

September 1, 1969

9100B CHEMICAL PROGRAM LISTING

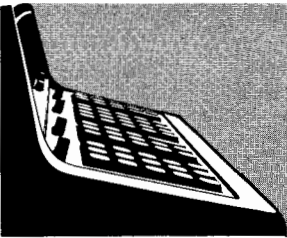
- 75502 - ELEMENTAL PERCENTAGE AND MOLECULAR WEIGHT - 6 ELEMENT
 Calculates percentages and molecular weight of compounds containing 6 elements or less.
- 75503 - CHN ANALYSIS [K VALUES]
 Calculates K values given C, H and N, blank values, and percentages for a known standard.
- 75504 - CHN PERCENTAGES
 Given C, H, and N values and using previously calculated K values and known blank values, calculates C, H and N percentages.
- 75505 - MOLECULAR WEIGHT BY VPO
 Calculates molecular weight for an unknown based on a series of vapor pressure osmometer (VPO) readings at various dilutions by extrapolating least squares curve fit to infinite dilution.
- 75506 - MEMBRANE OSMOMETER
 Determines the number-average molecular weight by extrapolating a least squares curve fit to infinite dilution.



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PART NO.
09100-75502

ELEMENTAL PERCENTAGE AND MOLECULAR WEIGHT
· 6 ELEMENT

This program calculates relative elemental percentages of up to and including 6 elements. The atomic weight of the elements are programmed into the calculator. The total molecular weight of the compound is also calculated.

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USER INSTRUCTIONS

ENTER PROGRAM (Starting Address is 0 - 0)

N_1 {
 PRESS: GO TO (0) (4)
 SET: PROGRAM
 Enter program steps for atomic weight of N_1 ;
 maximum of 6 steps is allowed.
 SET: RUN

N_2 {
 PRESS: GO TO (1) (4)
 SET: PROGRAM
 Enter program steps for atomic weight of N_2
 as before.
 SET: RUN

N_3 {
 PRESS: GO TO (2) (4)
 SET: PROGRAM
 Enter atomic weight of N_3 as before.
 SET: RUN

N_4 {
 PRESS: GO TO (3) (4)
 SET: PROGRAM
 Enter atomic weight of N_4 as before.
 SET: RUN

N_5 {
 PRESS: GO TO (4) (4)
 SET: PROGRAM
 Enter atomic weight of N_5 as before.
 SET: RUN

N_6 {
 PRESS: GO TO (5) (4)
 SET: PROGRAM
 Enter atomic weight of N_6 as before.
 SET: RUN

PRESS: GO TO (0) (0) [or End]

PRESS: CONTINUE

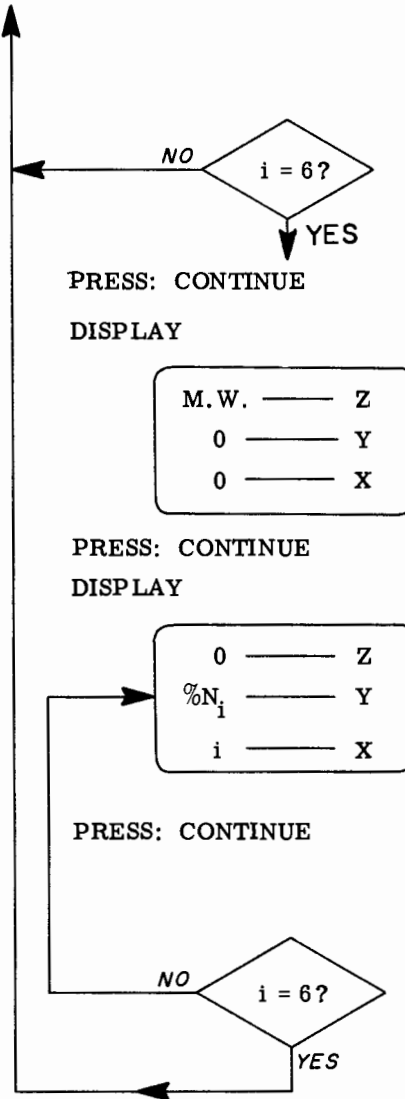
DISPLAY

| | | |
|---|---|---|
| 0 | — | Z |
| 0 | — | Y |
| i | — | X |

(i indicates number of element to be entered)

ENTER DATA: $N_i \rightarrow X$ (N_i = the number of atoms of each element.)

USER INSTRUCTIONS con't



Note: To reset problem with different elements, repeat user instructions; otherwise, enter new number of atoms of each element when initial display appears after completion of last problem.

EXAMPLE

| Elements: | N ₁ (C) | N ₂ (H) | N ₃ (S) | N ₄ (N) | N ₅ (O) | N ₆ (Si) |
|------------|--------------------|--------------------|--------------------|--------------------|--------------------|---------------------|
| At. Wt.: | 12.01 | 1.008 | 32.07 | 14.01 | 16.00 | 28.09 |
| # of Atoms | 6 | 2 | 8 | 1 | 2 | 3 |

Solution:

$$\% \text{ C} = 15.63\%$$

$$\% \text{ H} = .44\%$$

$$\% \text{ S} = 55.66\%$$

$$\% \text{ N} = 3.04\%$$

$$\% \text{ O} = 6.94\%$$

$$\% \text{ Si} = 18.28\%$$

$$\text{Molecular Weight} = 460.92$$

| Step | Key | Code | Display | | | Storage | | | | | | | | | | | | |
|------|----------|-------|---|---|---|----------------------|---|---|---|---|---|--|--|--|--|--|--|--|
| | | | x | y | z | f | e | d | c | b | a | | | | | | | |
| 0 | 0 | CLEAR | 20 | | | | | | | | | | | | | | | |
| 1 | 1 | 01 | | | | | | | | | | | | | | | | |
| 2 | STOP | 41 | N ₁ | 0 | 0 | ENTER N ₁ | | | | | | | | | | | | |
| 3 | ↑ | 27 | | | | | | | | | | | | | | | | |
| 4 | CONTINUE | 47 | | | | | | | | | | | | | | | | |
| 5 | | | | | | | | | | | | | | | | | | |
| 6 | | | AREA FOR INSERTING ATOMIC WEIGHT OF N ₁ | | | | | | | | | | | | | | | |
| 7 | | | | | | | | | | | | | | | | | | |
| 8 | | | | | | | | | | | | | | | | | | |
| 9 | CONTINUE | 47 | | | | | | | | | | | | | | | | |
| a | X | 36 | CALCULATE PARTIAL MOLECULAR WEIGHT | | | | | | | | | | | | | | | |
| b | ACC + | 60 | | | | | | | | | | | | | | | | |
| c | y→() | 40 | STORE X ₁ | | | | | | | | | | | | | | | |
| d | a | 13 | | | | | | | | | | | | | | | | |
| 1 | 0 | ↓ | 25 | | | | | | | | | | | | | | | |
| 1 | 2 | 02 | | | | | | | | | | | | | | | | |
| 2 | STOP | 41 | N ₂ | 0 | 0 | ENTER N ₂ | | | | | | | | | | | | |
| 3 | ↑ | 27 | | | | | | | | | | | | | | | | |
| 4 | CONTINUE | 47 | | | | | | | | | | | | | | | | |
| 5 | | | | | | | | | | | | | | | | | | |
| 6 | | | AREA FOR INSERTING ATOMIC WEIGHT OF N ₂ | | | | | | | | | | | | | | | |
| 7 | | | | | | | | | | | | | | | | | | |
| 8 | | | | | | | | | | | | | | | | | | |
| 9 | CONTINUE | 47 | | | | | | | | | | | | | | | | |
| a | X | 36 | CALCULATE PARTIAL MOLECULAR WEIGHT | | | | | | | | | | | | | | | |
| b | ACC + | 60 | | | | | | | | | | | | | | | | |
| c | y→() | 40 | STORE X ₂ | | | | | | | | | | | | | | | |
| d | b | 14 | | | | | | | | | | | | | | | | |
| 2 | 0 | ↓ | 25 | | | | | | | | | | | | | | | |
| 1 | 3 | 03 | | | | | | | | | | | | | | | | |
| 2 | STOP | 41 | N ₃ | 0 | 0 | ENTER N ₃ | | | | | | | | | | | | |
| 3 | ↑ | 27 | | | | | | | | | | | | | | | | |
| 4 | CONTINUE | 47 | | | | | | | | | | | | | | | | |
| 5 | | | | | | | | | | | | | | | | | | |
| 6 | | | AREA FOR INSERTING ATOMIC WEIGHT OF N ₃ | | | | | | | | | | | | | | | |
| 7 | | | | | | | | | | | | | | | | | | |
| 8 | | | | | | | | | | | | | | | | | | |
| 9 | CONTINUE | 47 | | | | | | | | | | | | | | | | |
| a | X | 36 | CALCULATE PARTIAL MOLECULAR WEIGHT | | | | | | | | | | | | | | | |
| b | ACC + | 60 | | | | | | | | | | | | | | | | |
| c | y→() | 40 | STORE X ₃ | | | | | | | | | | | | | | | |
| d | c | 16 | | | | | | | | | | | | | | | | |

| Step | Key | Code | Display | | | Storage | | | | | | |
|------|------|----------|------------------------|------------------------------------|---|---------|----------------------|---|---|---|---|--|
| | | | x | y | z | f | e | d | c | b | a | |
| 3 | 0 | ↓ | 25 | | | | | | | | | |
| | 1 | 4 | 04 | | | | | | | | | |
| | 2 | STOP | 41 | N ₄ | 0 | 0 | ENTER N ₄ | | | | | |
| | 3 | ↑ | 27 | | | | | | | | | |
| | 4 | CONTINUE | 47 | | | | | | | | | |
| | 5 | | | | | | | | | | | |
| | 6 | | | AREA FOR INSERTING | | | | | | | | |
| | 7 | | | ATOMIC WEIGHT OF N ₄ | | | | | | | | |
| | 8 | | | | | | | | | | | |
| | 9 | CONTINUE | 47 | | | | | | | | | |
| | a | X | 36 | CALCULATE PARTIAL MOLECULAR WEIGHT | | | | | | | | |
| | b | ACC + | 60 | | | | | | | | | |
| c | y→() | 40 | STORE X ₄ | | | | | | | | | |
| d | d | 17 | | | | | | | | | | |
| 4 | 0 | ↓ | 25 | | | | | | | | | |
| | 1 | 5 | 05 | | | | | | | | | |
| | 2 | STOP | 41 | N ₅ | 0 | 0 | ENTER N ₅ | | | | | |
| | 3 | ↑ | 27 | | | | | | | | | |
| | 4 | CONTINUE | 47 | | | | | | | | | |
| | 5 | | | | | | | | | | | |
| | 6 | | | AREA FOR INSERTING | | | | | | | | |
| | 7 | | | ATOMIC WEIGHT OF N ₅ | | | | | | | | |
| | 8 | | | | | | | | | | | |
| | 9 | CONTINUE | 47 | | | | | | | | | |
| | a | X | 36 | CALCULATE PARTIAL MOLECULAR WEIGHT | | | | | | | | |
| | b | ACC + | 60 | | | | | | | | | |
| c | y→() | 40 | STORE X ₅ | | | | | | | | | |
| d | f | 15 | | | | | | | | | | |
| 5 | 0 | ↓ | 25 | | | | | | | | | |
| | 1 | 6 | 06 | | | | | | | | | |
| | 2 | STOP | 41 | N ₆ | 0 | 0 | ENTER N ₆ | | | | | |
| | 3 | ↑ | 27 | | | | | | | | | |
| | 4 | CONTINUE | 47 | | | | | | | | | |
| | 5 | | | | | | | | | | | |
| | 6 | | | AREA FOR INSERTING | | | | | | | | |
| | 7 | | | ATOMIC WEIGHT OF N ₆ | | | | | | | | |
| | 8 | | | | | | | | | | | |
| | 9 | CONTINUE | 47 | | | | | | | | | |
| | a | X | 36 | | | | | | | | | |
| | b | e | 12 | | | | | | | | | |
| c | x↔y | 30 | CALCULATE AND STORE | | | | | | | | | |
| d | + | 33 | TOTAL MOLECULAR WEIGHT | | | | | | | | | |

CHN ANALYSIS - K VALUES

This program calculates the K values (K_C , K_H , and K_N), for compounds containing carbon (C), hydrogen (H), and nitrogen (N), from blank values (B_C , B_H , and B_N), percentages of C, H, and N from a known standard ($\%C_s$, $\%H_s$, and $\%N_s$), and measured quantities of C, H, and N of the known standard (C_{s_i} , H_{s_i} , and N_{s_i}).

Two sets of measurements of C-H-N quantities of the standard are normally taken, although one set of measurements is sufficient for operation of the program.

The following equations are used:

$$K_C = \frac{\%C_s}{\bar{C}_s - B_C}$$

$$K_H = \frac{\%H_s}{\bar{H}_s - B_H}$$

$$K_N = \frac{\%N_s}{\bar{N}_s - B_N}$$

where \bar{M}_s [M = C, H, or N] is the average of M_{s_1} and M_{s_2} .

If only one set of C-H-N quantities of the standard are used, then:

$$\bar{M}_s [M = C, H, \text{ or } N] = M_{s_1}$$

$$K_C = \frac{\%C_s}{C_1 - B_C}, \text{ etc.}$$

USER INSTRUCTIONS

USER INSTRUCTIONS (con't)

ENTER PROGRAM (Starting Address is 0 - 0)
 PRESS: GO TO (3) (1)
 SET:

ENTER: Program steps for the constant - %N_s
 (five spaces available).
 SET:

PRESS: GO TO (4) (3)
 SET:

ENTER: Program steps for the constant - %C_s
 (five spaces available).
 SET:

PRESS: GO TO (5) (3)
 SET:

ENTER: Program steps for the constant - %H_s
 (five spaces available).
 SET:

PRESS: GO TO (0) (0) [or END]
 PRESS: CONTINUE

DISPLAY

| | | |
|---|-------|---|
| 0 | _____ | Z |
| 0 | _____ | Y |
| 0 | _____ | X |

ENTER DATA: B_N → Z, B_H → Y, B_C → X

PRESS: CONTINUE

DISPLAY

| | | |
|---|-------|---|
| 0 | _____ | Z |
| 0 | _____ | Y |
| 1 | _____ | X |

ENTER DATA: N_{s1} → Z, H_{s1} → Y, C_{s1} → X

PRESS: CONTINUE

DISPLAY

| | | |
|---|-------|---|
| 0 | _____ | Z |
| 0 | _____ | Y |
| 2 | _____ | X |

ENTER DATA: N_{s2} → Z, H_{s2} → Y, C_{s2} → X

PRESS: CONTINUE

DISPLAY

| | | |
|----------------|-------|---|
| K _N | _____ | Z |
| K _H | _____ | Y |
| K _C | _____ | X |

Note: If only one set of standard values is to be used, N_{s2}, H_{s2}, and C_{s2} must be set to zero. Do not press "clear" at any time during program operation.

To reset program for a different standard, repeat user instructions.

EXAMPLES

(A) Only 1 set of standard values is available

Given: %C_s = 51.79, %H_s = 5.07, %N_s = 20.14
 B_C = 1.6, B_H = 30, B_N = 1.0
 C_{s1} = 125.0, H_{s1} = 119.5, N_{s1} = 88.0

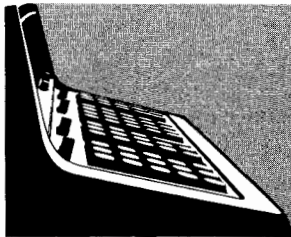
Note: Since only 1 set of standards is available, the 2nd set of standards must be set to zero at the appropriate data input of the program. Do not press "CLEAR" to zero the 2nd set of standards.

Solution: K_C = .420, K_H = .057, K_N = .231

(B) Given: %C_s = 51.79, %H_s = 5.07, %N_s = 20.14

B_C = 1.6, B_H = 30, B_N = 1.0
 C_{s1} = 121.0, H_{s1} = 121.5, N_{s1} = 79.5
 C_{s2} = 120.5, H_{s2} = 115.5, N_{s2} = 79.5

Solution: K_C = .435, K_H = .057, K_N = .257



PART NO.
09100-75504

CHN PERCENTAGES

Percentages of carbon (C), hydrogen (H), and nitrogen (N) in an unknown substance are calculated from measured quantities of C, H, and N, blank values (B_C , B_H , and B_N), and K values (K_C , K_H , K_N) which may be calculated with the K value program (09100-75503). K and B values must be stored prior to program operation either manually by the operator, or automatically by the use of the K value program.

The following equations are used:

$$\% C_1 = K_C (C_1 - B_C)$$

$$\% C_2 = K_C (C_2 - B_C)$$

or, in general:

$$\% M_1 [M = C, H, \text{ or } N] = K_M (M_1 - B_M)$$

$$\% M_2 [M = C, H, \text{ or } N] = K_M (M_2 - B_M)$$

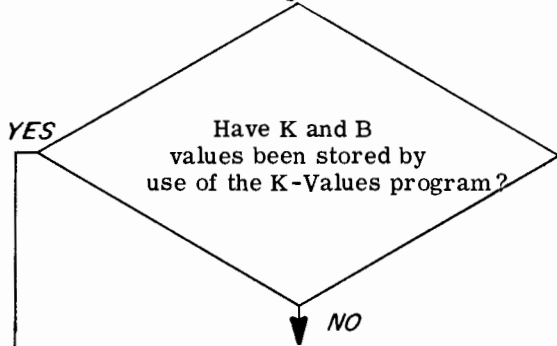
The percentage evaluation is considered successful if M_1 and M_2 differ by .3% or less.

If only one set of CHN measurements are available, then C_2 , H_2 , and N_2 may be made any value at the corresponding data input. In this case only $\% C_1$, $\% H_1$, and $\% N_1$ are useful information; disregard answers for $\% C_2$, $\% H_2$, and $\% N_2$.

USER INSTRUCTIONS

USER INSTRUCTIONS (con't)

ENTER PROGRAM [(Starting Address is 0 - 0)]



ENTER DATA: $K_N \rightarrow Z, K_H \rightarrow Y, K_C \rightarrow X$

PRESS: { x →
f →
y →
e →
R ↓
y →
d →

ENTER DATA: $B_N \rightarrow Z, B_H \rightarrow Y, B_C \rightarrow X$

PRESS: { x →
a →
y →
b →
R ↓
y →
c →

PRESS: GO TO (0) (0) [or END]

PRESS: CONTINUE

DISPLAY

| | | |
|---|---|---|
| 0 | — | Z |
| 0 | — | Y |
| 1 | — | X |

ENTER DATA: $N_1 \rightarrow Z, H_1 \rightarrow Y, C_1 \rightarrow X$

PRESS: CONTINUE

DISPLAY

| | | |
|---|---|---|
| 0 | — | Z |
| 0 | — | Y |
| 2 | — | X |

ENTER DATA: $N_2 \rightarrow Z, H_2 \rightarrow Y, C_2 \rightarrow X$

Note: If only one C-H-N set is available, N_2 , H_2 , and C_2 may be set to zero or any other value--Simply disregard the solutions for $\% C_2$, $\% H_2$, and $\% N_2$.

PRESS: CONTINUE

DISPLAY

| | | |
|----------|---|---|
| $\% C_2$ | — | Z |
| $\% C_1$ | — | Y |
| 1 | — | X |

PRESS: CONTINUE

DISPLAY

| | | |
|----------|---|---|
| $\% H_2$ | — | Z |
| $\% H_1$ | — | Y |
| 2 | — | X |

PRESS: CONTINUE

DISPLAY

| | | |
|----------|---|---|
| $\% N_2$ | — | Z |
| $\% N_1$ | — | Y |
| 3 | — | X |

To reset problem for different C, H, and N samples.

To reset program for different sets of K and B, repeat user instructions.

EXAMPLES

(A)

Example (A) of the K-value program (09100-75503) has previously been run, and the K and B values have already been stored.

Data: $C_1 = 118.3$, $H_1 = 75.0$, $N_1 = 49.1$
 $C_2 = 128.6$, $H_2 = 69.7$, $N_2 = 53.4$

Solution: $\%C_1 = 48.98$, $\%C_2 = 53.30$
 $\%H_1 = 2.55$, $\%H_2 = 2.25$
 $\%N_1 = 11.13$, $\%N_2 = 12.13$

(B)

The K-value program (09100-75503) has not been run; K and B values must therefore be stored manually. (see "user instructions").

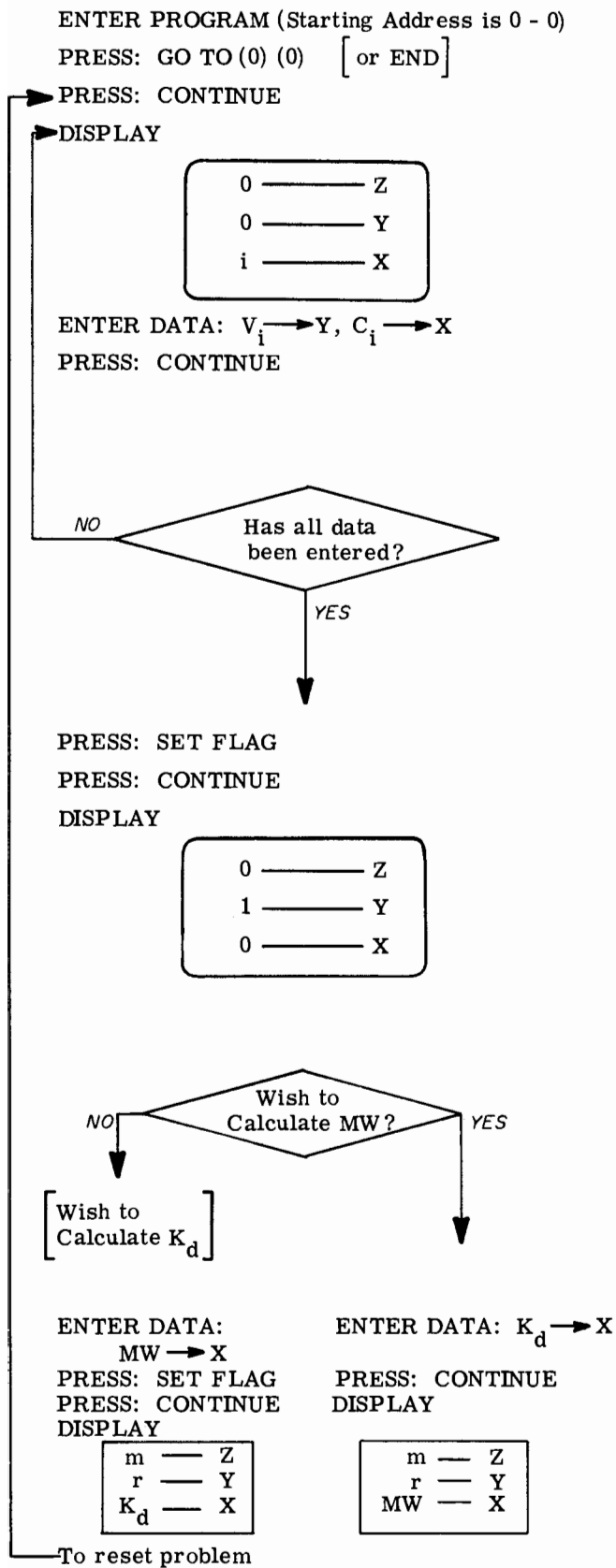
Data: $B_C = 2.1$, $B_H = 28$, $B_N = 3$
 $K_C = .520$, $K_H = .102$, $K_N = .235$
 $C_1 = 132.1$, $H_1 = 92.0$, $N_1 = 57.9$

Solution: $\%C_1 = 67.6$
 $\%H_1 = 6.53$
 $\%N_1 = 12.90$

Note: Disregard answers for $\%C_2$, $\%H_2$, and $\%N_2$ since a second set of C-H-N was not available.

USER INSTRUCTIONS

EXAMPLES



(A) Calculate K_d for the following standard molecular weight, and set of VPO and C readings.

Data: MW = 1500

| i | V_i | C_i |
|---|-------|-------|
| 1 | 500 | 34 |
| 2 | 330 | 24 |
| 3 | 205 | 16 |
| 4 | 125 | 8 |

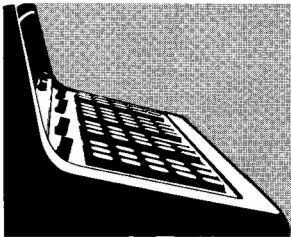
Solution: $m = -.017$
 $r = -.156$
 $K_d = 21858.377$

(B) Calculate MW for the following data:

Data: $K_d = 337.576$

| i | V_i | C_i |
|---|-------|--------|
| 1 | 56.10 | 121.95 |
| 2 | 23.85 | 57.32 |
| 3 | 11.45 | 27.85 |
| 4 | 5.68 | 13.72 |

Solution: $m = .0005$
 $r = .9419$
 MW = 843.5813



MEMBRANE OSMOMETER

PART NO.
09100-75506

The membrane osmometer is used to obtain data for calculation of either the constant RT (R = gas constant, T = absolute temperature), or the number average molecular weight (\bar{M}_n). In normal application, osmotic pressure (P) measurements are taken for various concentrations (C) of a substance with known \bar{M}_n , and RT is subsequently calculated. The number average molecular weight of an unknown substance may then be determined from membrane osmometer measurements of P obtained from various concentrations of the unknown, and from the previously determined RT .

The same procedure is used to calculate either RT or \bar{M}_n . In both cases, a linear regression is performed with $(P/C)^{1/2}$ and C as the dependent and independent variables respectively. The regression is similar to that of the regression program (09100-70803) for equations of the form $y = mx + b$; in this case the defining equation is $P/C = mc + \frac{RT}{\bar{M}_n}$, where m is the slope of the (P/C) versus C curve. The $(P/C)^{1/2}$ versus C curve is then extrapolated to infinite dilution ($c=0$) to obtain the $Y = P/C$ intercept (b), i. e. $\lim_{c \rightarrow 0} P/C = b$. $(P/C)^{1/2}$ rather than P/C is used in the regression to avoid extrapolation error when the P/C and C data results in a P/C versus C plot with pronounced curvature. In many cases where the first power plot has pronounced curvature, the square-root plot will produce a straight line suitable for extrapolation. The desired intercept (b) of the P/C versus C curve is then the square of the $(P/C)^{1/2}$ versus C intercept.

RT is calculated using the equations:

$$RT = \bar{M}_n (b) \quad \text{where } \bar{M}_n \text{ is a known number average molecular weight.}$$

Likewise, \bar{M}_n may be calculated by the equation:

$$\bar{M}_n = \frac{RT}{b} \quad \text{where now } \bar{M}_n \text{ is the number average molecular weight (of an unknown substance) which is to be determined.}$$

A correlation coefficient (r) is also calculated. r is a measure of reproducibility and also how ideal the system is.

ENTER PROGRAM (Starting Address is 0 - 0)

PRESS: END

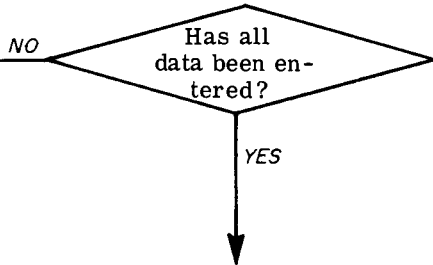
PRESS: CONTINUE

DISPLAY

| | | |
|---|---|---|
| 0 | — | Z |
| 0 | — | Y |
| i | — | X |

ENTER DATA: $P_i \rightarrow Y, C_i \rightarrow X$

PRESS: CONTINUE

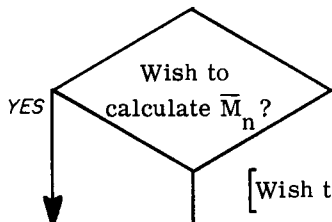


PRESS: SET FLAG

PRESS: CONTINUE

DISPLAY

| | | |
|---|---|---|
| 0 | — | Z |
| 1 | — | Y |
| 0 | — | X |



ENTER DATA: $RT \rightarrow X$

ENTER DATA: $\bar{M}_n \rightarrow X$

PRESS: SET FLAG PRESS: CONTINUE

PRESS: CONTINUE

DISPLAY

DISPLAY

| | | |
|-------------|---|---|
| m | — | Z |
| r | — | Y |
| \bar{M}_n | — | X |

| | | |
|----|---|---|
| m | — | Z |
| r | — | Y |
| RT | — | X |

To reset problem:

(A) Determine RT for a substance with known number average molecular weight (\bar{M}_n) using the following data:

Data: $\bar{M}_n = 1.2 \times 10^5$

| i | P_i | C_i |
|---|-------|-------|
| 1 | .58 | 2 |
| 2 | 1.75 | 5 |
| 3 | 4.45 | 10 |
| 4 | 12.64 | 20 |

Solution: $m = .014$
 $r = .998$
 $RT = 32,185.017$

(B) Calculate \bar{M}_n for an unknown substance using the following data:

Data: $RT = 3.65 \times 10^4$

| i | P_i | C_i |
|---|-------|-------|
| 1 | .67 | 2.2 |
| 2 | 1.50 | 4.3 |
| 3 | 3.72 | 8.4 |
| 4 | 10.41 | 18.6 |

Solution: $m = .012$
 $r = .977$
 $\bar{M}_n = 124,403.599$

