

# ACHARYA NARENDRA DEV COLLEGE

## APPLICATIONS OF COMPUTERS IN CHEMISTRY

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**Problem 1: Write a program in BASIC to find the value of factorial of a number.**

Program:

```
10 CLS
20 REM*VALUE OF FACTORIAL*
30 INPUT "The number"; N
40 IF N > 34 THEN 100
50 P = 1
60 FOR I = 1 TO N
70 P = P * I
80 NEXT I
90 PRINT "The factorial of "; N; "is "; P: GOTO 110
100 PRINT "The value of the factorial exceeds computer memory"
110 END
```

Output:

```
The number? 10
The factorial of 10 is 3628800
The number? 36
The value of the factorial exceeds computer memory
```

**Program 2: Write a program in BASIC to calculate pressure of an ideal gas at different temperatures.**

```
10 CLS
20 REM Pressure of an ideal gas at different temperatures
30 R = 8.314: N = 1: V = .0245
40 PRINT "Pressure of an ideal gas at various temperatures"
50 PRINT "Amount of gas="; N; "mol", "Volume of gas="; V; "m^3"
55 PRINT "Temperature(K)"; "Pressure(Pa)"
60 FOR T = 300 TO 400 STEP 20
70 P = N * R * T / V
80 PRINT T, P
90 NEXT T
95 PRINT "Pressure of an ideal gas increases with increase in T at constant V & n"
100 END
```

**Program 3: Write a program in BASIC to print the capital and small alphabet**

In this program, as long as X is < or = 26, statements 50,60,70 are executed. As soon as X>26, the control goes to the next statement after WEND, that is, 90.

```
10 CLS
15 A$ = "A": B$ = "a"
20 I = ASC(A$): J = ASC(B$)
30 X = 1
40 WHILE X <= 26
50 PRINT CHR$(I); CHR$(J); ", ";
60 X = X + 1
70 I = I + 1: J = J + 1
80 WEND
90 END
```

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### Program 12: Write a program in BASIC to decide the risk factor using SELECT CASE

```
INPUT "Enter acceptable level of risk (1-5): ", Total
SELECT CASE Total

CASE IS >= 5
    PRINT "Maximum risk and potential return."
    PRINT "Choose stock investment plan."

CASE 2 TO 4
    PRINT "Moderate to high risk and potential return."
    PRINT "Choose mutual fund or corporate bonds."

CASE 1
    PRINT "No risk, low return."
    PRINT "Choose PPF."
END SELECT
END
```

### Problem 4: Write a program in BASIC to find the roots of the given quadratic equation.

Program:

```
10 CLS
20 REM* ROOTS OF QUADRATIC EQUATION*
30 INPUT "A,B,C IN EQUATION ax^2+bx+c=0 ARE"; A, B, C
40 IF A = 0 THEN 150 ELSE 50
50 D = B ^ 2 - 4 * A * C
55 E = ABS(D): F = SQR(E)
60 IF D < 0 THEN 170 ELSE 70
70 IF D = 0 THEN 80 ELSE 110
80 PRINT "EQUAL ROOTS"
90 R = (-B) / (2 * A)
100 PRINT "ROOT IS "; R: GOTO 210
110 X1 = (-B + F) / (2 * A)
120 X2 = (-B - F) / (2 * A)
130 PRINT "REAL ROOTS ARE "; X1; "AND"; X2
140 GOTO 210
150 PRINT " THE EQUATION IS LINEAR"
160 GOTO 210
170 PRINT "ROOTS ARE IMAGINARY"
180 X = (-B) / (2 * A): Y = F / (2 * A)
190 PRINT "FIRST ROOT IS "; X; "+i"; Y
200 PRINT "SECOND ROOT IS "; X; "-i"; Y
210 END
```

Output:

```
A,B,C IN EQUATION ax^2+bx+c=0 ARE? 1,2,3
ROOTS ARE IMAGINARY
FIRST ROOT IS -1 +i 1.414214
SECOND ROOT IS -1 -i 1.414214
A,B,C IN EQUATION ax^2+bx+c=0 ARE? 4,10,4
REAL ROOTS ARE -.5 AND-2
A,B,C IN EQUATION ax^2+bx+c=0 ARE? 0,1,2
THE EQUATION IS LINEAR
```

### Problem 4 (b): Another method using select case

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```
10 CLS
20 REM *to find the roots of quadratic equation*
30 INPUT a, b, c
35 IF a = 0 THEN 36 ELSE 40
36 PRINT "Equation is not linear": GOTO 210
40 d = b ^ 2 - 4 * a * c
50 SELECT CASE d
    CASE IS > 0                                don't give any statement number here
60 PRINT "roots are real"
70 r1 = (-b + SQR(d)) / (2 * a)
80 r2 = (-b - SQR(d)) / (2 * a)
90 PRINT r1; r2
100 CASE IS = 0
110 r = -b / (2 * a)
120 PRINT "equal roots"
130 PRINT "root="; r1
140 CASE IS < 0
150 e = ABS(d)
160 x = -b / (2 * a)
170 y = SQR(e) / (2 * a)
180 PRINT "Roots are imaginary"
190 PRINT "r1="; x; "+i"; y
200 PRINT "r2="; x; "-i"; y
205 END SELECT
210 END
```

**Problem 5: Write a program in BASIC to determine the greatest of the three given numbers.**

**Program:**

```
10 CLS
20 REM* TO FIND GREATEST OF THREE NUMBERS*
30 INPUT "ENTER THE THREE NUMBERS X1,X2,X3"; X1, X2, X3
40 IF X1 > X2 THEN G = X1 ELSE G = X2
50 IF G < X3 THEN G = X3
60 PRINT "The greatest of three numbers "; X1; X2; X3; "IS", G
70 INPUT "DO YOU WISH TO CONTINUE?ENTER Y OR N "; A$
80 IF A$ = "Y" OR A$="y" THEN 30 else 90
90 END
```

OPTIONAL  
STATEMENTS

**Output:**

```
ENTER THE THREE NUMBERS X1,X2,X3? 10,5,100
The greatest of three numbers 10 5 100 IS 100
DO YOU WISH TO CONTINUE?ENTER Y OR N ? Y
ENTER THE THREE NUMBERS X1,X2,X3? -10,-6,-20
The greatest of three numbers -10 -6 -20 IS -6
DO YOU WISH TO CONTINUE?ENTER Y OR N ? N
```

**Problem 6: Write a program in BASIC to print the given name as initial of first name and last name. Also, print the name in a column.**

**Program:**

```
10 CLS
20 INPUT "Enter First Name, Last name "; N$, S$
30 A$ = LEFT$(N$, 1)
40 PRINT A$; "."; S$
50 L = LEN(N$): M = LEN(S$)
60 FOR I = 1 TO L
70 X$ = MID$(N$, I, 1)
80 PRINT X$
```

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```
90 NEXT I
100 FOR K = 1 TO M
110 Y$ = MID$(S$, K, 1)
130 PRINT Y$
140 NEXT K
150 END
```

#### Output:

```
Name, Last name ? NEETI,MISRA
N.MISRA
N
E
E
T
I
M
I
S
R
A
```

**Problem 7: Write a program in BASIC to generate prime numbers up to N. Take N as 20 or 50 or 100.**

#### Program:

```
10 CLS
20 REM* GENERATE PRIME NUMBERS
30 INPUT "Generate prime numbers upto "; N
40 PRINT "THE PRIME NUMBERS UPTO ";N;"ARE"
50 PRINT 1, 2,
60 FOR I = 3 TO N
70 FOR J = 2 TO I - 1
80 Q = I / J
90 IF Q = INT(Q) THEN 120 ELSE 100
100 NEXT J
110 PRINT I,
120 NEXT I
130 END
```

#### Output:

Generate prime numbers upto ? 100

THE PRIME NUMBERS UPTO 100 ARE

1	2	3	5	7
11	13	17	19	23
29	31	37	41	43
47	53	59	61	67
71	73	79	83	89
97				

**Problem 8: Write a program in BASIC to generate prime numbers up to N using Mod command. Take N as 20 or 50 or 100.**

```
10 CLS
20 REM generate prime numbers using mod command
30 INPUT "Enter the number up to which prime nos. to be found =", N
40 PRINT "Prime numbers up to "; N; "are"
50 PRINT 1, 2,
60 FOR I = 3 TO N
70 FOR J = 2 TO I - 1
80 IF I MOD J = 0 THEN 110 ELSE 90
```

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```
90 NEXT J
100 PRINT I,
110 NEXT I
120 END
```

**Problem 9:** Write a program in BASIC to generate 10 random numbers between 0 and N. Take N as 20 or 50 or 100.

```
10 CLS
20 REM Generate 10 random numbers
30 INPUT N
40 FOR I = 1 TO N
50 Y = RND * N
60 PRINT Y,
70 NEXT I
80 END
```

**Problem 10:** Write a program in BASIC to generate 10 integers between 0 and N. Take as 50 and 100. Use Randomize command to get different random numbers.

```
10 CLS
20 REM Generate 10 random numbers
30 INPUT N
35 RANDOMIZE
40 FOR I = 1 TO N
50 Y = RND * N
60 PRINT INT(Y),
70 NEXT I
80 END
```

Modify the program using RANDOMIZE TIMER in place of RANDOMIZE