Applications of computers in Chemistry

Some miscellaneous programs

1. Write a program in BASIC to print the capital and small alphabet

In this program WHILE and WEND commands have been used. These two commands are used for conditional branching.

WHILE <condition>
----WEND

As long as the condition is true, the steps before wend are repeated. When the condition becomes false, the program comes out of the loop.

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

2. Write the program in BASIC to determine the value of $\cos \Theta$ using Taylor series.

$$\cos x = 1 - x^{2} / 2! + x^{4} / 4! - x^{6} / 6! + x^{8} / 8! - \dots$$

$$\cos x = \sum_{n=0}^{\infty} (-1)^{n} \frac{x^{2k}}{2k!}$$

Here x is the angle in radians. In our program we will enter the value of angle in degrees and the program will convert it into radians.

Program:

5 REM taylor series for cos

10 INPUT "enter the angle in degree"; D

$$15 X = D * 22 / (7 * 180)$$
: PRINT X

20 I = -1

30 C = 0: N = 0

35 K = 2 * N

40 GOSUB 500

50 A = P

 $60 \text{ C1} = \text{C} + (-1) ^ N * ((X ^ K) / A)$

65 IF N = 0 THEN 80

70 IF ABS((C1 - C) / C) < .000001 THEN 100 ELSE 80

80 C = C1: N = N + 1

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90 GOTO 35

100 PRINT C1, N

110 END

500 P = 1

510 FOR J = 1 TO K

520 P = P * J

530 NEXT J

540 RETURN

3. Write the program in BASIC to determine the value of $\sin \Theta$ using Taylor series.

$$\sin x = x - x^3/3! + x^5/5! - x^7/7! + x^9/9! - \dots$$

$$\sin x = \sum_{n=1}^{\infty} (-1)^{n-1} \frac{x^{2n-1}}{(2n-1)!}$$

or

$$\sin x = \sum_{n=0}^{\infty} (-1)^n \frac{x^{2n+1}}{(2n+1)!}$$

10 CLS

20 INPUT x

Here the value of x is in radians

30 N = 0: C = 0

35 K = 2 * N + 1

40 GOSUB 500

50 A = P

 $60 \text{ C1} = \text{C} + (-1) ^ N * ((x ^ K) / A)$

70 IF ABS((C1 - C)) < .0001 THEN 100 ELSE 80

80 C = C1: N = N + 1

90 GOTO 35

100 PRINT C1

110 END

500 P = 1

510 FOR I = 1 TO K

520 P = P * I

530 NEXT I

540 RETURN

4. Write a program in BASIC to separate odd-even numbers from the list.

Program 1:

5 REM Separate odd and even numbers

10 INPUT n

20 FOR i = 1 TO n

30 READ x

40 IF INT(x / 2) = x / 2 THEN 50 ELSE 60

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50 PRINT x, "even number": GOTO 70
        60 PRINT x, "odd number"
        70 NEXT i
        80 DATA 2,5,19,81,10,11
        90 END
Program 2:
CLS
5 REM Separate odd and even numbers
10 INPUT n
DIM A(n), B(n)
J = 0: K = 0
20 \text{ FOR i} = 1 \text{ TO n}
30 READ x
40 \text{ IF INT}(x / 2) = x / 2 \text{ THEN } 50 \text{ ELSE } 60
50 J = J + 1: A(J) = x: GOTO 70
60 \text{ K} = \text{K} + 1 : \text{B(K)} = \text{x}
70 NEXT i
80 DATA 2,5,19,81,10,11,110
90 PRINT "even nos."
100 \text{ FOR } i = 1 \text{ TO J}
110 PRINT A(i),
120 NEXT i
PRINT
130 PRINT "odd nos."
140 \text{ FOR } i = 1 \text{ TO K}
150 PRINT B(i),
160 NEXT i
170 END
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5. Write a program in BASIC to print the matrix, by entering the values using input

command. $\begin{vmatrix} 1 & 2 \\ 3 & 4 \end{vmatrix}$

The ASCII code for line | is 179.

Program:

10 CLS

20 REM printing marices

30 INPUT m, n

40 DIM a(m, n)

50 FOR i = 1 TO m

60 FOR j = 1 TO n

70 INPUT a(i, j)

80 NEXT j

90 NEXT i

100 FOR i = 1 TO m

105 PRINT CHR\$(179);

110 FOR j = 1 TO n

120 PRINT a(i, j);

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130 NEXT j 140 PRINT CHR\$(179) 150 NEXT i 160 END

6. Write the output of the following commands

a.	CINT (3.4)	INT(3.4)	FIX(3.4)
b.	CINT (3.8)	INT (3.8)	FIX(3.8)
c.	CINT(-3.4)	INT(-3.4)	FIX(-3.4)
d.	CINT(-3.8)	INT(-3.8)	FIX(-3.8)

This will give you an idea about difference in CINT, INT and FIX

7. Write the output of the following program

Y = Z MOD Xfor X=2 2 2 3 3.6 4 Z=15 14.4 14.8 15 15 15

Z MOD X means z is divided by x and the answer is the value of remainder.

However, first z and x are rounded off to the nearest integer.