```
RUN
? 5
 FACTORIAL OF THIS NUMBER IS  120
Ok_
```

11. Program to compute the value of area and circumference of a circle:

```
170 VISC = X/Y
180 PRINT "VISCOSITY OF THE LIQUID IS "VISC
190 END
Ok_
```

Its output is:

```
RUN
PROGRAM FOR CAL OF VISCOSITY ON POSULIE'S EQUATION
ENTER THE VALUE OF RADIUS OF CAPILLARY
? 0.5
ENTER THE VALUE OF PRESSURE HEAD
? 760
ENTER THE VALUE OF TIME OF FLOW
? 20
ENTER THE VALUE OF LENGTH OF LIQUID FLOW
? 5
ENTER THE VALUE OF VOLUME OF LIQUID FLOW
? 3
VISCOSITY OF THE LIQUID IS  24.85834
Ok_
```

31. Program for computation of value of β and hence to find out the value of n_i on the basis of Boltzmann's statistics:

According to the Boltzmann Statistics number of particles in the I^{th} level is given by

$$n_i = n_0 e^{-\beta \epsilon_i}$$

Where n_0 is the number of particles in the ground state or in the zeroth state and β is a constant equal to 1/kT and ϵ_i is the energy of i^{th} level. Program for this computation can is as follows, considering n_0 as N_A (the Avogadro's number):

```
5 REM PROGRAM FOR MAXWELL DISTRIBUTION
10 K = 1.38E-16
20 NA = 6.023E+23
30 PRINT " PROGRAM FOR MAXWELL DISTRIBUTION"
40 PRINT " ENTER THE VALUE OF TEMP"
50 INPUT T
60 PRINT "ENTER THE VALUE OF ENERGY OF LEVEL"
70 INPUT E
80 B = 1/(K*T)
90 X =-(E*B)
```

```
100 Y = EXP(X)
110 NI = NA*Y
120 PRINT "VALUE OF B IS "B
130 PRINT "NO OF PARTICLES IN THE LEVEL ARE "NI
140 END
Ok_
```

Its output is:

```
RUN
 PROGRAM FOR MAXWELL DISTRIBUTION
 ENTER THE VALUE OF TEMP
? 373
ENTER THE VALUE OF ENERGY OF LEVEL
? 3E4
VALUE OF B IS  1.942728E+13
NO OF PARTICLES IN THE LEVEL ARE  1.701412E+38
Ok_
```

32. Program for computation of K_a for weak acid (say acetic acid):

For any weak acid like acetic acid when C is the concentration and α is the degree of ionization of acid, the K_a value can be predicted on the basis of Ostwald's dilution law as

$$K_a = c\alpha^2/(1-\alpha)$$

Its program is as follows:

```
5 REM PROGRAM FOR DILUTION LAW
10 PRINT "PROGRAM FOR OSTWALD DITUTION LAW"
20 PRINT "ENTER THE VALUE OF DEGREE OF DISOCIATION"
30 INPUT ALP
40 PRINT "ENTER THE VALUE OF CONCENTRATION"
50 INPUT C
60 IF ALP > 1 THEN 70 ELSE 90
70 PRINT "YOU ARE JOCKING"
80 GOTO 130
90 X = C*(ALP^2)
100 Y = 1-ALP
110 KA = X/Y
120 PRINT " THE VALUE OF DISOCIATION CONSTANT IS "KA
130 END
Ok_
```

PROGRAM TO CALL μ S + L

Its program is as follows:

```
5 REM PROGRAM FOR CALCULATION OF MAGNETIC MOMENT
10 PRINT " PROGRM FOR CALCULATION OF MAGNETIC MOMENT
WITH ORBITAL CONTROBUTION
20 PRINT " ENTER THE VALUES FOR SPIN QUAMTUM NUMBER"
30 INPUT S
40 PRINT " ENTER THE VALUE FOR ORBITAL QUANTUM NUMBER"
50 INPUT L
60 X = 4*S*(S+1)
70 Y = L*(L+1)
80 Z = X+Y
90 MU = SQR(Z)
100 PRINT "MAGNETIC MOMENT WITH ORBITAL CONTRIBUTION IS
";MU
110 END
Ok_
```

Its output is:

```
RUN
 PROGRM FOR CALCULATION OF MAGNETIC MOMENT WITH
ORBITAL CONTROBUTION
 ENTER THE VALUES FOR SPIN QUAMTUM NUMBER
? 0.5
 ENTER THE VALUE FOR ORBITAL QUANTUM NUMBER
? 2
MAGNETIC MOMENT WITH ORBITAL CONTRIBUTION IS  3
Ok_
```

35 .Program for computation of value of Bohr magneton:

```
10 REM PROGRAM FOR BOHR MAGNETON
20 E = 1.6020E-19
30 H = 6.636E-34
40 PI = 3.14159
50 M = 9.1091E-31
60 C = 2.99E 8
70 BM = (E*H)/(4*PI*M*C)
80 PRINT "BOHR MAGNETON IS ";BM
90 END
```

```
 ENTER THE HEAT OF FORMATION
? 98
 ENTER THE HEAT OF SUBLIMATION
? 26
 ENTER THE IONIZATION POTENTIAL
? 118
 ENTER THE DISSOCIATION ENERGY
? 58
 ENTER THE VALUE OF ELECTRON AFFINITY
? 87
 LATTICE ENERGY FOR THE NACL IS 184
Ok_
```

46. Program for computation of lattice energy on the basis of Born Lande's Equation:

As Born Lande's equation is

$$U = \frac{N_A A e^2 Z + Z -}{r_0}\left(1 - \frac{1}{n}\right)$$

So, program for this computation is as follows:

```
LIST
10 PRINT "PROGRAM TO CALCULATE LATTICE ENERGY ON THE BASIS
OF BORN LANDE EQ"
20 PRINT " ENTER CHARGES"
30 INPUT Z1,Z2
40 PRINT " ENTER THE NAME OF CRYSTAL"
45 B = 8
50 INPUT C$
52 PRINT " ENTER THE BOND DISTANCE"
55 INPUT DIST
60 NA = 6.023E+23
65 MAC = 1.74
70 C1 = 4.8E-10
80 C2 = 1E-10
90 P = Z1*Z2
100 X1 = NA*MAC*P
110 Y = 1/B
120 X2 = C1*C2*(1-Y)
130 LE = X1*(X2/DIST)*C2
140 PRINT " LATTICE ENERGY IS " LE
150 END
Ok_
```

```
WANT TO CALCULATE WAVE LENGTH OR FREQUENCY OR ENERGY
ENTER THE DATA KEEPING UNKNOWN ZERO
? 2.4E4,3E-9,0
 ENERGY IS  1.59264E-29
Ok_
```

48. Program for computation of surface tension on the basis of capillary action:

For capillary action

$$\gamma = \frac{r h \rho g}{2 \cos \theta}$$

Where r is the radius of capillary, h is the height ρ is the density of the liquid, g is the acceleration due to gravity and θ is the angle that the liquid makes with the walls of capillary. Program for this computation is:

```
LIST
5 REM PROGRAM FOR CAPILLARY ACTION
10 PRINT " PROGRAM FOR CAPILLARY ACTION "
20 PRINT " ENTER ANGLE"
30 G = 980
40 INPUT AN
60 PRINT " ENTER RADIUS OF CAPILLARY"
70 INPUT R
```

```
80 PRINT " ENETR HEIGHT UPTO WHICH LIQUID RISE"
90 INPUT H
100 PRINT " ENTER DENSITY OF LIQUID "
110 INPUT D
120 IF AN = 0 THEN 130 ELSE 140
130 Y = (R*H*D*G)/2
135 GOTO 180
140 RAN = 3.14/180
150 A = RAN*AN
160 CA = COS(A)
170 Y = (R*H*D*G)/(2*CA)
180 PRINT " SURFACE TENSION IS " Y
190 END
Ok_
```

Its output is:

```
RUN
 PROGRAM FOR CAPILLARY ACTION
 ENTER ANGLE
? 0
```

Here in this program matrix elements are given as data points in the data card in line no. 130,which can be changed according to requirement. This program will print the matrix and its transpose on the screen.

61.Program to evaluate any integral on the basis of Monte Carlo's method:

It is a numerical integration technique for which the program in the BASIC language is as follows. This program asks the number of iterations or the number of times the user wants to solve the integral and after getting the input from the user as 'N' it generates a random number and solve the integral for 'N' iterations and finally prints the result.

```
LIST
10 PRINT" PROGRM TO SOLVE AN INTEGRAL ON THE BASIS OF
MONTECARLO METHOD"
20 PRINT" ENTER THE NUMBER OF TIMES YOU WANT TO CYCLIZE THE
INTEGRAL"
30 INPUT N
40 S = 0
50 FOR I = 1 TO N
60 Z = RND
70 F = 1/(1+Z^2)
80 S = S+F
90 NEXT I
100 IN = S/N
110 PRINT IN
120 END
Ok_
```

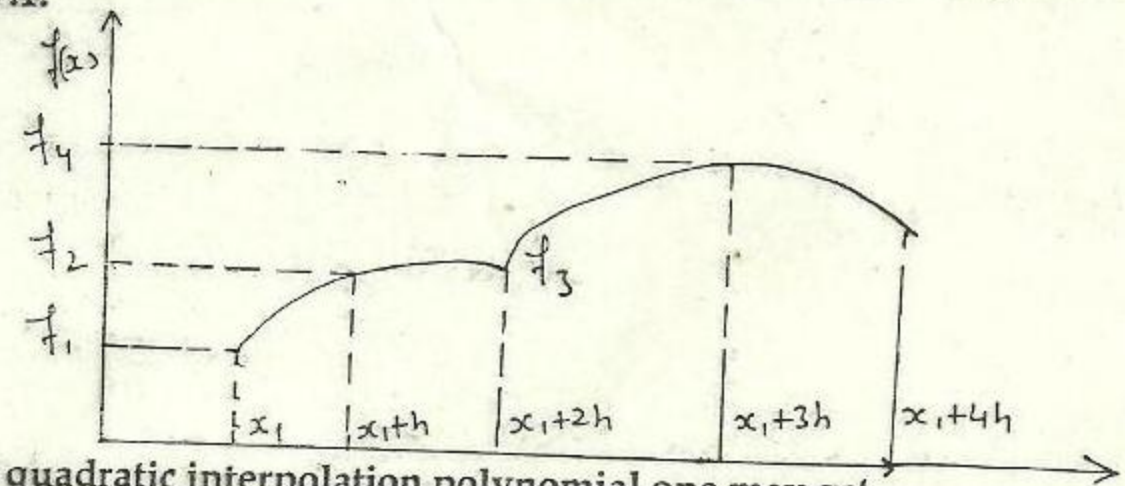
Output of this program is:

```
RUN
 PROGRM TO SOLVE AN INTEGRAL ON THE BASIS OF MONTECARLO
METHOD
 ENTER THE NUMBER OF TIMES YOU WANT TO CYCLIZE THE
INTEGRAL
? 1000
 .7817735
Ok_
```

62. Program to solve the integral on the basis of Simpson's rule:

Simpson's rule is a popular numerical integration method. It is based on the approximating the function f(x) by fitting quadratics through sets of three

points. These points are illustrated graphically as per according the following figure 7.1.



Using a quadratic interpolation polynomial one may get

$$S = \int_{x_1}^{x_1+nh} f(x)\,dx = \sum_{i=1,3\ldots n-2} \int_{x_i}^{x_i+2h} \left[f_i + \frac{\Delta f_i}{h}(x-x_i) + \frac{\Delta^2 f_i}{2h^2}(x-x_i)(x-x_i-h) \right] dx$$

Integrating the above expression we obtain

$$S = \sum_{i=1,3,5\ldots n-2} h/3\,(f_i + 4f_{i+1} + f_{i+2})$$

$$= h/3\,[f_1 + 4f_2 + 2f_3 + 4f_4 + 2f_5 + 4f_6 + \ldots + f_{n+1}]$$

In using the above formula it is implied that f is tabulated at an odd number of points. The exact value of any integral on the basis of Simpson's rule may also be zero as Simpson's rule is exact up to a cubic. The Simpson's formula may also be derived by a technique called the method of undetermined coefficients. In this method we seek an integration formula of the type

$$S = af_1 + bf_2 + cf_3$$

Where f1,f2 and f3 are the values of the function being integrated at the three points viz. x1, x1+h and x1+2h and a, b and c are constants to be determined. Program for evaluation of integral on the basis of Simpson's rule is as follows:

```
. LIST
5 REM SIMPSON'S RULE PROGRAM
10 PRINT " PROGRM FOR INTEGRATION ON THE BASIS OF SIMPSON
RULE"
20 INPUT A,E
30 DEF FNA(X) = X*X
40 N = 4
50 S = 0
60 H = (E-A)/N
70 S = FNA(X)
80 FOR I = 1 TO N-1 STEP 2
90 X = A+I*H
100 S = S+4*FNA(X)
110 NEXT I
```

? 3E8
THE VALUE OF WAVE LENGTH ON THE BASIS OF DEBROGLIE EQ FOR THE
PARTICLE IS 2.430769E-05
Ok_

53. To compute the slope and the Intercept for the given set of data of straight line:

As for computation of slope and intercept for a best fit straight line on the basis method of least squares, formulae are

$$m(\text{slope}) = \frac{(n \times \Sigma x_i y_i) - (\Sigma x_i)(\Sigma y_i)}{(n \times \Sigma x_i^2) - (\Sigma x_i)^2} \quad \& \quad c(\text{intercept}) = \frac{1}{n}\left(\Sigma y_i - m \times \Sigma x_i\right)$$

For x_i, y_i set of points. These two parameters for the best fit line can e computed using computer. In most of the experiments in the analytical and physical chemistry straight line graphs are to be plotted. Therefore, this computation is useful and beneficial for chemists. Program for this computation is as follows:

```
LIST
10 PRINT " PROGRM FOR LEAST SQUARE FIT"
20 DIM X(100), Y(100)
30 S1 = 0
40 S2 = 0
50 S3 = 0
60 S4 = 0
70 INPUT N
80 FOR I = 1 TO N
90 READ X(I)
100 READ Y(I)
110 S1 = S1+X(I)
120 S2 = S2+Y(I)
130 S3 = S3+X(I)*Y(I)
140 S4 = S4 +X(I)^2
150 NEXT I
160 M = (N*S3-S1*S2)/(N*S4-S1^2)
170 C = (S2-M*S1)/N
180 PRINT "SLOPE OF THE GIVEN DATA IS" M
190 PRINT " INTERCEPT OF THE GIVEN DATA IS "C
200 DATA 3,2,4,7,3,5,9,20
210 END
Ok_
```

Its output is :

```
RUN
 PROGRM FOR LEAST SQUARE FIT
? 4
SLOPE OF THE GIVEN DATA IS 2.727273
 INTERCEPT OF THE GIVEN DATA IS -4.454546
Ok_
```

Data point are given in the data card in the program itself in line number 200.

54. To compute correlation coefficient for the given set of data :

Correlation coefficient is also a parameter which is useful for estimating the correlation between set of data (i.e. experimental observations) in any scientific field. This coefficient can be computed on the basis of following formula

$$\rho = \frac{\Sigma xy}{\sqrt{\Sigma x^2}\sqrt{\Sigma y^2}}$$

where $x = X_i - \bar{X}$ (x average)

$y = Y_i - \bar{Y}$ (y average)

Program for this computation is given below:

```
LIST
10 PRINT " PROGRAM FOR COMPUTATION OF CORRELATION COEFF."
20 S = 0
30 S1 = 0
40 S2 = 0
50 S3 = 0
60 S4 = 0
70 PRINT "ENTER THE LIMIT"
80 INPUT N
90 FOR I = 1 TO N
100 READ X(I),Y(I)
110 S = S+X(I)
120 S1 = S1+Y(I)
130 NEXT I
140 XB = S/N
150 YB = S1/N
160 FOR I = 1 TO N
170 S2 = S2+(X(I)-XB)*(Y(I)-YB)
180 S3 = S3+(X(I)-XB)^2
190 S4 = S4+(Y(I)-YB)^2
200 NEXT I
210 NUM1 = SQR(S3)
220 NUM2 = SQR(S4)
230 CC = S2/(NUM1*NUM2)
```

```
240 PRINT " AVERAGE OF X(I) DATA IS " ;XB
250 PRINT " AVERAGE OF Y(I) DATA IS " ;YB
260 PRINT " CORRELATION COEFFICIENT BETWEEN X(I) AND Y(I) IS
";CC
265 DATA 2,3,2,3,4,5,4,5,6,7,6,7,8,7,8,8,3,9,20
270 END
Ok_
```

Output of this program is :

```
RUN
 PROGRAM FOR COMPUTATION OF CORRELATION COEFF.
ENTER THE LIMIT
? 5
 AVERAGE OF X(I) DATA IS  3
 AVERAGE OF Y(I) DATA IS  3.8
 CORRELATION COEFFICIENT BETWEEN X(I) AND Y(I) IS  .874 0074
Ok_
```

Data points are given in line number 265 in the program itself. One can change these data points according to requirements.

These are some programs for which flowcharts are given in chapter 2(ref. section 2.2). Now, some programs are given which are also useful in Chemistry and for some numerical analysis.

55. Program for computation of iso-electric point :

As iso-electric point for any amino acid is given by the following formula:

$pH = pI_{so} = (pK_1 + pK_2)/2$ where pK_1 & pK_2 are dissociation constants for $\overset{+}{N}H_3CH_2COO^-$ & $NH_2CH_2COO^-$ ions.

Program for computation of this point is given below:

```
LIST
10 PRINT " PROGRAM FOR CALCULATION OF ISOELECTRIC POINT"
20 PRINT " ENTER NAME OF ACID"
30 INPUT N$
40 PRINT " ENTER DISSOCIATION CONSTANTS"
50 INPUT K1,K2
60 H = SQR(K1*K2)
70 H1 = -LOG(K1/2.303)
80 H2 = -LOG(K2/2.303)
90 I1 = (H1+H2)/2
100 PRINT " HYDROGEN ION CONCENTRATION IS " H
```

Further Reading

- Computers For Chemists by K. V. Raman, Tata McGraw Hill Publication.
- Computer Applications in Chemistry by Kishor Arora, Anmol Publications New Delhi's Publication.

Feel Free to contact for further information

- Via College's email: pgcdatia@rediffmail.com

- Best Of Luck

Computers Applications In Chemistry Part -II

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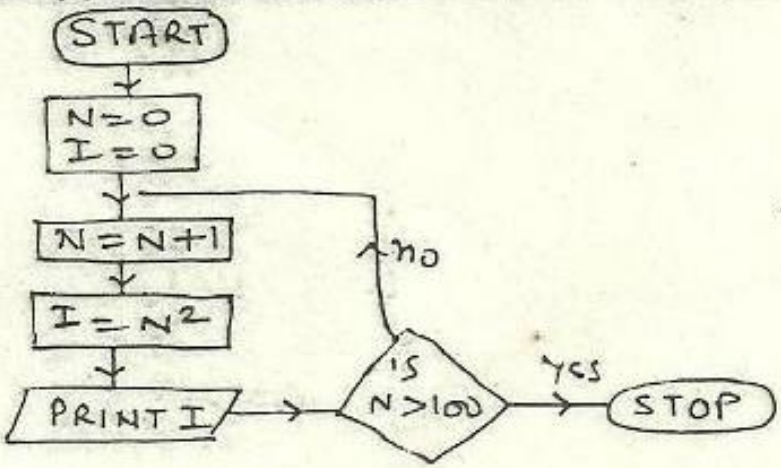
(M.P.) 475 661

Topics Covered

- Some More Examples – Programmes in BASIC
- Introduction to Computer Softwares used for teaching and research in Chemistry
- Classification of these Softwares.
- A little bit of uses of these softwares.

8. To print the squares of first 100 natural numbers the flow chart is :



9. To compute the value of X and Y variables in the solution of simultaneous equations :

As system of simultaneous equations are

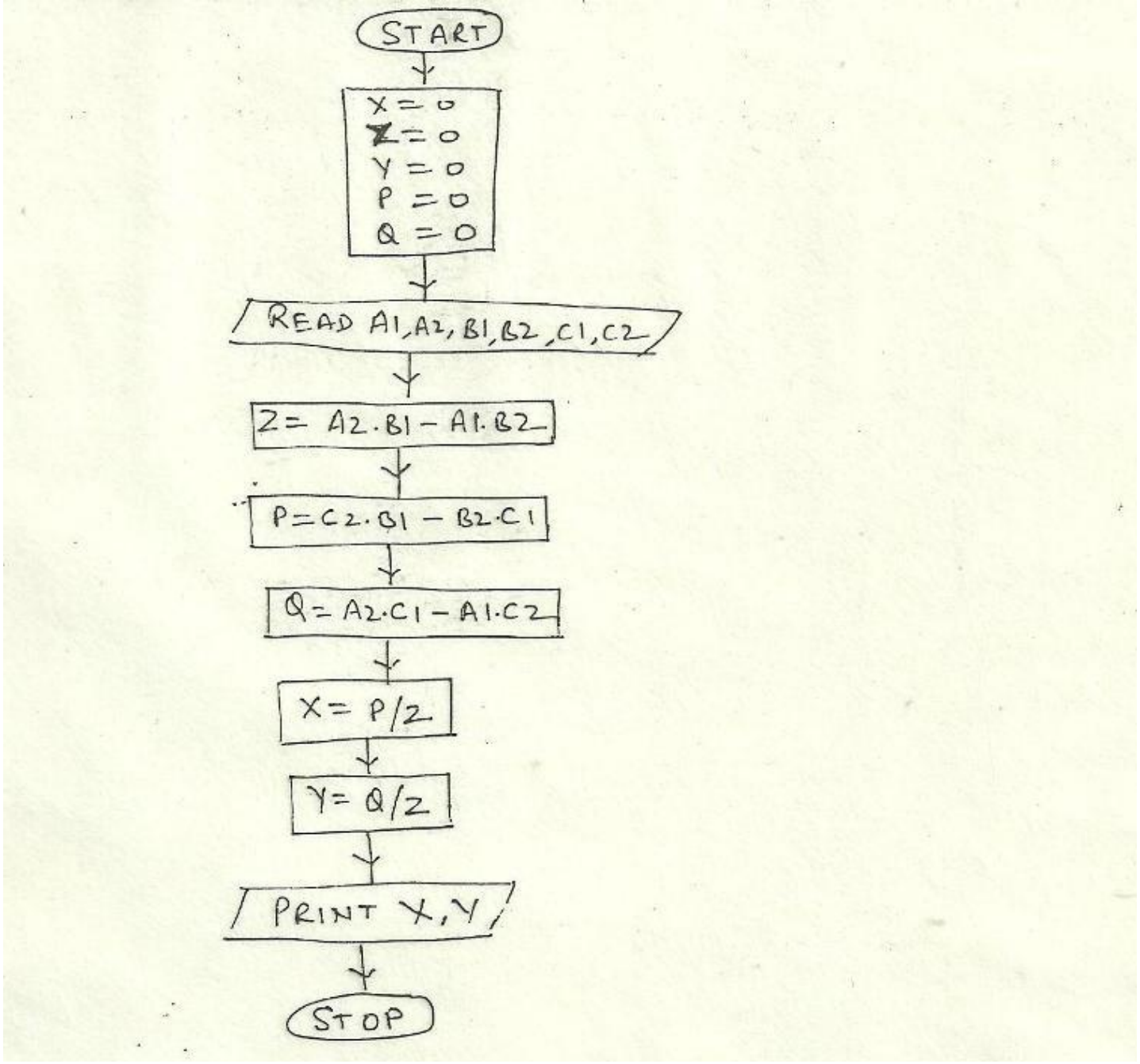
A1X + B1Y = C1

A2 X+ B2 Y = C2

These equations on solution gives

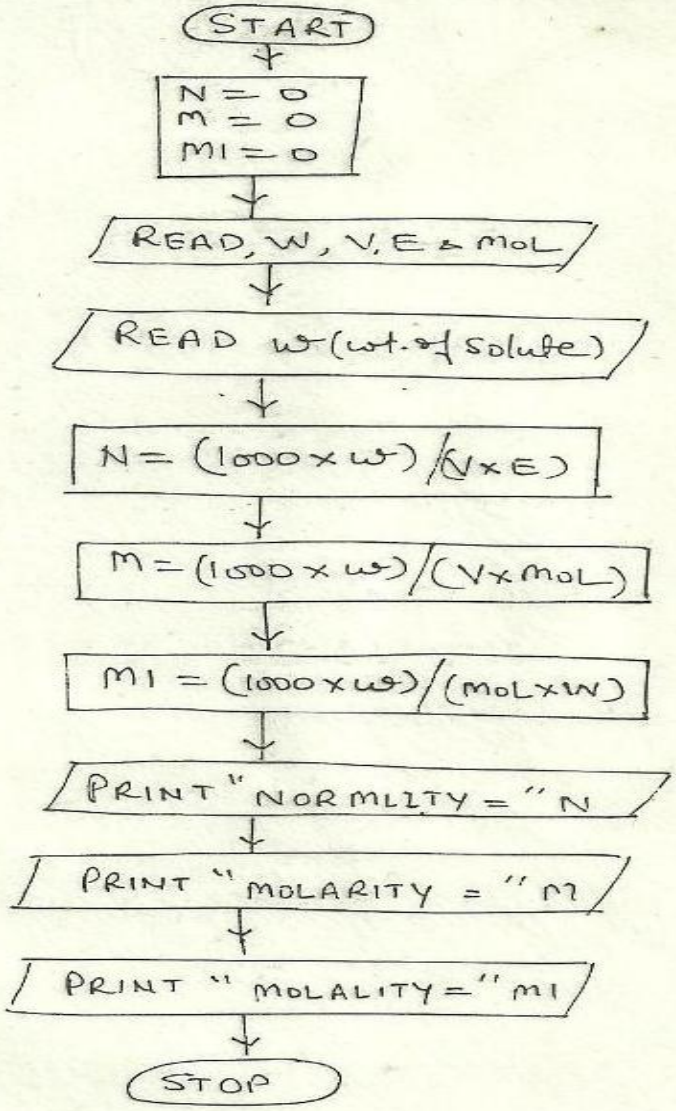
X = (B1C2 – B2C1)/(A2B1-A1B2) and Y = (A2C1 – A1 C2)/(A2B1- A1 B2).

So, flow chart for this problem.is


START
X = 0
Z = 0
Y = 0
P = 0
Q = 0
READ A1, A2, B1, B2, C1, C2
Z = A2 · B1 − A1 · B2
P = C2 · B1 − B2 · C1
Q = A2 · C1 − A1 · C2
X = P/Z
Y = Q/Z
PRINT X, Y
STOP

14. To compute normality, molarity and molality values for a given solution:

As normality is N = (1000×w)/ (V×E) ; molarity is M = (1000×w)/(V×Mol) and molality is m = (1000×w)/ (Mol×W) where W is the weight of solvent, V is the volume of solution, E is the equivalent weight of solute and Mol is the molecular weight of solute. Flow chart for computing these quantities is:

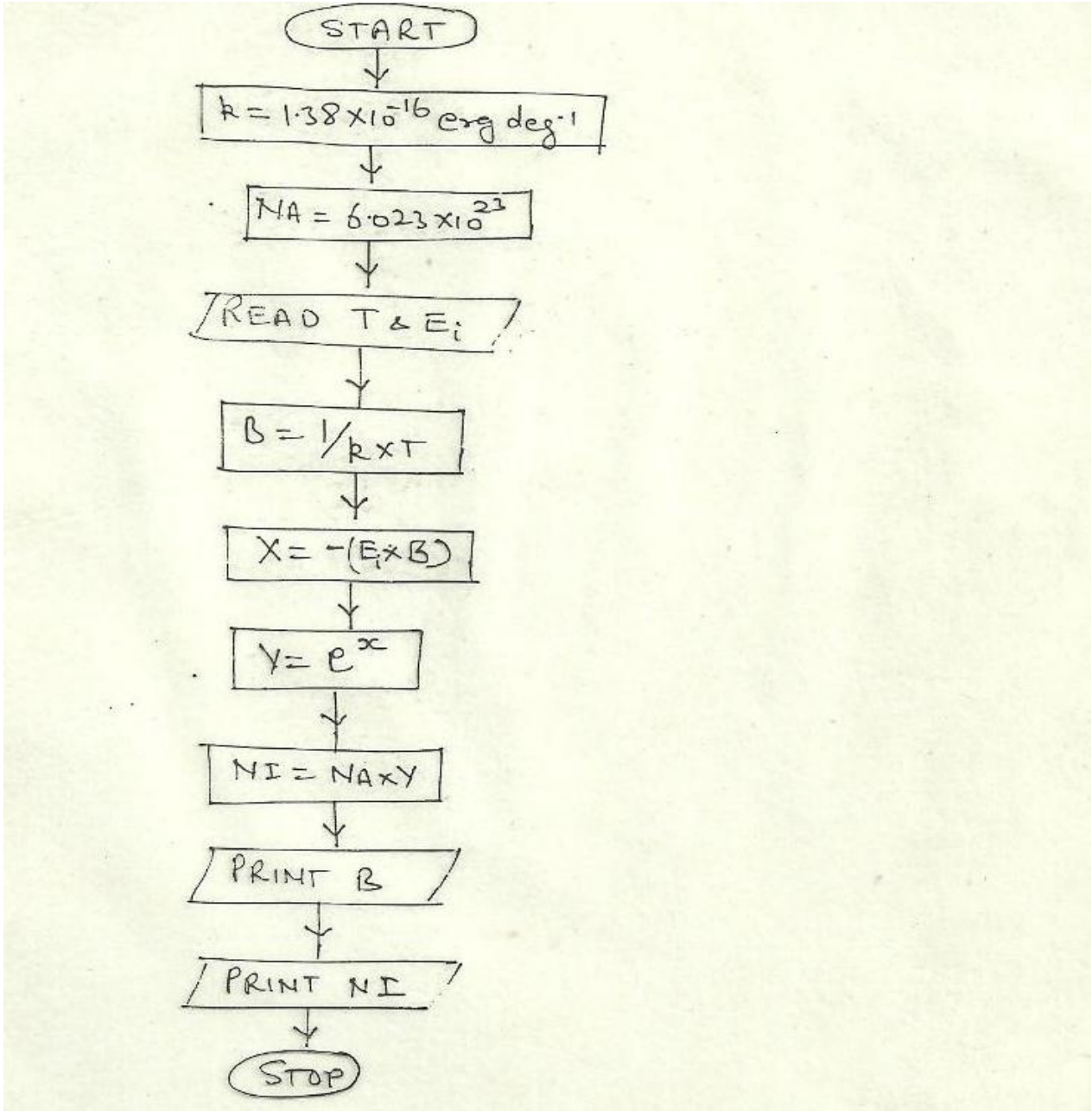


31 To compute the value of and hence to find out the value of n_i on the basis of Boltzmann Statistics

According to the Boltzmann Statistics number of particles in the I[th] level is given by

$$n_i = n_0 e^{-\beta \epsilon_i}$$

Where n_0 is the number of particles in the ground state or in the zeroth state and β is a constant equal to 1/kT and ϵ_i is the energy of i^{th} level. Flow chart for this computation can be drawn as follows, considering n_0 as N_A (the Avogadro's number)

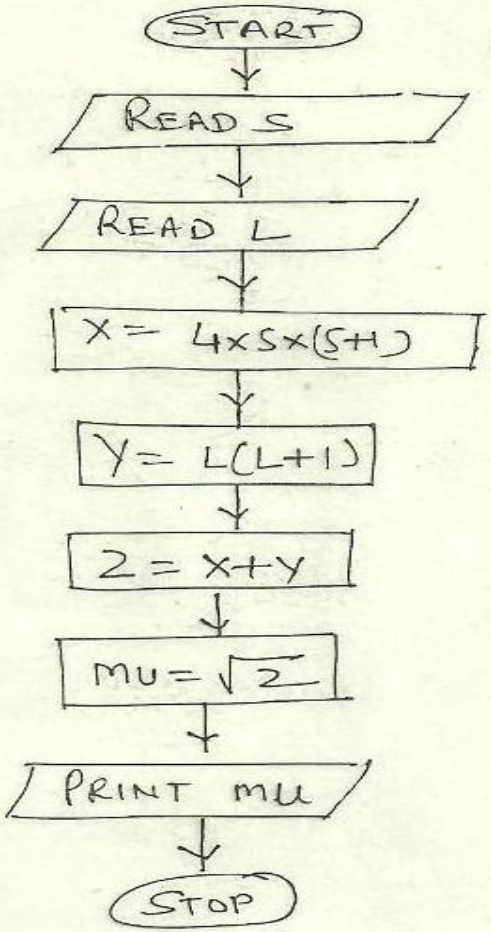

START
k = 1.38 x 10^-16 erg deg^-1
NA = 6.023 x 10^23
READ T & Ei
B = 1/k x T
X = -(Ei x B)
Y = e^x
NI = NA x Y
PRINT B
PRINT NI
STOP

34. To compute the value of magnetic moment of a substance on the basis of μ_{s+l} formula:

Magnetic moment of a substance can be calculated on the basis of μ_{s+l} formula as

$$\mu_{s+l} = \sqrt{4s(s+1) + l(l+1)} \text{ BM}$$

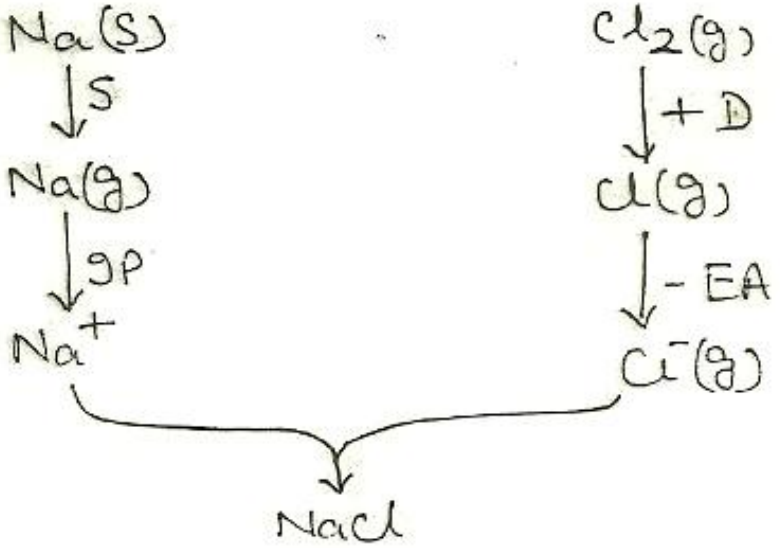
Its flow chart can be drawn as follows:



46 To compute the value of Lattice Energy on the basis of Born Haber's Cycle:

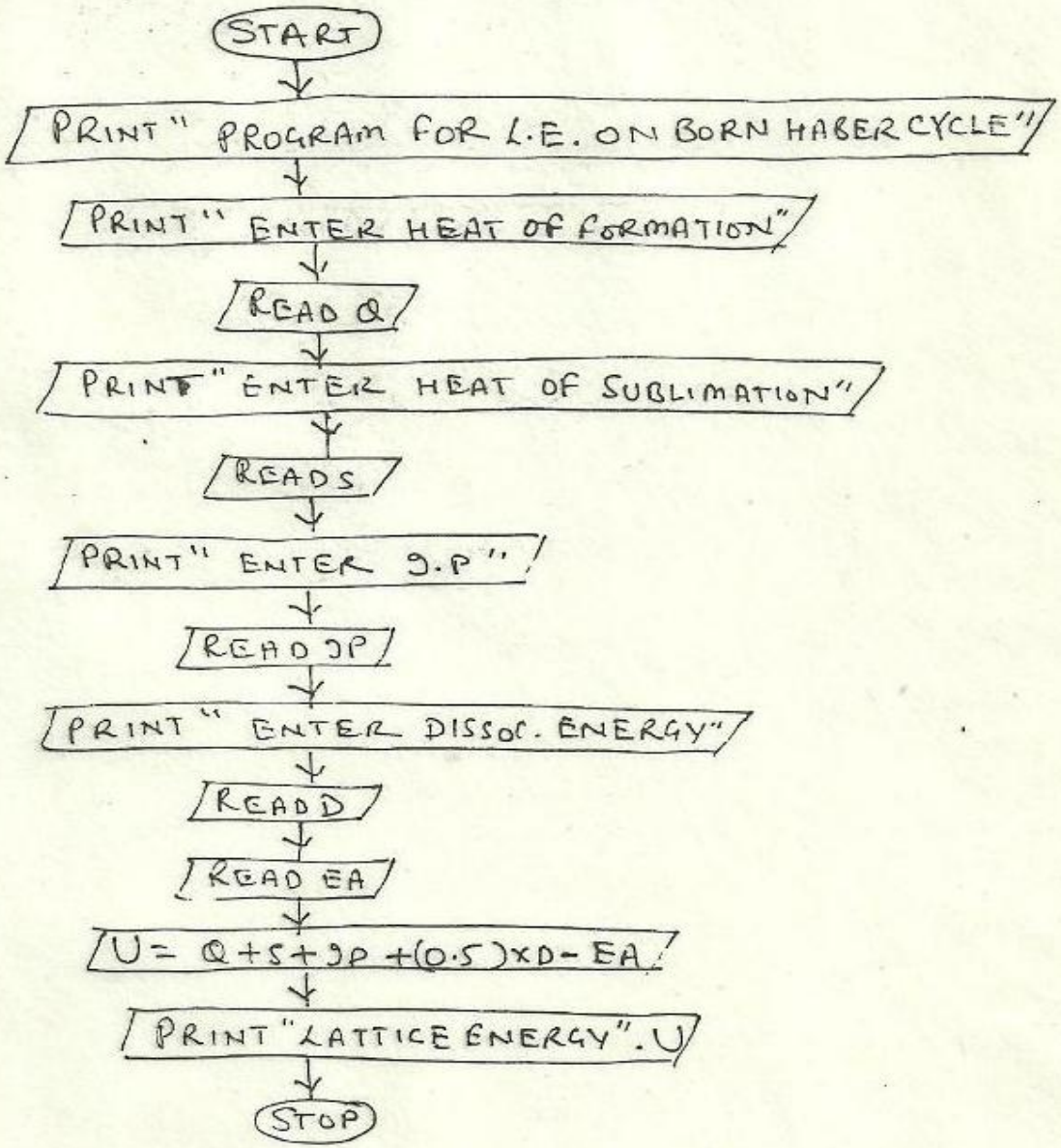
Lattice energy on the basis of Born Haber's Cycle can be calculated for a reaction as follows :

e.g. for the reaction $Na(g) + Cl_2(g) \xrightarrow{-Q} NaCl$ this cycle is as follows



So, $-Q = S + IP + \frac{1}{2}D - EA - U$, where S is the heat of sublimation, IP is the ionization potential of Na, D is the dissociation energy, EA is the electron affinity, U is the lattice energy and Q is the heat of formation. On rearranging it

$-U = -Q - S - IP - \frac{1}{2}D + EA$ or $U = Q + S + IP + \frac{1}{2}D - EA$. Its flow chart is :

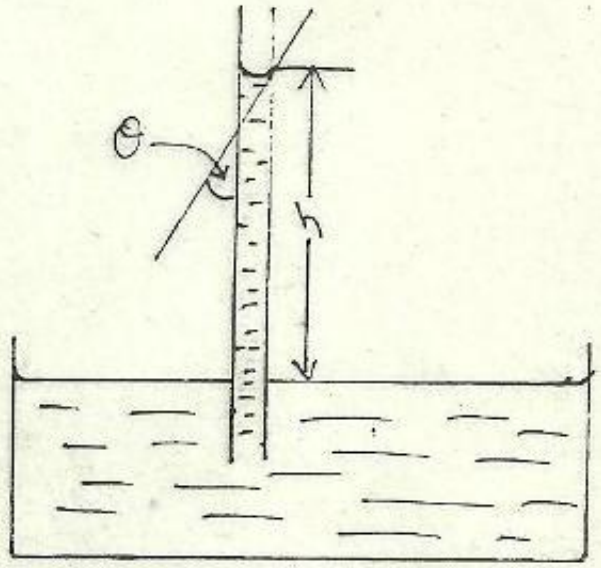


48 To calculate the value of surface tension on the basis of capillary action

For capillary action

$$\gamma = \frac{r h \rho g}{2 \cos\theta}$$

Where r is the radius of capillary, h is the height ρ is the density of the liquid, g is the acceleration due to gravity and θ is the angle that the liquid makes with the walls of capillary.

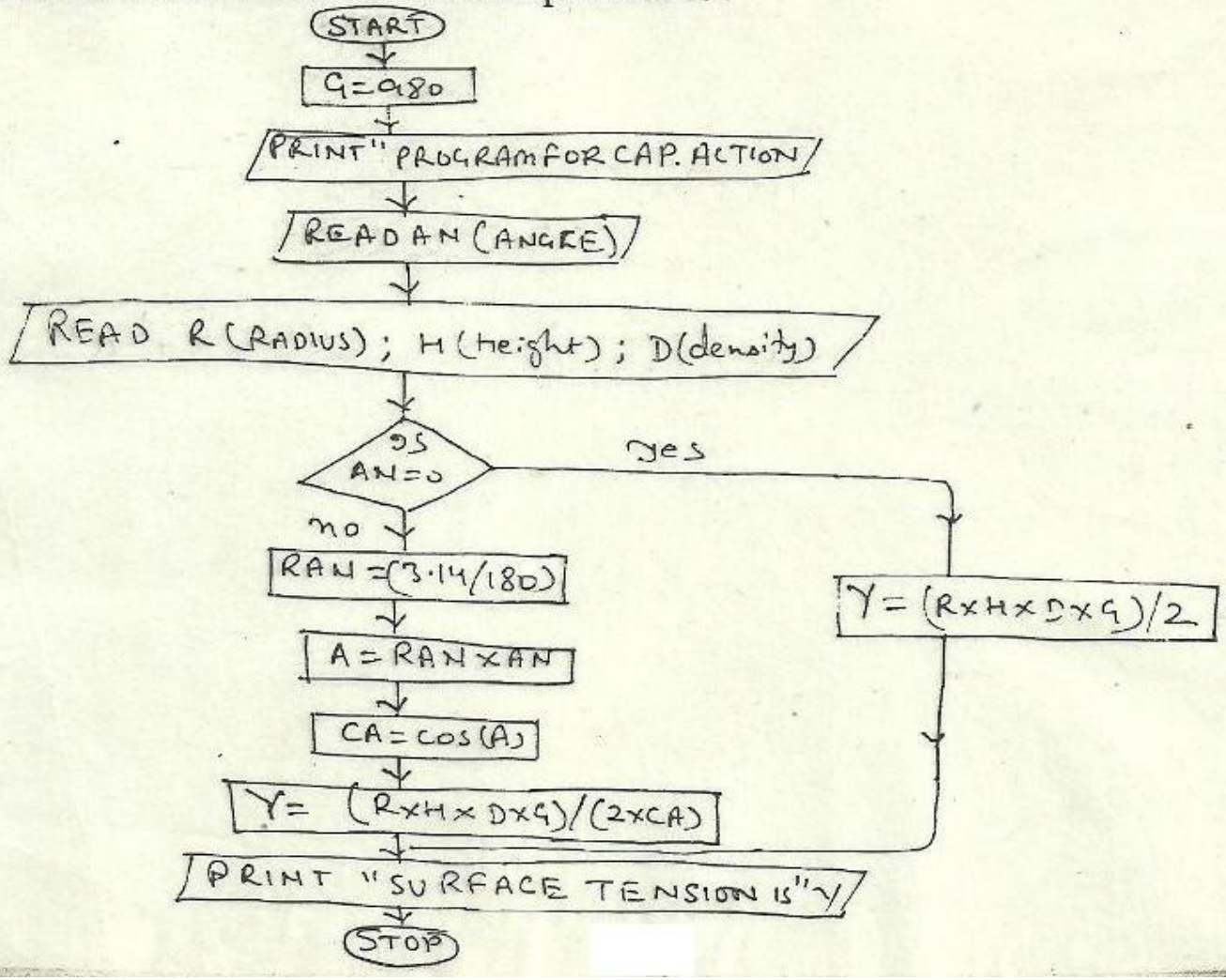


Figure

For $\theta = 0^{\circ}$ i.e. for $\cos\theta = 1$

$$\gamma = \frac{rh\rho g}{2}$$

Therefore the flow chart for this computation is :

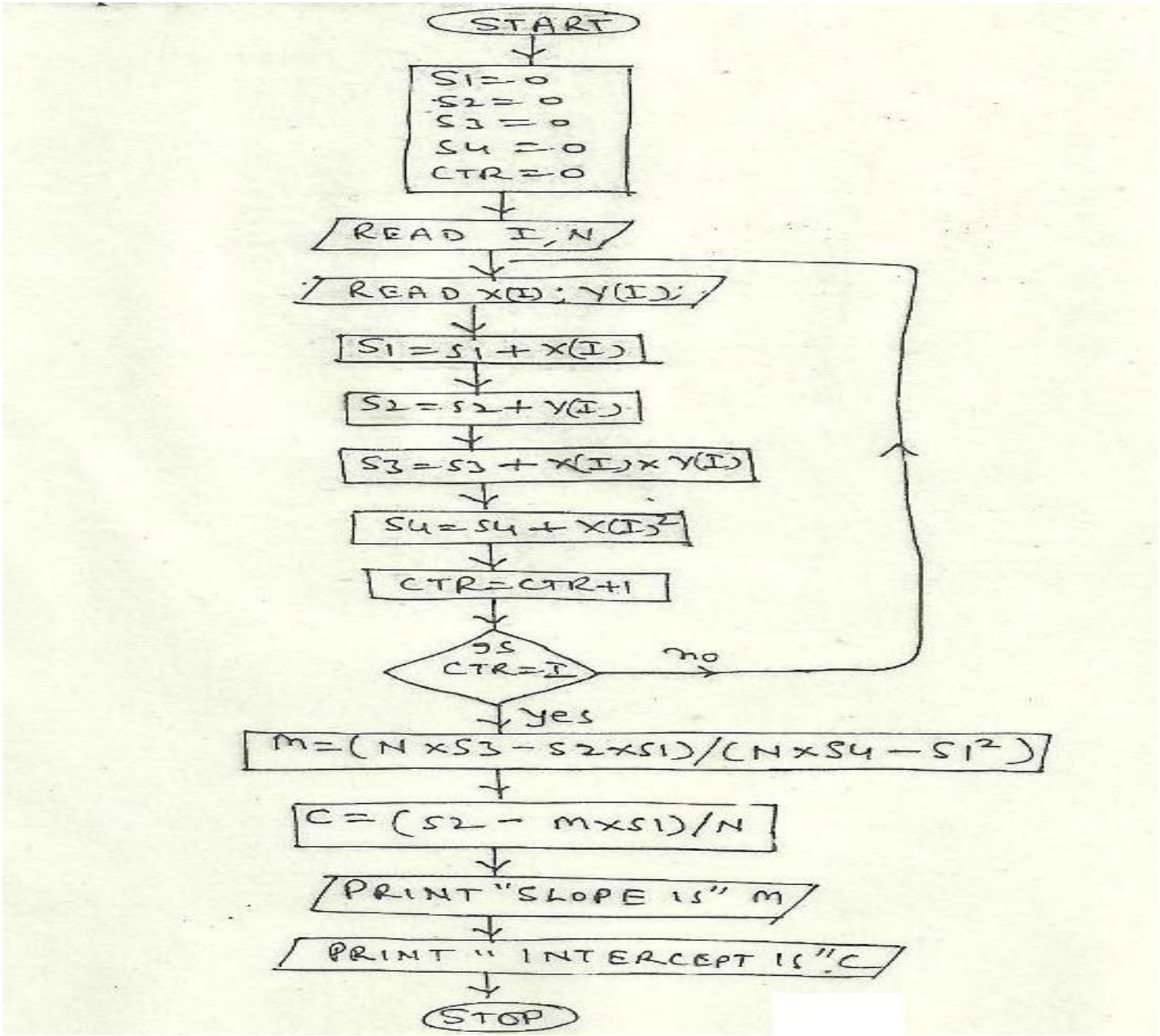


53. *To compute the slope and the intercept for the given set of data of straight line:*

As for computation of slope and intercept for a best fit straight line on the basis method of least squares, formulae are

$$m(\text{slope}) = \frac{(n \times \Sigma x_i y_i) - (\Sigma x_i)(\Sigma y_i)}{(n \times \Sigma x_i^2) - (\Sigma x_i)^2} \quad \& \quad C(\text{intercept}) = \frac{1}{n}\left(\Sigma y_i - m \times \Sigma x_i\right)$$

For x_i, y_i set of points. These two parameters for the best fit line can e computed using computer. In most of the experiments in the analytical and physical chemistry straight line graphs are to be plotted. Therefore, this computation is useful and beneficial for chemists. Flow chart for this computation is as follows:


START
S1 = 0
S2 = 0
S3 = 0
S4 = 0
CTR = 0
READ I, N
READ X(I); Y(I);
S1 = S1 + X(I)
S2 = S2 + Y(I)
S3 = S3 + X(I) x Y(I)
S4 = S4 + X(I)²
CTR = CTR + 1
IS CTR = I
no
yes
M = (N x S3 - S2 x S1) / (N x S4 - S1²)
C = (S2 - M x S1) / N
PRINT "SLOPE IS" M
PRINT "INTERCEPT IS" C
STOP

Program for COL or Normality & Molarity

molecular wt of solute. Flow chart for this computation has been included in chapter 2 (section 2.2). Its program listing in BASIC is given below:

```
10 N = 0
20 M = 0
30 M1 = 0
40 PRINT "GIVE WT OF SOLUTE"
50 INPUT W
60 PRINT "GIVE VOLUME OF SOLUTION"
70 INPUT V
80 PRINT "ENTER EQ WT OF SOLUTE"
90 INPUT E
100 PRINT "ENTER MOL WT OF SOLUTE"
110 INPUT MOL
120 PRINT "ENTER WT OF SOLVENT"
130 INPUT WT
140 N = (1000*W)/(V*E)
150 M = (1000*W)/(V*MOL)
160 M1 = (1000*W)/(MOL*WT)
170 PRINT "NORMALITY OF THE SOLUTION IS "N
180 PRINT "MOLARITY OF THE SOLUTION IS "M
190 PRINT "MOLALITY OF THE SOLUTION IS "M1
200 END
Ok_
```

Its output is :

```
RUN
GIVE WT OF SOLUTE
? 6.3
GIVE VOLUME OF SOLUTION
? 1000
ENTER EQ WT OF SOLUTE
? 63
ENTER MOL WT OF SOLUTE
? 126
ENTER WT OF SOLVENT
? 1000
NORMALITY OF THE SOLUTION IS  .1
MOLARITY OF THE SOLUTION IS  .05
MOLALITY OF THE SOLUTION IS  .05
Ok_
```

PROGRAM FOR AV & SD OF DATA

```
10 DIM X(100)
20 S = 0
30 S1 = 0
35 INPUT N
40 FOR I = 1 TO N
50 READ X(I)
60 S = S+X(I)
70 NEXT I
80 A = S/N
90 FOR I = 1 TO N
100 S1 = S1+(X(I)-A)^2
110 NEXT I
120 V = S1/(N-1)
130 SD = SQR(V)
140 PRINT A,V,SD
150 DATA 2,3,4,4,4,5,6,7,8,9
160 END
Ok_
```

Out put is

```
RUN
? 5
 3.4          .8          .8944272
Ok_
```

7. Program to compute and print the roots of quadratic equation

As quadratic equation is $AX^2 + BX + C = 0$ for which roots can be computed when D , the discriminant is greater than zero. Flow chart for this computation is given in chapter 2 (ref. 2.2). Its program in BASIC is given below:

```
5 REM PROGRAM FOR COMPUTING ROOTS OF QUADRATIC
EQUATION
10 D = 0
20 S = 0
25 PRINT " ENTER A,B,C"
30 INPUT A,B,C
40 D = (B^2)-(4*A*C)
50 IF D > 0 THEN 60 ELSE 100
60 S = SQR(D)
70 X1 = (-B+S)/(2*A)
80 X2 = (-B-S)/(2*A)
90 PRINT "ROOTS ARE "X1,X2
95 GOTO 110
100 PRINT "ROOTS ARE IMAGINARY"
```

```
110 END
Ok_
```

Output is

```
RUN
 ENTER A,B,C
? 1,3,2
ROOTS ARE -1  -2
Ok_
```

8. Program for printing squares of first 100 natural numbers:

Program listing for this computation is given below in BASIC and its flow chart has already given in chapter2.

```
5 REM PROGRAM FOR PRINTING SQUARES OF FIRST 100 NATURAL
NUMBERS
10 N = 0
20 I = 0
30 N = N+1
40 I = N^2
50 PRINT I
60 IF N > 100 THEN 70 ELSE 30
70 END
Ok_
```

Output is :

This program on execution will print the squares of first 100 natural numbers.

9. Program to compute the values of X and Y variables in the solution of system of simultaneous equations:

As system of simultaneous equations are

A1X + B1Y = C1

A2X + B2Y = C2

Flow chart for computation of the values of X and Y has already been given in chapter 2 and its program in BASIC is given below:

```
5 REM PROGRAM FOR SYSTEM OF SIMULTANEOUS EQUATION
10 X = 0
20 Y = 0
30 Z = 0
40 P = 0
50 Q = 0
60 PRINT "GIVE THE VALUES FOR A1,A2,B1,B2,C1,C2"
```

```
70 INPUT A1,A1,B1,B2,C1,C2
80 Z = (A2*B1)-(A1*B2)
90 P = (C2*B1)-(B2*C1)
100 Q = (C1*A2)-(A1*C2)
110 X = P/Z
120 Y = Q/Z
130 PRINT " THE VALUE OF X IS ";X
135 PRINT "THE VALUE OF Y IS " ;Y
140 END
Ok_
```

Out put is

```
RUN
GIVE THE VALUES FOR A1,A2,B1,B2,C1,C2
? 2,3,4,4,3,5
 THE VALUE OF X IS -.6666667
THE VALUE OF Y IS  1.25
Ok_
```

10. To print the factorial of a number N:

As factorial for a number is N(N-1)(N-2).....1. For this computation flow chart has already been given in chapter 2 and here program listing for this computation in BASIC is given.

```
5 REM PROGRAM FOR COMPUTING FACTORIAL OF A NUMBER
10 F = 1
20 INPUT N
30 F = F*N
40 N = N-1
50 IF N = 0 THEN 60 ELSE 30
60 PRINT " FACTORIAL OF THIS NUMBER IS " F
70 END
Ok_
```

Output is

```
RUN
? 5
 FACTORIAL OF THIS NUMBER IS  120
Ok_
```

11. Program to compute the value of area and circumference of a circle:

```
170 VISC = X/Y
180 PRINT "VISCOSITY OF THE LIQUID IS "VISC
190 END
Ok_
```

Its output is:

```
RUN
PROGRAM FOR CAL OF VISCOSITY ON POSULIE'S EQUATION
ENTER THE VALUE OF RADIUS OF CAPILLARY
? 0.5
ENTER THE VALUE OF PRESSURE HEAD
? 760
ENTER THE VALUE OF TIME OF FLOW
? 20
ENTER THE VALUE OF LENGTH OF LIQUID FLOW
? 5
ENTER THE VALUE OF VOLUME OF LIQUID FLOW
? 3
VISCOSITY OF THE LIQUID IS  24.85834
Ok_
```

31. Program for computation of value of β and hence to find out the value of n_i on the basis of Boltzmann's statistics:

According to the Boltzmann Statistics number of particles in the I^{th} level is given by

$$n_i = n_0 e^{-\beta \epsilon_i}$$

Where n_0 is the number of particles in the ground state or in the zeroth state and β is a constant equal to 1/kT and ϵ_i is the energy of i^{th} level. Program for this computation can is as follows, considering n_0 as N_A (the Avogadro's number):

```
5 REM PROGRAM FOR MAXWELL DISTRIBUTION
10 K = 1.38E-16
20 NA = 6.023E+23
30 PRINT " PROGRAM FOR MAXWELL DISTRIBUTION"
40 PRINT " ENTER THE VALUE OF TEMP"
50 INPUT T
60 PRINT "ENTER THE VALUE OF ENERGY OF LEVEL"
70 INPUT E
80 B = 1/(K*T)
90 X =-(E*B)
```

```
100 Y = EXP(X)
110 NI = NA*Y
120 PRINT "VALUE OF B IS "B
130 PRINT "NO OF PARTICLES IN THE LEVEL ARE "NI
140 END
Ok_
```

Its output is:

```
RUN
 PROGRAM FOR MAXWELL DISTRIBUTION
 ENTER THE VALUE OF TEMP
? 373
ENTER THE VALUE OF ENERGY OF LEVEL
? 3E4
VALUE OF B IS  1.942728E+13
NO OF PARTICLES IN THE LEVEL ARE  1.701412E+38
Ok_
```

32. *Program for computation of K_a for weak acid (say acetic acid):*

For any weak acid like acetic acid when C is the concentration and α is the degree of ionization of acid, the K_a value can be predicted on the basis of Ostwald's dilution law as

$$K_a = c\alpha^2/(1-\alpha)$$

Its program is as follows:

```
5 REM PROGRAM FOR DILUTION LAW
10 PRINT "PROGRAM FOR OSTWALD DITUTION LAW"
20 PRINT "ENTER THE VALUE OF DEGREE OF DISOCIATION"
30 INPUT ALP
40 PRINT "ENTER THE VALUE OF CONCENTRATION"
50 INPUT C
60 IF ALP > 1 THEN 70 ELSE 90
70 PRINT "YOU ARE JOCKING"
80 GOTO 130
90 X = C*(ALP^2)
100 Y = 1-ALP
110 KA = X/Y
120 PRINT " THE VALUE OF DISOCIATION CONSTANT IS "KA
130 END
Ok_
```

PROGRAM TO CALL μ S + L

Its program is as follows:

```
5 REM PROGRAM FOR CALCULATION OF MAGNETIC MOMENT
10 PRINT " PROGRM FOR CALCULATION OF MAGNETIC MOMENT
WITH ORBITAL CONTROBUTION
20 PRINT " ENTER THE VALUES FOR SPIN QUAMTUM NUMBER"
30 INPUT S
40 PRINT " ENTER THE VALUE FOR ORBITAL QUANTUM NUMBER"
50 INPUT L
60 X = 4*S*(S+1)
70 Y = L*(L+1)
80 Z = X+Y
90 MU = SQR(Z)
100 PRINT "MAGNETIC MOMENT WITH ORBITAL CONTRIBUTION IS
";MU
110 END
Ok_
```

Its output is:

```
RUN
 PROGRM FOR CALCULATION OF MAGNETIC MOMENT WITH
ORBITAL CONTROBUTION
 ENTER THE VALUES FOR SPIN QUAMTUM NUMBER
? 0.5
 ENTER THE VALUE FOR ORBITAL QUANTUM NUMBER
? 2
MAGNETIC MOMENT WITH ORBITAL CONTRIBUTION IS  3
Ok_
```

35 .Program for computation of value of Bohr magneton:

```
10 REM PROGRAM FOR BOHR MAGNETON
20 E = 1.6020E-19
30 H = 6.636E-34
40 PI = 3.14159
50 M = 9.1091E-31
60 C = 2.99E 8
70 BM = (E*H)/(4*PI*M*C)
80 PRINT "BOHR MAGNETON IS ";BM
90 END
```

```
 ENTER THE HEAT OF FORMATION
? 98
 ENTER THE HEAT OF SUBLIMATION
? 26
 ENTER THE IONIZATION POTENTIAL
? 118
 ENTER THE DISSOCIATION ENERGY
? 58
 ENTER THE VALUE OF ELECTRON AFFINITY
? 87
 LATTICE ENERGY FOR THE NACL IS 184
Ok_
```

46. Program for computation of lattice energy on the basis of Born Lande's Equation:

As Born Lande's equation is

$$U = \frac{N_A A e^2 Z + Z -}{r_0}\left(1 - \frac{1}{n}\right)$$

So, program for this computation is as follows:

```
LIST
10 PRINT "PROGRAM TO CALCULATE LATTICE ENERGY ON THE BASIS
OF BORN LANDE EQ"
20 PRINT " ENTER CHARGES"
30 INPUT Z1,Z2
40 PRINT " ENTER THE NAME OF CRYSTAL"
45 B = 8
50 INPUT C$
52 PRINT " ENTER THE BOND DISTANCE"
55 INPUT DIST
60 NA = 6.023E+23
65 MAC = 1.74
70 C1 = 4.8E-10
80 C2 = 1E-10
90 P = Z1*Z2
100 X1 = NA*MAC*P
110 Y = 1/B
120 X2 = C1*C2*(1-Y)
130 LE = X1*(X2/DIST)*C2
140 PRINT " LATTICE ENERGY IS " LE
150 END
Ok_
```

```
WANT TO CALCULATE WAVE LENGTH OR FREQUENCY OR ENERGY
ENTER THE DATA KEEPING UNKNOWN ZERO
? 2.4E4,3E-9,0
 ENERGY IS  1.59264E-29
Ok_
```

48. Program for computation of surface tension on the basis of capillary action:

For capillary action

$$\gamma = \frac{r h \rho g}{2 \cos \theta}$$

Where r is the radius of capillary, h is the height ρ is the density of the liquid, g is the acceleration due to gravity and θ is the angle that the liquid makes with the walls of capillary. Program for this computation is:

```
LIST
5 REM PROGRAM FOR CAPILLARY ACTION
10 PRINT " PROGRAM FOR CAPILLARY ACTION "
20 PRINT " ENTER ANGLE"
30 G = 980
40 INPUT AN
60 PRINT " ENTER RADIUS OF CAPILLARY"
70 INPUT R
```

```
80 PRINT " ENETR HEIGHT UPTO WHICH LIQUID RISE"
90 INPUT H
100 PRINT " ENTER DENSITY OF LIQUID "
110 INPUT D
120 IF AN = 0 THEN 130 ELSE 140
130 Y = (R*H*D*G)/2
135 GOTO 180
140 RAN = 3.14/180
150 A = RAN*AN
160 CA = COS(A)
170 Y = (R*H*D*G)/(2*CA)
180 PRINT " SURFACE TENSION IS " Y
190 END
Ok_
```

Its output is:

```
RUN
 PROGRAM FOR CAPILLARY ACTION
 ENTER ANGLE
? 0
```

Here in this program matrix elements are given as data points in the data card in line no. 130,which can be changed according to requirement. This program will print the matrix and its transpose on the screen.

61.Program to evaluate any integral on the basis of Monte Carlo's method:

It is a numerical integration technique for which the program in the BASIC language is as follows. This program asks the number of iterations or the number of times the user wants to solve the integral and after getting the input from the user as 'N' it generates a random number and solve the integral for 'N' iterations and finally prints the result.

```
LIST
10 PRINT" PROGRM TO SOLVE AN INTEGRAL ON THE BASIS OF
MONTECARLO METHOD"
20 PRINT" ENTER THE NUMBER OF TIMES YOU WANT TO CYCLIZE THE
INTEGRAL"
30 INPUT N
40 S = 0
50 FOR I = 1 TO N
60 Z = RND
70 F = 1/(1+Z^2)
80 S = S+F
90 NEXT I
100 IN = S/N
110 PRINT IN
120 END
Ok_
```

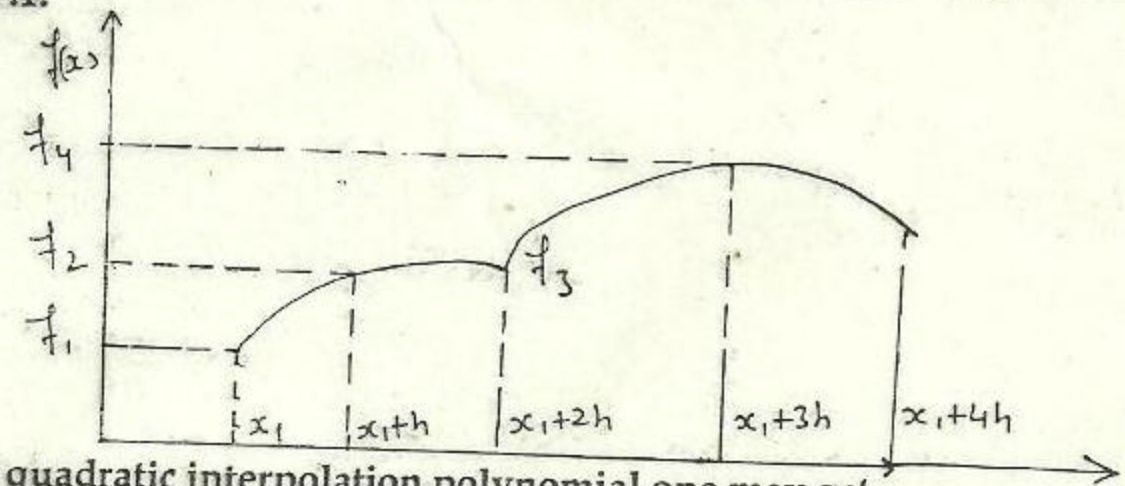
Output of this program is:

```
RUN
 PROGRM TO SOLVE AN INTEGRAL ON THE BASIS OF MONTECARLO
METHOD
 ENTER THE NUMBER OF TIMES YOU WANT TO CYCLIZE THE
INTEGRAL
? 1000
 .7817735
Ok_
```

62. Program to solve the integral on the basis of Simpson's rule:

Simpson's rule is a popular numerical integration method. It is based on the approximating the function f(x) by fitting quadratics through sets of three

points. These points are illustrated graphically as per according the following figure 7.1.



Using a quadratic interpolation polynomial one may get

$$S = \int_{x_1}^{x_1+nh} f(x)\,dx = \sum_{i=1,3\ldots n-2} \int_{x_i}^{x_i+2h} \left[f_i + \frac{\Delta f_i}{h}(x-x_i) + \frac{\Delta^2 f_i}{2h^2}(x-x_i)(x-x_i-h) \right] dx$$

Integrating the above expression we obtain

$$S = \sum_{i=1,3,5\ldots n-2} h/3\,(f_i + 4f_{i+1} + f_{i+2})$$

$$= h/3\,[f_1 + 4f_2 + 2f_3 + 4f_4 + 2f_5 + 4f_6 + \ldots + f_{n+1}]$$

In using the above formula it is implied that f is tabulated at an odd number of points. The exact value of any integral on the basis of Simpson's rule may also be zero as Simpson's rule is exact up to a cubic. The Simpson's formula may also be derived by a technique called the method of undetermined coefficients. In this method we seek an integration formula of the type

$$S = af_1 + bf_2 + cf_3$$

Where f1,f2 and f3 are the values of the function being integrated at the three points viz. x1, x1+h and x1+2h and a, b and c are constants to be determined. Program for evaluation of integral on the basis of Simpson's rule is as follows:

```
. LIST
5 REM SIMPSON'S RULE PROGRAM
10 PRINT " PROGRM FOR INTEGRATION ON THE BASIS OF SIMPSON
RULE"
20 INPUT A,E
30 DEF FNA(X) = X*X
40 N = 4
50 S = 0
60 H = (E-A)/N
70 S = FNA(X)
80 FOR I = 1 TO N-1 STEP 2
90 X = A+I*H
100 S = S+4*FNA(X)
110 NEXT I
```

? 3E8
THE VALUE OF WAVE LENGTH ON THE BASIS OF DEBROGLIE EQ FOR THE
PARTICLE IS 2.430769E-05
Ok_

53. To compute the slope and the Intercept for the given set of data of straight line:

As for computation of slope and intercept for a best fit straight line on the basis method of least squares, formulae are

$$m(\text{slope}) = \frac{(n \times \Sigma x_i y_i) - (\Sigma x_i)(\Sigma y_i)}{(n \times \Sigma x_i^2) - (\Sigma x_i)^2} \quad \& \quad c(\text{intercept}) = \frac{1}{n}\left(\Sigma y_i - m \times \Sigma x_i\right)$$

For x_i, y_i set of points. These two parameters for the best fit line can e computed using computer. In most of the experiments in the analytical and physical chemistry straight line graphs are to be plotted. Therefore, this computation is useful and beneficial for chemists. Program for this computation is as follows:

```
LIST
10 PRINT " PROGRM FOR LEAST SQUARE FIT"
20 DIM X(100), Y(100)
30 S1 = 0
40 S2 = 0
50 S3 = 0
60 S4 = 0
70 INPUT N
80 FOR I = 1 TO N
90 READ X(I)
100 READ Y(I)
110 S1 = S1+X(I)
120 S2 = S2+Y(I)
130 S3 = S3+X(I)*Y(I)
140 S4 = S4 +X(I)^2
150 NEXT I
160 M = (N*S3-S1*S2)/(N*S4-S1^2)
170 C = (S2-M*S1)/N
180 PRINT "SLOPE OF THE GIVEN DATA IS" M
190 PRINT " INTERCEPT OF THE GIVEN DATA IS "C
200 DATA 3,2,4,7,3,5,9,20
210 END
Ok_
```

Its output is :

```
RUN
 PROGRM FOR LEAST SQUARE FIT
? 4
SLOPE OF THE GIVEN DATA IS 2.727273
 INTERCEPT OF THE GIVEN DATA IS -4.454546
Ok_
```

Data point are given in the data card in the program itself in line number 200.

54. To compute correlation coefficient for the given set of data :

Correlation coefficient is also a parameter which is useful for estimating the correlation between set of data (i.e. experimental observations) in any scientific field. This coefficient can be computed on the basis of following formula

$$\rho = \frac{\Sigma xy}{\sqrt{\Sigma x^2}\sqrt{\Sigma y^2}}$$

where $x = X_i - \bar{X}$ (x average)

$y = Y_i - \bar{Y}$ (y average)

Program for this computation is given below:

```
LIST
10 PRINT " PROGRAM FOR COMPUTATION OF CORRELATION COEFF."
20 S = 0
30 S1 = 0
40 S2 = 0
50 S3 = 0
60 S4 = 0
70 PRINT "ENTER THE LIMIT"
80 INPUT N
90 FOR I = 1 TO N
100 READ X(I),Y(I)
110 S = S+X(I)
120 S1 = S1+Y(I)
130 NEXT I
140 XB = S/N
150 YB = S1/N
160 FOR I = 1 TO N
170 S2 = S2+(X(I)-XB)*(Y(I)-YB)
180 S3 = S3+(X(I)-XB)^2
190 S4 = S4+(Y(I)-YB)^2
200 NEXT I
210 NUM1 = SQR(S3)
220 NUM2 = SQR(S4)
230 CC = S2/(NUM1*NUM2)
```

```
240 PRINT " AVERAGE OF X(I) DATA IS " ;XB
250 PRINT " AVERAGE OF Y(I) DATA IS " ;YB
260 PRINT " CORRELATION COEFFICIENT BETWEEN X(I) AND Y(I) IS
";CC
265 DATA 2,3,2,3,4,5,4,5,6,7,6,7,8,7,8,8,3,9,20
270 END
Ok_
```

Output of this program is :

```
RUN
 PROGRAM FOR COMPUTATION OF CORRELATION COEFF.
ENTER THE LIMIT
? 5
 AVERAGE OF X(I) DATA IS  3
 AVERAGE OF Y(I) DATA IS  3.8
 CORRELATION COEFFICIENT BETWEEN X(I) AND Y(I) IS  .874 0074
Ok_
```

Data points are given in line number 265 in the program itself. One can change these data points according to requirements.

These are some programs for which flowcharts are given in chapter 2(ref. section 2.2). Now, some programs are given which are also useful in Chemistry and for some numerical analysis.

55. Program for computation of iso-electric point :

As iso-electric point for any amino acid is given by the following formula:

$pH = pI_{so} = (pK_1 + pK_2)/2$ where pK_1 & pK_2 are dissociation constants for $\overset{+}{N}H_3CH_2COO^-$ & $NH_2CH_2COO^-$ ions.

Program for computation of this point is given below:

```
LIST
10 PRINT " PROGRAM FOR CALCULATION OF ISOELECTRIC POINT"
20 PRINT " ENTER NAME OF ACID"
30 INPUT N$
40 PRINT " ENTER DISSOCIATION CONSTANTS"
50 INPUT K1,K2
60 H = SQR(K1*K2)
70 H1 = -LOG(K1/2.303)
80 H2 = -LOG(K2/2.303)
90 I1 = (H1+H2)/2
100 PRINT " HYDROGEN ION CONCENTRATION IS " H
```

Introduction to Quantum – Chemical Packages:-

Ab-Initio

Uses all electron Hamiltonian

- Based on Hartree-Fock Quantum Chemical Approach
- Optimize Geometry
- Minimize energy

Semi-Empirical

Uses Valance electron Hamiltonian

Predict the results like :-

1. Heat of formation
2. Electronic energy
3. Core-Core Repulsion energy
4. Ionization potential
5. Total energy
6. Dipole moment
7. Eigen Values
8. Homo-Lumo gap
9. Moment of inertia/force constants
10. Normal modes with force constants in spectral analysis

- Near exact values with m::ximum iterations
- Visualize the molecule/giant molecules easily in various fashions
- Predicts the bond-angles/bond lengths after optimization of geometry

Some of the commonly used Ab-Initio Packages now-a-days are :

***GAUSSIAN**

***GAMESS**

Etc.

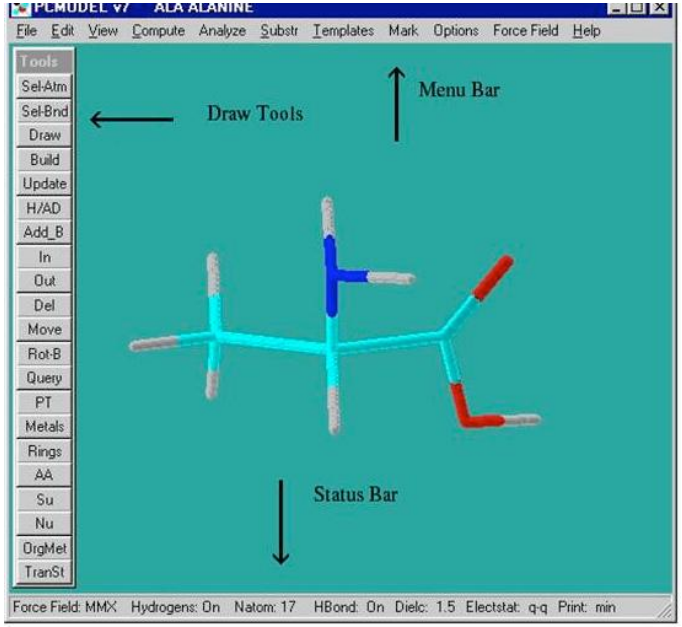
Some of the commonly used Semi-empirical Packages now-a-days are:

- **PCMODEL (Serena Software pvt. Ltd.)**
- **MOPAC**
- **WINMOPAC**
- **HYPERCHEM**

Etc.

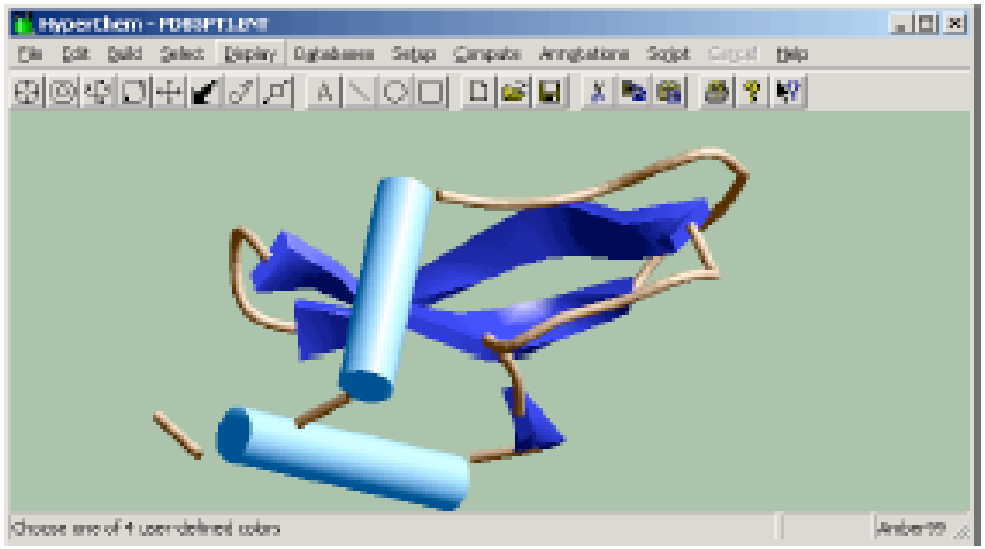
PC-MODEL

- *PC-Model, from Serena Software (http://www.serenasoft.com/pcm8.html) is* a less well-known commercial molecular modeling software package. *PCModel* is primarily a *molecular mechanics (MM) computational package, but* it can also serve as a *front-end, or interface, to other packages such as* Gaussian, GAMESS, MOPAC, and others. *PC-Model can also read output* files from most of the other codes, and display the results of those calculations as visualizations.
- *PC-Model is a cross-platform software package, meaning that it runs on* most types of computers, including Windows, Macintosh, and UNIX/Linux operating systems. It should be noted that most, but not all, software packages are cross-platform to ensure competitiveness in an increasingly challenging marketplace. Many of these codes have their origin as UNIX programs, and many have been *ported, or* re-written, to run on the more commonly found Windows machines. More and more packages, however, are being ported to Macintosh computers.



HYPERCHEM

HyperChem, produced by HyperCube, Inc. (http://www.hyper.com/), is the last of the "featured" software packages described in this chapter. *HyperChem is a cross-platform* computational package that provides a full-range of computational methods (molecular mechanics, semi-empirical, *ab initio, and DFT) in a user-friendly graphical interface*. A window from hyperchem is shown below :



Feel free to Contact for further Questions

- Through College email: pgcdatia@rediffmail.com

REFERENCES AND ACKNOWLEDGEMENTS

1. Computers In Chemistry; K.V. Raman; Tata McGraw Hill;
2. Computer Applications In Chemistry; Kishor Arora; Anmol Publications Pvt. Ltd. (2004).

http://en.wikipedia.org/

https://www.google.com

Best of Luck