AR – 7143

MSc – IV Semester, 2013

Chemistry

Paper: CMT – 401

(Computer Applications in Chemistry)

Maximum Marks: 60

(i) Write the rules for variables.

Ans. → Rules for variables :—

① A variable Name can be atmost 6 characters long.

② It can consist of both alphabet & digit.

③ The first character has to be alphabet.

④ In an integer variable, the first character started on I, J, K, L, M, N.

⑤ In Real variable first character must be A to Z.

(ii) How many type of expressions are used in FORTRAN

Ans → 3 type of expressions are used :—

① Arithmetic Expression → The expression which is used airthmetic operators like +, −, *, /, ** . It perform the simple calculation.

② Relational Expression → It performs the comparison b/w two variables, constants & also two airthmetic expressions. .LT., .GT., .LE., .GE., .NE., .EQ. these are the Relational operators.

③ Logical Expression → It performs more than one comparision. It is possible to combine two relational expressions. .AND., .OR., .NOT. these are the logical expressions.

(iii) write the syntax for DO stmts with example.

Ans. → Syntax of DO stmts :—

```
      DO  n  i = e1, e2, e3
          ⋮        ←——— Body of
                        the loop.
      n  CONTINUE
```

where

n → number of the last stmt in loop.
i → loop control variable
e_1 → initial value of control variable.
e_2 → final value of —"—
e_3 → increament value.

Exa. →

```
      DO 100 I = 1, 100, 2
         PRINT *, I
100   CONTINUE
```

(iv) what are the logical operators are used in FORTRAN.

Ans. → 3 logical operators are used :—

① .AND. ② .OR. ③ .NOT.

① .AND. → IF (A .GT. B .AND. C .GT. D)
② .OR. → IF (A .GT. B .OR. C .GT. D)
③ .NOT. → IF (.NOT. A)

(v) what is the character data type & write 5 example.

Ans. → character data type is the data type which is represent the data is character or string.

For exa → CHARACTER*10A means A is the variable which stores

a. character or maximum 10 characters in a string. Exa :—

1) CHARACTER * 20 NAME
2) CHARACTER * 30 COLG_NAME
3) CHARACTER * 50 CITY
4) CHARACTER * 100 ADDRESS.
5) CHARACTER * 10 CLASS.

vi) Perform A×B where

$A = \begin{matrix} 6 & 2 \\ 4 & 8 \end{matrix}$ $B = \begin{matrix} 3 & 2 \\ 9 & 4 \end{matrix}$

Solve $A \times B = \begin{bmatrix} 18+18 & 12+8 \\ 12+72 & 8+32 \end{bmatrix} = \begin{bmatrix} 36 & 20 \\ 84 & 40 \end{bmatrix}$ Ans.

vii) Write the method of Romberg method.

Ans. → Romberg method :—

$$I\left(h, \frac{h}{2}\right) = \frac{1}{3}\left[4I\left(\frac{h}{2}\right) - I(h)\right]$$

we use the trapezoidal rule several times successively having h & apply (4) to each pair of values as per the following scheme :-

$I(h)$

$I(h/2)$ $I(h, h/2)$

$I(h/4)$ $I\left(\frac{h}{2}, \frac{h}{4}\right)$ $I\left(h, \frac{h}{2}, \frac{h}{4}\right)$

$I(h/8)$ $I\left(\frac{h}{4}, \frac{h}{8}\right)$ $I\left(\frac{h}{2}, \frac{h}{4}, \frac{h}{8}\right)$ $I\left(h, \frac{h}{2}, \frac{h}{4}, \frac{h}{8}\right)$

(viii) Find a root of equation $x^3 - 4x - 9 = 0$ using Regula Falsi method. (Find only one Iteration)

Ans. → $x^3 - 4x - 9 = 0 = f(x)$

$f(0) = 0 - 0 - 9 = -9$

$f(1) = 1 - 4 - 9 = -12$

$f(2) = 8 - 8 - 9 = -9$

$f(3) = 27 - 12 - 9 = 6$

So $x_1 = 2$ & $x_2 = 3$, $f(x_1) = -9$, $f(x_2) = 6$

$$x_0 = x_1 - f(x_1) \times \frac{x_2 - x_1}{f(x_2) - f(x_1)}$$

$$x_0 = 2 + 9 \times \frac{3 - 2}{6 + 9} = 2.6$$

Root is $\boxed{x_0 = 2.6}$ Ans.

(ix) write the method of factorization method.

Ans. → $A = \begin{bmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{bmatrix}$, $X = \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix}$ & $B = \begin{bmatrix} b_1 \\ b_2 \\ b_3 \end{bmatrix}$

let $A = LU$ where $L = \begin{bmatrix} 1 & 0 & 0 \\ l_{21} & 1 & 0 \\ l_{31} & l_{32} & 1 \end{bmatrix}$ & $U = \begin{bmatrix} u_{11} & u_{12} & u_{13} \\ 0 & u_{22} & u_{23} \\ 0 & 0 & u_{33} \end{bmatrix}$

So $LUX = B$

write $UX = V$ than $LV = B$

than Comparision & take the values of V_1, V_2 & V_3

Put into the Original system $UX = V$

than taking 3 eq^n & solve it.

By back substitution, we have take the values of x, y, z.

(X) Differentiate $x^5+6x^3+3x^2+1$

Solve

$\Rightarrow x^5+6x^3+3x^2+1$

$\Rightarrow \frac{d}{dx}(x^5+6x^3+3x^2+1)$

$\Rightarrow \frac{d}{dx}x^5+\frac{d}{dx}6x^3+\frac{d}{dx}3x^2+\frac{d}{dx}1$

$\Rightarrow 5x^4+18x^2+6x+0$

$\Rightarrow 5x^4+18x^2+6x$ Ans.

Que. 2 → How many type of operators are used in FORTRAN. Explain.

Ans. → 3 type of operators are used in FORTRAN.
① Arithmetic Operators ② Relational Operators
③ Logical Operators.

① Arithmetic Operators → This operator's are used to simple Calculation.

(i) Addition (+) → For addition two digit, Constants, variables.

Exa → 4 + 8 , a + b , A + D , X + Y + Z.

(ii) Substraction (-) → For subtraction two digit, constants & variables.

Exa → 8 - 4, A - D, X - Y - Z.

(iii) Multiplication (*) → To multiply digits, Constants & variables.

Exa → 8 * 4 , A * D, X * Y * Z.

(iv) Division (/) → To devide digits, Constants & variables.

Exa → 8/4, A/D, X/Y

(iv) Exponentation (* *) → To perform exponent of digit, Constant & variables.

Exa → 8 ** 4 (8^4), A ** D (A^D).

② Relational Operators → Relational operators are used for Comparing the values of two airthmetic expressions. They Produce logical values .TRUE. or .FALSE. as result.

6 relational operators are there:—

(i) .LT. → Less than (<)

Exa → IF(X .LT. Y)
    THEN
        Stmt ___
    ELSE
        Stmt ___
    END IF

(ii) .LE. → Less than or equal to (<=)

Exa → IF(X .LE. Y)
    THEN
        Stat ___
    ELSE
        Stmt ___
    END IF

(iii) .EQ. → Equal to (=)

Exa → IF (X .EQ. Y)
    THEN
        Stmts —
    ELSE
        Stmts —
    END IF

(iv) .NE. → Not equal to (!=)

Exa → IF (X .NE. Y)
    THEN
        Stmts —
    ELSE
        Stmts —
    END IF

(v) .GT. → Greater than (>)

Exa → IF(X .GT. Y)
    THEN
        Stmts —
    ELSE
        Stmts —
    END IF

(vi) .GE. → Greater than or equal to (>=)

Exa → IF(C-D .GE. A-B)
THEN
stmts —
ELSE
stmts —
END IF

③ Logical Operators → we may need to make more than one comparision. It is possible to combine two relational exp. using the following logical operators :-

(i) .AND. → Both relations are true

Exa → IF (SUM .GT. 100 **.AND.** N .GT. 20)
THEN
≡
ELSE
≡
END IF

(ii) .OR. → one or both of the relations are true

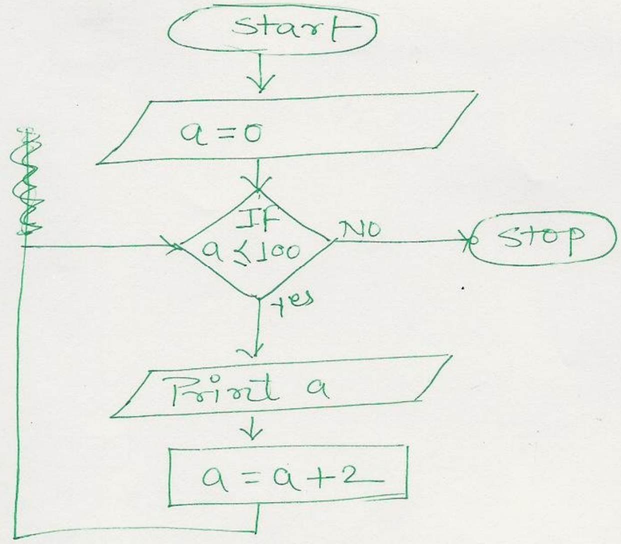
Exa → IF(AGE .LT. 30 .AND. DEGREE .EQ. 'ME')
THEN ≡
ELSE ≡
END IF

iii) .NOT. → Opposite is true

Exa → IF(.NOT. A .EQ. B)
THEN
≡
ELSE
≡
END IF

Que. 3 → Draw flow chart to print First 50 even numbers & their program.

Ans. → **Flow chart :-**



Program :-

```
FIRST_50_EVEN_NO.
INTEGER A=0
PRINT *, 'FIRST 50 EVEN NO'S'
DO 100 I = 1 , 98 , 2
     PRINT *, I
100 CONTINUE
END
```

Que. 4 → Perform $(A \times B) + (C \times D) - E$ where

$A = \begin{matrix} 4 & 2 & 0 \\ 9 & 1 & 3 \\ 2 & 5 & 7 \end{matrix}$ $B = \begin{matrix} 8 & 9 & 0 \\ 7 & 5 & 1 \\ 2 & 3 & 4 \end{matrix}$ $C = \begin{matrix} 1 & 5 & 7 \\ 5 & 6 & 0 \\ 3 & 8 & 4 \end{matrix}$

$D = \begin{matrix} 4 & 0 & 6 \\ 5 & 8 & 9 \\ 2 & 3 & 7 \end{matrix}$ $E = \begin{matrix} 5 & 3 & 0 \\ 1 & 8 & 4 \\ 2 & 6 & 4 \end{matrix}$

Solve →
$$\begin{bmatrix} 4 & 2 & 0 \\ 9 & 1 & 3 \\ 2 & 5 & 7 \end{bmatrix} \times \begin{bmatrix} 8 & 9 & 0 \\ 7 & 5 & 1 \\ 2 & 3 & 4 \end{bmatrix} + \begin{bmatrix} 1 & 5 & 7 \\ 5 & 6 & 0 \\ 3 & 8 & 4 \end{bmatrix} \times \begin{bmatrix} 4 & 0 & 6 \\ 5 & 8 & 9 \\ 2 & 3 & 7 \end{bmatrix} - \begin{bmatrix} 5 & 3 & 0 \\ 1 & 8 & 4 \\ 2 & 6 & 4 \end{bmatrix}$$

$$\Rightarrow \begin{bmatrix} 46 & 46 & 2 \\ 85 & 95 & 13 \\ 65 & 64 & 33 \end{bmatrix} + \begin{bmatrix} 43 & 61 & 100 \\ 50 & 48 & 84 \\ 60 & 76 & 118 \end{bmatrix} - \begin{bmatrix} 5 & 3 & 0 \\ 1 & 8 & 4 \\ 2 & 6 & 4 \end{bmatrix}$$

$$\Rightarrow \begin{bmatrix} 89 & 107 & 102 \\ 135 & 143 & 97 \\ 125 & 140 & 151 \end{bmatrix} - \begin{bmatrix} 5 & 3 & 0 \\ 1 & 8 & 4 \\ 2 & 6 & 4 \end{bmatrix}$$

$$\Rightarrow \begin{bmatrix} 84 & 104 & 102 \\ 134 & 135 & 93 \\ 123 & 134 & 147 \end{bmatrix}$$

Ans

Que. 5 → Find a root equation $x^2 - x - 2 = 0$ using False position method.

Solve. Given equation:-

$$x^2 - x - 2 = 0$$

$F(0) = 0 - 0 - 2 = -2$

$F(1) = 1 - 1 - 2 = -2$

$F(2) = 4 - 2 - 2 = 0$

$F(3) = 9 - 3 - 2 = 4$

So. $f(x_1) = f(1) = -2$

Iteration 1 $f(x_2) = f(3) = 4$

$$x_0 = x_1 - f(x_1) \times \frac{x_2 - x_1}{f(x_2) - f(x_1)}$$

$$x_0 = 1 + 2 \times \frac{3-1}{4+2} = 1.6667$$

$F(x_0) = -0.8889$

x_0 -ve & x_2 +ve

So root lies b/w x_0 & x_2 [2nd iteration]

$$x_0 = 1.6667 + 0.8889 \times \frac{3 - 1.6667}{4 + 0.8889} = 1.909$$

$F(x_0) = 0.2345$

Root lies b/w $x_0 = 1.909$ & $x_2 = 3$ [3rd iteration]

$$x_0 = 1.909 + 0.2647 \times \frac{3 - 1.909}{4 - 0.2647}$$

$$= 1.986$$

The estimated root after third iteration is 1.986 means that root is approximately 2,

$\boxed{x = 2}$ Ans.

Que.6 → Solve the system

$3x + y + 2z = 3$, $2x - 3y - z = -3$, $x + 2y + z = 4$

using Matrix inversion method.

Solve Given that

$$A = \begin{bmatrix} 3 & 1 & 2 \\ 2 & -3 & -1 \\ 1 & 2 & 1 \end{bmatrix}, \quad X = \begin{bmatrix} x \\ y \\ z \end{bmatrix}, \quad D = \begin{bmatrix} 3 \\ -3 \\ 4 \end{bmatrix}$$

By matrix inversion method :-

$$X = A^{-1} D$$

then

$$A^{-1} = \frac{\text{Adj } A}{|A|}$$

$$\text{Adj } A = \begin{bmatrix} -1 & 3 & 5 \\ -3 & 1 & 7 \\ 7 & -5 & -11 \end{bmatrix}, \quad |A| = 8$$

So

$$\Rightarrow \begin{bmatrix} x \\ y \\ z \end{bmatrix} = \frac{1}{8} \begin{bmatrix} -1 & 3 & 5 \\ -3 & 1 & 7 \\ 7 & -5 & -11 \end{bmatrix} \times \begin{bmatrix} 3 \\ -3 \\ 4 \end{bmatrix}$$

$$\Rightarrow \begin{bmatrix} x \\ y \\ z \end{bmatrix} = \begin{bmatrix} 1 \\ 2 \\ -1 \end{bmatrix}$$

Hence

$x = 1$

$y = 2$

$z = -1$ Ans

Que. 7 → Apply Euler – Maclaurin formula to evaluate:-

$$\cancel{\frac{1}{51^2}} * \cancel{\frac{1}{15^2}} * \frac{1}{51^2} + \frac{1}{53^2} + \frac{1}{55^2} + \cdots + \frac{1}{99^2}$$

Solve Taking $y = \frac{1}{x^2}$, $x_0 = 51$, $h = 2$, $n = 24$

we have $y' = \frac{-2}{x^3}$, $y''' = \frac{-24}{x^5}$

Then Euler – Maclaurin formula gives

$$\int_{51}^{99} \frac{dx}{x^2} = \frac{2}{2}\left[\frac{1}{51^2} + \frac{2}{53^2} + \frac{2}{55^2} + \cdots \frac{2}{97^2} + \frac{1}{99^2}\right]$$

$$- \frac{(2)^2}{12}\left[\frac{-2}{99^3} - \frac{-2}{51^3}\right] + \frac{(2)^4}{720}\left[\frac{-24}{99^5} - \frac{-24}{51^5}\right]$$

$$= [0.000384 + 0.0007119 + 0.0006611 + 0.000615 + 0.000574 + 0.000537 + 0.000503 + 0.000478 + 0.000445 + 0.000420 + 0.000396 + 0.000375 + 0.000355 + 0.000337 + 0.00032 + 0.000304 + 0.00029 + 0.000276 + 0.000264 + 0.000252 + 0.000241 + 0.000231 + 0.000221 + 0.000212 + 0.000204] - 0.33[-0.000002 + 0.00001] + 0.022[\cdots\cdots]$$

$$= [0.009565 - 0.00000264] + 0.022$$

$$= 0.00315 \text{ (Approx)}$$

Ans